ABSTRACT BOOK

Chemical Reaction Engineering toward Carbon-Neutral Future

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Oral Presentation

Plenary Lecture

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PL0393

Advanced Model-based Reaction Engineering for Circular Economy

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Abstract Category: Invited Lecture - Plenary Lecture

Keywords: first principles, equation-oriented, data-driven, circular economy, scale-up, autonomous operation

Abstract Body.

Chemical Reaction Engineering (CRE) is central to the transformation of industries toward circularity, decarbonization, and greater operational excellence. Recent study(1) emphasizes that future advances in CRE will depend on improved reactor design and scale‑up, process intensification, electrification of reaction systems, and integration of mechanistic understanding with data‑driven methods. Despite significant innovation in catalysis and sustainable process concepts, persistent challenges remain in translating laboratory discoveries into industrial practice, driven by reactor complexity, uncertainty during scale‑up, and fragmented use of experimental and digital data. Addressing these challenges requires more comprehensive and detailed modeling approaches that consistently link reaction kinetics, catalysis, transport phenomena, and process‑level decision making across scales. Advanced Model-based Reaction Engineering has therefore emerged as a critical enabler for implementing circular economy principles, waste valorization strategies, and low‑carbon chemical manufacturing pathways.

This work presents an Advanced Model-based Reaction Engineering framework based on first‑principles, equation‑oriented process modeling. Detailed representations of reaction kinetics, thermodynamics, and mass and energy transport are embedded within reactor and flowsheet models to ensure consistency from laboratory and pilot studies through to industrial design. The methodology supports steady‑state and dynamic simulation, parameter estimation, sensitivity analysis, and rigorous optimization. These capabilities enable systematic evaluation of conventional and non‑standard reactor concepts, including intensified and dynamically operated systems, as well as electrochemical reaction technologies. The modeling framework further allows integration of emerging data‑driven techniques, providing a balanced combination of mechanistic insight and data utilization while preserving interpretability, robustness, and predictive capability from design to operation(2,3).

Advanced Model-based Reaction Engineering demonstrates clear benefits in addressing the innovation priorities and challenges identified in recent CRE roadmap. Mechanistic reactor models reduce scale‑up risk by enabling quantitative assessment of performance, operability, and safety under realistic operating constraints. Dynamic simulations and optimizations reveal opportunities for process intensification and flexible and optimized operation. Integrated reactor–flowsheet studies support circular economy objectives by enabling systematic evaluation of carbon utilization, waste valorization, and energy integration strategies. Moreover, the ability to deploy validated models beyond process design—such as soft-sensing,

optimization, and operational decision support—extends their impact across the process lifecycle. Overall, Advanced Model-based Reaction Engineering emerges as a central pillar of modern reaction engineering, bridging innovation and industrial implementation while supporting the transition toward circular economy and autonomous operation.

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PL0726

Electrified, High temperature Thermocatalytic Reactor Technologies

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Abstract Category: *Invited Lecture - Plenary Lecture*

Keywords: electrification, chemical reactors, AI, multiscale modeling, experiments

Abstract Body.

Purpose

Advanced manufacturing increasingly relies on processing complex feedstocks—such as plastics and textiles for recycling, as well as remote biomass and biogas resources—which demands new catalytic materials, intensified reactors, and efficient modes of heat delivery. This talk will discuss various electrification technologies for various applications.

Methods

We will outline the key challenges to enable these transformations on a large scale. We will then examine emerging electrification technologies, including plasmas, microwaves, and Joule heating, with a particular focus on high-temperature applications and the potential for retrofitting and scaling these approaches within existing industrial infrastructure. In addition, we will highlight recent advances in AI-enabled multiscale modeling for accelerated materials discovery, process optimization, and scale-up. These concepts will be illustrated through case studies in shale-gas upgrading, textiles recycling, and plastics upcycling.

Results

Process intensification and electrification offer significant advantages over conventional technologies. We will outline these advantages.

Conclusions

This plenary will review high-temperature thermocatalytic reactors and provide a roadmap for future work.

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PL0158

Reactor Engineering for Converting CO2 and Biogas to Carbon Nanofibers

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Abstract Category: Invited Lecture - Plenary Lecture

Keywords: tandem reactor, CO2, biogas

Abstract Body.
Upgrading decentralized biogas represents a sustainable route to produce valuable products while mitigating two potent greenhouse gases, namely methane (CH4) and carbon dioxide (CO2). Conventional dry reforming of CH4 with CO2 yields syngas with low H2:CO ratios (≤1) and requires high temperatures (>800 °C) to overcome equilibrium constraints and abate coke deposition. In this work, we demonstrate the conversion of biogas into valueadded carbon nanofibers via reactor engineering using tandem thermochemical reactors, while reducing the reaction temperature, shifting equilibrium limits, and yielding H2-enriched syngas (H2:CO=2-3) as a byproduct [1]. Furthermore, we also discuss the utilization of electrochemical-thermochemical tandem reactors to convert CO2 and H2O to carbon nanofibers with H2 as a byproduct [2]. The tandem strategies can also be applied to convert CO2 and H2O to aromatics and oxygenates [3].

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PL0069

From Fossil Feedstocks to Renewable Carbon: Rethinking the Petrochemical Value Chain

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Abstract Category: Invited Lecture - Plenary Lecture

Keywords: Electrification, Olefins, Process Intensification, Shockwave Heating, Circular Economy, Life Cycle Assessment.

Abstract Body.

The petrochemical industry is at a crossroad: while light olefins such as ethylene and propylene remain indispensable building blocks for modern society, their production via conventional steam cracking accounts for over 240 Mt CO_2-equivalent emissions annually. Current approaches to decarbonization—such as carbon capture and storage—address emissions downstream but fail to tackle their root cause. This work introduces a disruptive alternative: electrification of steam cracking combined with valorization of renewable feedstocks, including biomass and plastic waste.

Electrifying steam cracking furnaces can reduce greenhouse gas emissions by up to 90%, eliminating more than 200 Mt CO_2-equivalent per year if powered by renewable electricity. However, conventional electric heating concepts (resistive, induction, microwave) remain constrained by heat transfer limitations and material challenges. To overcome these barriers, we propose the High Mach e-CRACKER, a novel electrified reactor concept inspired by aerospace engineering. This modular turbomachine achieves volumetric heating through supersonic flow and controlled shockwave generation, enabling temperature rises of >1000°C in less than 10 milliseconds—an order of magnitude faster than state-of-the-art technologies. By eliminating surface-heating constraints, the design allows for ultra-compact reactors, higher selectivity, and unprecedented process intensification.

Experimental and modeling studies demonstrate that this approach can increase olefin yields by 10 wt% compared to conventional cracking, translating into significant economic benefits and reduced coke formation. Life Cycle Assessment (LCA) confirms that electrification, combined with renewable grids and advanced feedstocks, can drastically lower Scope 1 and Scope 3 emissions while enabling circularity through the integration of plastic waste-derived pyrolysis oils. Furthermore, the technology's modular design facilitates rapid deployment and scalability, with pilot-scale TRL-5 units planned by 2027 and industrial testing by 2030.

Beyond technical innovation, this work emphasizes the necessity of supportive legislation and market incentives to create viable business cases for sustainable technologies. Electrification of steam cracking, coupled with advanced chemical recycling, represents a transformative pathway toward a carbon-neutral petrochemical value chain.

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PL0517

Modular Technologies for Decentralised PtX Applications

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Abstract Category: Invited Lecture - Plenary Lecture

Keywords: Micro Process Technology, Additive Manufacturing, Electro-Fuels

Abstract Body.

Introduction.

In the global energy transition, “electrification” is a megatrend because at point of use, electrical energy is often the most efficient among all forms of final energy. Renewable power generation from solar photovoltaics and wind turbines has seen strong cost reductions in the past, and its worldwide deployment is on a steep rise. However, solar and wind energy are highly variable, and large quantities of electrical energy can neither economically be stored in batteries nor be transported via transmission lines over long distances to bridge the mismatch of demand and supply. In addition, some applications such as long-distance air transport and shipping call for high energy density which rules out the use of batteries there in the foreseeable future. Moreover, non-fossil chemical feedstocks are needed in industry. This is where “Power-to-X” (PtX) comes into play, as a means for seasonal energy storage, long-distance energy transport, sustainable fuels and chemical feedstocks, and optimization of the energy system via sector coupling.

Methods.

With the aim of enabling load-flexible PtX plants, modular microstructured reactors were developed at the IMVT over the past 10 years both for Fischer-Tropsch synthesis and methanation from lab-scale devices to prototypes for demonstration. They are based on stacked metal plates where the repeating unit accommodates a 2D micro packed bed of a powder catalyst sandwiched between cooling plates having a patented fluid distribution channel design which enables an efficient 2D evaporation cooling pattern. In addition, metal additive manufacturing is being investigated at IMVT for industrial fabrication of compact modular reactors for Fischer-Tropsch synthesis, ammonia synthesis, and methanol synthesis. Two different routes are followed here: thin-walled 3D-printed structured parts as inserts for conventional pressure vessels and entirely 3D printed reactors which include a pressure-resistant shell. Moreover, compact helical distillation units were fabricated by metal 3D printing targeting containerized distillation units.

Results and discussion.

The prototypes were successfully tested in the lab and in PtX container plants established at KIT’s Energy Lab. The microreactor technology has been further developed and scaled up by our spin-off company INERATEC and is used in the World’s first commercial Power-toLiquid plant in Frankfurt Höchst, Germany. The presentation will highlight the design principles for microstructured and 3D printed reactors and devices for the different applications and summarize their status as well as selected results on their performance.

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PL0033

Engineering Chemical Process by Capsule Catalyst and 3D Printed Self-Catalytic Reactor

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Abstract Category: Invited Lecture - Plenary Lecture
Keywords: Capsule Catalyst, 3D printing, C1 Chemistry

Abstract Body.

Direct conversion of CO2 by hydrogenation as well as carbon-neutral syngas (CO+H2) conversion is a key technology for carbon neutral society because most of the organic compounds, either chemicals or energy products, are composing of C, H, O, obtainable from syngas or CO2+H2, whereas powerful catalyst and simple / highly efficient catalytic process are key factors.

Here as a typical chemical product with huge market and higher price, para-xylene (PX) direct synthesis from CO2+H2 or syngas, with our tailor-made capsule catalyst technology (1), is reported (2, 3). We are now scaling up this new C1 chemistry, being added by Japanese government and 6 Japanese companies, aiming full commercialization in 2028, as PX is easily oxidized to form T of PET plastics.

Butadiene is a key product for tires and plastics. We invented a new carbon-neutral tire production technology from CO2+H2, where ethanol synthesis from CO2 plays a key role (4, 5).

LPG is a promising energy product and carbon neutral LPG will have great impact. Beyond conventional zeolite-mixed methanol-based catalysts, we invented a new catalyst where Fe-Co-Cx confined in graphene fence, exhibiting high and stable activity for LPG synthesis from CO2+H2 (6).

Furthermore, we innovated self-catalytic reactor (SCR) fabrication by metal 3D print technology (7, 8), where catalyst and high-pressure reactor are printed simultaneously. The down-sized SCR without catalyst pellet loading, is also employed for CO2 conversion, as a new concept of micro-reactor as well as mobile factory.

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Oral Presentation

Reaction Mechanism and Kinetics

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MKF0088

Kinetic study of the impact of electric field on the liquid phase oxidation of technical fluids

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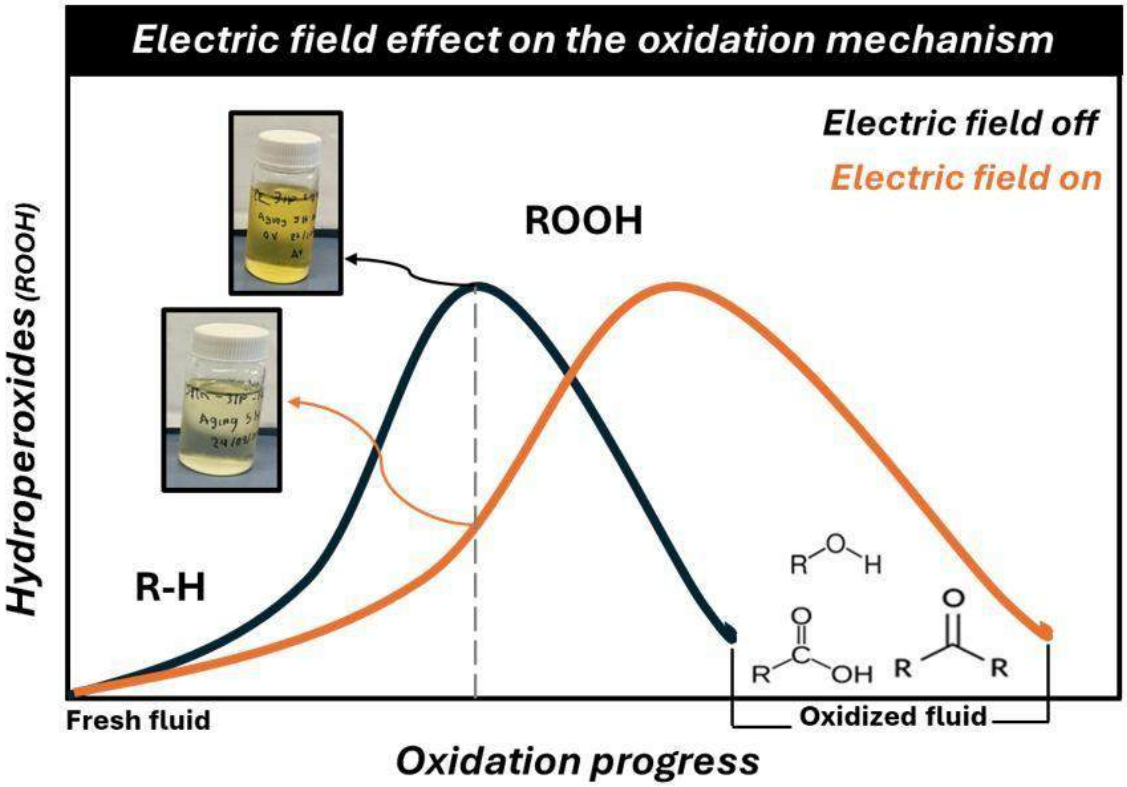
Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Fundamental

Keywords: oxidation mechanism, electric field, HPLC-PcR, hydroperoxides, hydrocarbons

Abstract Body.

Today, a quarter of energy consumption in all sectors, from mobility to energy production, is related to tribology. The fight against climate change is driving the development of decarbonized technologies, such as electric motors and transformers, which are essential for achieving this goal. However, these new technologies alter the environment in which technical fluids, used for lubrication or cooling, operate and their required properties. A major factor in these environments is long-term exposure to electric fields, whose effect on fluid oxidation kinetics remains unexplored. This study presents a new experimental approach to determine the influence of an electric field on the oxidation mechanism and kinetics of a technical fluid. Representative molecules of technical fluids were first identified, and a twostep methodology was established to study the effect of the electric field on the oxidation pathway. The methodology coupled a standardized oxidation reactor (autoclave) and a rheometer HR20, which were used as successive oxidation reactors under controlled conditions. UV spectroscopy, HPLC-PcR, GC-MS, and iodometric titration were used to analyze the oxidized samples. Our results revealed that the reactivity and the viscosity of oxidized fluids may be influenced by an electric field, depending on their molecular structures. The results showed, for the first time in the literature, that the electric field could affect the oxidation process and limit the loss of viscosity. This, combined with the fact that pre-oxidized samples exhibited a stronger response to the electric field, establishes its primary influence on intermediate reactions. Coupling the standardized autoclave and the rheometer constitutes an approach enabling a controlled reaction framework to be defined, capable of characterizing the effect of an electric field on the oxidation mechanisms and kinetics of a fluid.

Figure 1. Electric field effect on the oxidation process of a technical fluid.



ISCRE29 & APCRE11
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MKF0202

The Reaction Mechanism and Kinetics of the Deacon Process on Cu-K-La/γ-Al2O3 Catalyst under Harsh Conditions

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Fundamental

Keywords: Deacon process; Cu-based catalyst; Deactivation mechanism; Microkinetic modeling.

Abstract Body.

Introduction.

The Deacon process efficiently recycles HCl into Cl2, with Cu-based catalysts offering a cost-effective alternative to Ru-based ones. However, severe deactivation at high temperatures (over 700 K in adiabatic reactor) hinders industrial use. While traditionally attributed to active phase volatilization, this study demonstrates that irreversible deactivation under harsh conditions (500 °C) is primarily driven by the formation of inert delafossite CuAlO2.

Methods.

Using a high-performance Cu-K-La/γ-Al2O3 catalyst, contrastive samples with varying deactivation levels (83% to 69% conversion) were obtained through reaction, and prepared under Ar atmosphere for quasi-in-situ characterization (ICP, BET, XRD, XPS, and SEM). Reaction mechanisms were explored via thermodynamic analysis and chlorination experiments. DFT calculations and Langmuir-type microkinetic modeling were employed to evaluate adsorption energies of HCl and identify the rate-determining step (RDS).

Results and discussion.

ICP and BET analysis ruled out Cu loss and sintering as primary deactivation causes. Instead, XRD and XPS confirmed that surface CuAlO2 formation correlates positively with activity decline. Thermodynamic and DFT results revealed that high temperatures facilitate the transition from CuO to CuAlO2, which significantly weakens HCl adsorption and inhibits the essential chlorination step in the redox cycle. Microkinetic modeling identified a fundamental kinetic shift: the RDS changes from the surface reaction (fresh catalyst) to the chlorination step (deactivated catalyst). The shift is statistically validated by residual analysis, proves that CuAlO2 formation triggers chlorination inhibition. These insights provide a theoretical framework for developing stable Cu-based catalysts by suppressing the formation of monovalent copper-aluminum oxides.

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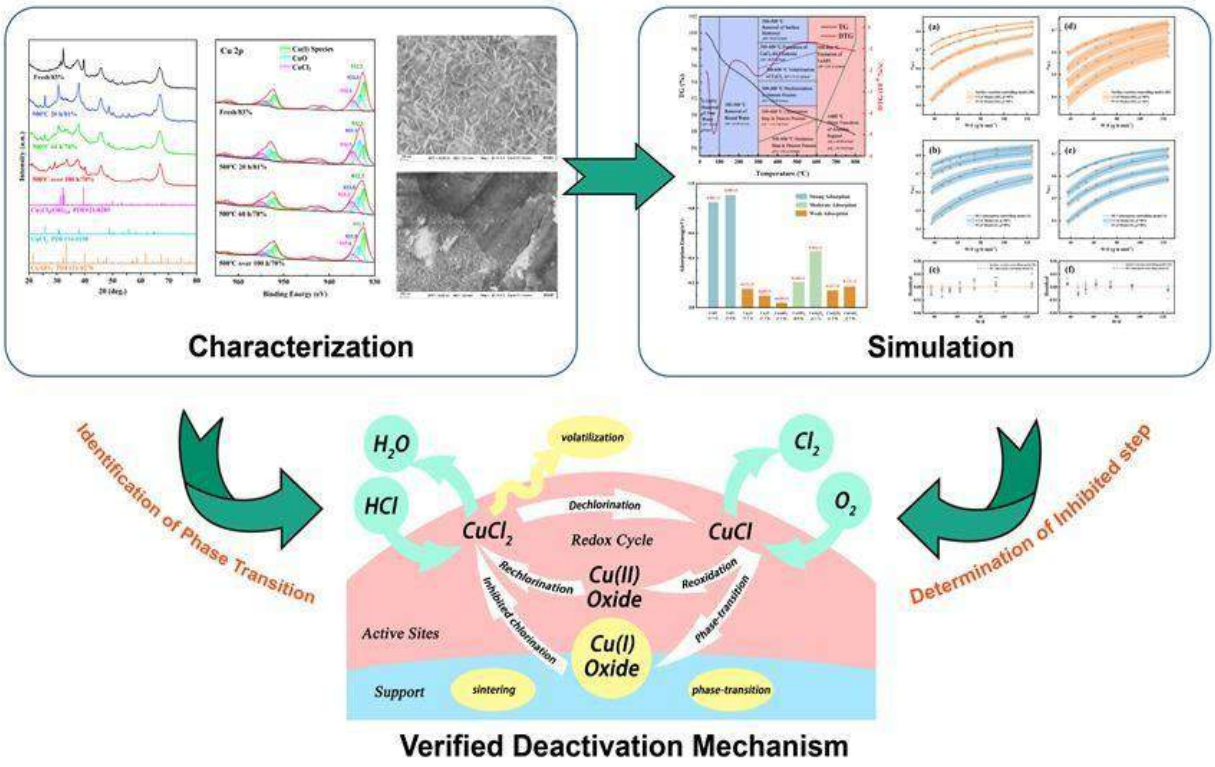

The deactivation of Cu-based Deacon catalysts: from CuAlO2 identification to simulation validation

ISCRE29 & APCRE11
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KN0107

Molecular modeling of plastic co-pyrolysis: Effects of polystyrene and its fragments on product yields, dispersion, and reaction mechanisms

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Abstract Category: Invited Lecture - Keynote Lecture

Keywords: co-pyrolysis, plastic recycling, polymer melt, molecular dynamics simulation, ReaxFF

Abstract Body.
We simulate mixtures of polyethylene (PE), polypropylene (PP), polystyrene (PS), and their fragments such as ethylbenzene (EB) and linear alpha-olefins (LAOs) at various ratios using classical and reactive force fields. All-atom models are validated by calculating conformations and diffusivities of PE melts with different chain lengths, in good agreement with experimental data. Simulations are then performed at 450 and 513 K, which mimic lowtemperature thermal co-pyrolysis conditions, showing that the decomposition of PE into LAOs influences the densities and diffusivities of PE, with the effect depending on PE chain length. In PE/PP/PS simulations, PS polymers aggregate at PS concentrations of 20 wt% or higher, leading to phase separation between PS and the other polymers. When EB, assumed to originate from PS decomposition, is included, polymer aggregation is not observed. To investigate reaction mechanisms, reactive simulations of PE and PS are conducted, showing increased heavy-oil and decreased gas yields at higher PS concentrations, consistent with experimental observations, because PS fragments such as benzene, EB, and methylbenzene bind to PE and are incorporated into heavy or light oil products. In particular, the transfer of hydrogen radicals between PE and PS not only suppresses further polymer decomposition but also generates polymer-based free radicals that can accelerate co-pyrolysis. These simulation findings help explain experimental observations regarding liquid and gas product yields and suggest an optimal PS concentration that avoids aggregation under thermal co-pyrolysis conditions, interpreted by reaction mechanisms involving hydrogen-radical transfer and benzene-derived fragments.

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MKF0260

Chemical looping oxidative dehydrogenation of methanol as a probe for oxygen reactivity

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Keywords: chemical looping; selective oxidation; oxygen reactivity; *in-situ* DRIFTS; perovskites

Introduction: Selective oxidation reactions account for the production of many highvalue and commodity chemicals. However, incumbent processes are constrained by the non-selective formation of CO_2 and strict operating limits imposed by flammability risks[1]. A chemical looping (CL) approach replaces gaseous oxygen with lattice oxygen (O_{latt}) supplied from metal oxides, eliminating explosive mixtures and associated limitations. The reactivity of the O_{latt} can be tuned by manipulating process conditions and the structure of the metal oxide[2]. Here, we use the chemical looping oxidative dehydrogenation (CL-ODH) of methanol as a probe reaction to assess how the chemical potential of oxygen (μ_O) delivered by $SrFeO_3$ (SFO) perovskite affects reaction pathways and selectivity to formaldehyde.

Methods: Strontium ferrite prepared *via* solid-state synthesis[3] was impregnated with Au or Ag. Samples were heated to 270-330°C in a packed bed, cycling the feed gas to drive reduction (2vol%CH_3OH/N_2) and reoxidation (0.21-21vol% O_2/N_2) of SFO. Outlet gases were monitored with an online Fourier Transform Infrared Spectrometer. Diffuse Reflectance Infrared Fourier Transform Spectroscopy (DRIFTS) was used to identify intermediate species during reduction, and the temperature-induced release of O_2 under N_2 was measured by thermogravimetric analysis (TGA).

Results: Production of formaldehyde achieved over SFO yielded ~0.5 $g_{HCHO}\,g^{-1}_{cat}\,h^{-1}$, comparable to Fe-Mo catalysts in studies with O_2(g)[4]. Among all samples, the Ag(15wt%)/SFO sample was the most active, leading to 15% conversion of methanol, but the least selective to formaldehyde (21%). By contrast, Au(10wt%)/SFO gave superior selectivities (80%) but little conversion (3%). The observed performance correlated to the ease of O_2 removal during TGA. Materials that released O_2 at lower temperatures (indicative of higher μ_O) were more active, but less selective in packed-bed experiments. Temporal analysis of the products (**Fig. 1**) showed that initially only CO_2 was produced over Ag(15wt%)/SFO with formaldehyde appearing when SFO partially reduced and oxygen release slowed down. Conversely, Au(10wt%)/SFO gave stable selectivity to HCHO: >80% throughout. *In situ* DRIFTS confirmed that intermediates were rapidly oxidised to CO and CO_2 over Ag(15wt%)/SFO, whereas Au and reduced SFO stabilised selective adsorbates. Increasing the pO_2 during regeneration improved the yield of formaldehyde over SFO but promoted further overoxidation on Ag/SFO.

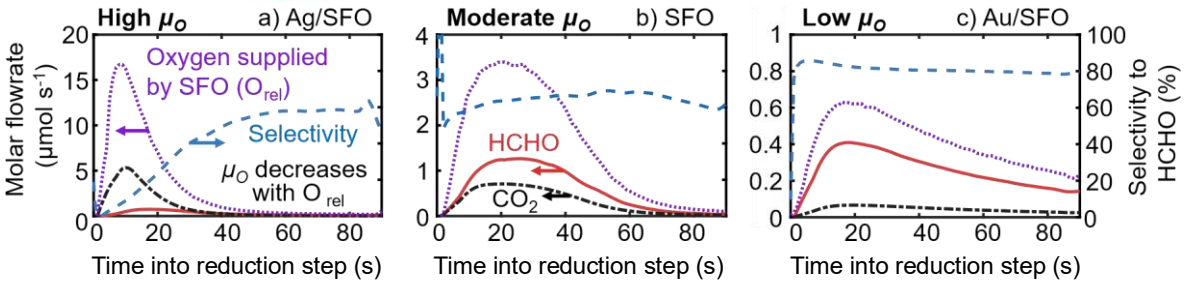

Figure 1 Product concentrations during reduction at 310°C over a) Ag(15wt%)/SFO, b) SFO, and c) Au(10wt%)/SFO. Left y-axis varies in range between a-c.

Conclusions: The chemical potential of $SrFeO_3$-based materials governs selectivity during CL-ODH of methanol. High μ_O accelerates oxygen transfer, promoting overoxidation, whereas moderate μ_O stabilises intermediates and favours formaldehyde formation. Surface modifications (Au, Ag) and altering regeneration pO_2 readily tune the μ_O, offering promising strategies to optimise selectivity in chemical looping catalysis.

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ISCRE29 & APCRE11
2026 / SEOUL, KOREA

MKF0657

Ethylene-Vinyl Acetate Copolymer Alcoholysis: Kinetic Study and Mechanism Exploration

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Fundamental

Keywords: Ethylene-vinyl acetate copolymer; Alcoholysis; In situ FTIR spectroscopy; Kinetic model; Reaction mechanism

Abstract Body.
Controlled alcoholysis of ethylene–vinyl acetate copolymer (EVA) is of great significance in both industrial production and academic research. Traditional methods for studying polymer reaction kinetics are cumbersome and time-consuming due to the requirement of product purification. Herein, we developed a new method based on in situ FTIR spectroscopy to study the alcoholysis of EVA with 32 mol% ethylene content, and verified its feasibility and accuracy. A kinetic model for predicting the reaction rate was established, and its applicability was further confirmed by flow alcoholysis experiments in a microflow reactor, showing high accuracy for conversions up to around 60% even at relatively high temperatures. Additionally, combined experimental and computational investigations were conducted to explore the kinetics and mechanism of EVA alcoholysis. The results indicate that the overall polymer chain structure has little effect on the alcoholysis rate, while the local structure of the acetate group, closely related to ethylene content, significantly influences the overall reaction rate. An empirical model was developed to predict the effect of ethylene content on the overall Kapp through detailed triad kinetic studies. The self-acceleration phenomenon in EVA alcoholysis was observed, though less pronounced than in polyvinyl acetate. Density functional theory (DFT) calculations revealed the structure-effect relationship in EVA alcoholysis, and for the first time theoretically confirmed the effect of neighboring hydroxyl groups on the self-acceleration phenomenon. This work provides valuable insights into EVA alcoholysis and offers guidance for exploring its reaction mechanism and designing production processes of EVA-related polymer materials.

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MKF0683

Direct reduction of iron: an overarching experimental modeling framework

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Fundamental

Keywords: Direct Iron Reduction, Porous Pellets Experiments, Gas-Solid Kinetics, Intrinsic mass transfer

Abstract Body.

Direct reduction of iron: an overarching experimental modelling framework

The reduction of porous iron oxide solids for industrial steel production is gaining momentum as an alternative to the conventional liquid-phase blast furnace route, driven by the need to reduce greenhouse gas emissions. A detailed understanding of the intrinsic processes occurring within porous solids at the single-pellet level is essential for reliable plant-scale design. To this end, an experimental setup was developed to investigate the reduction of individual spherical iron oxide pellets with diameters of 7, 9, and 11 mm. Reduction experiments were performed using H_2 and CO, both as pure gases and in mixed compositions, over an industrially relevant temperature range of 600–1000 °C and pressures from 1 to 10 bar(a).

This work builds upon existing single-pellet studies by combining conventional characterization techniques—SEM, EDX, XRF, microCT—for chemical and microstructural analysis and particle-scale gravimetric measurements with in-situ optical spectroscopy and off-gas analysis. This combined methodology enables quantitative assessment of the effects of pressure, temperature, and pellet chemistry on solid- and gas-phase kinetics and masstransfer phenomena, together with associated microstructural evolution, including particle swelling, pore development, carbon deposition, and cementite formation. State-of-the-art models [1, 2] for gas–solid reactions in porous media were applied to extract apparent kinetic and diffusion parameters as functions of temperature, pressure, and gas composition.

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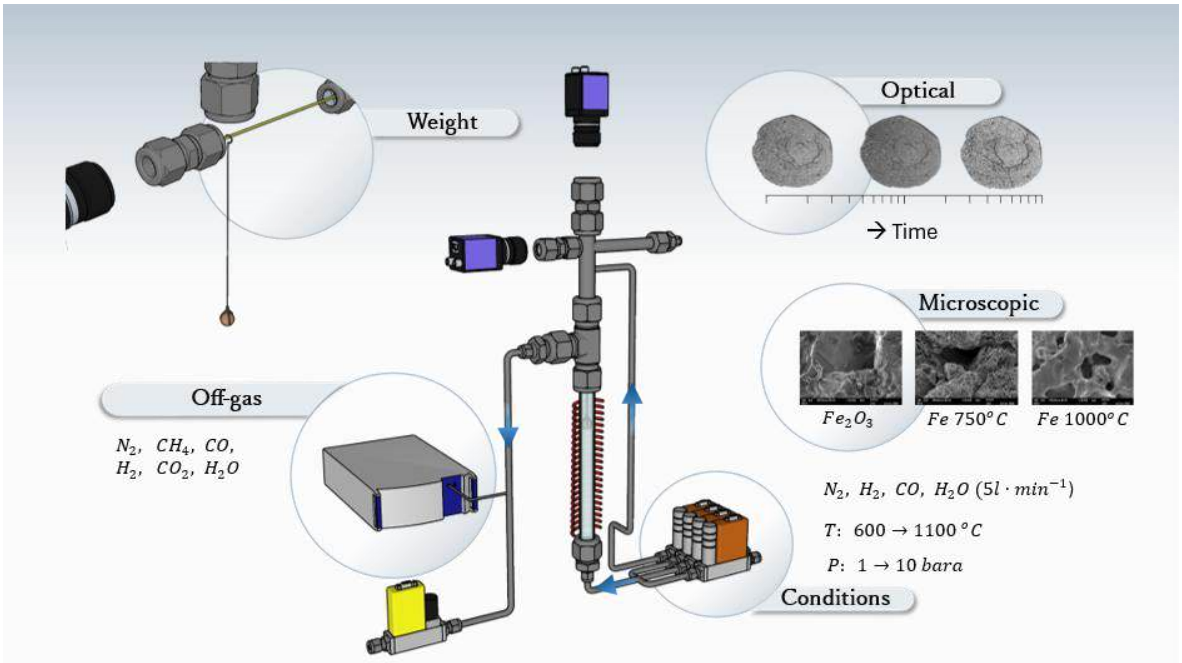
Weight
Optical
→ Time
Microscopic
Fe_2O_3
Fe 750°C
Fe 1000°C
Off-gas
N_2, CH_4, CO,
H_2, CO_2, H_2O
N_2, H_2, CO, H_2O $(5l \cdot min^{-1})$
T: 600 → 1100 °C
P: 1 → 10 $bara$
Conditions

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MKF0215

Deactivation of a Ni/Al2O3 catalyst during CO2 methanation studied in a concentration-controlled recycle reactor

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Fundamental

Keywords: Heterogeneous catalysis, Catalyst deactivation, CO2 methanation

Abstract Body.
Introduction: Catalyst deactivation negatively affects the economic efficiency of a chemical plant due to increased energy and reactant consumption during the production process and downtime costs during catalyst exchange [1]. Simulation and optimization studies can assist in developing strategies to reduce these costs. For this, however, knowledge of the deactivation kinetics is required. In the case of CO2 methanation, accurate descriptions of the reaction kinetics are available [2], yet literature lacks in detailed descriptions of deactivation kinetics. Therefore, this work investigates the deactivation of a Ni/Al2O3 catalyst during CO2 methanation, examining how the temperature and partial pressures influence the deactivation rate, identifying the dominant deactivation mechanism and developing a deactivation model.
Methods: In order to develop appropriate deactivation kinetics based on experimental data, it is necessary to decouple the catalyst activity from the concentration effects on the reaction rates. With constant inlet flow rates to the recycle reactor, partial pressures of species, and thus reaction rates, change due to deactivation, requiring exact knowledge of reaction kinetics to determine catalyst activity. To avoid additional uncertainties from kinetic models, the decoupling of catalyst activity and reaction rates is achieved by measures in the experimental design. Keeping the concentrations constant by adjusting the inlet flow rates allows for observing the catalyst activity [3].
Results and discussion: Utilizing this concentration-controlled recycle reactor (CCRR), the catalyst activity is observed over time. As shown in Figure 1a, the temperature significantly influences the deactivation rate and the deactivation is caused by sintering of the nickel particles. Furthermore, the deactivation is influenced by the partial pressures in the reactor. Figure 1b shows that an increased partial pressure of water increases the deactivation rate under otherwise constant conditions. Based on these investigations, a first deactivation model was developed. Systematic experimental studies and extension of the deactivation model will enable optimization studies on reactor design and operating strategies.

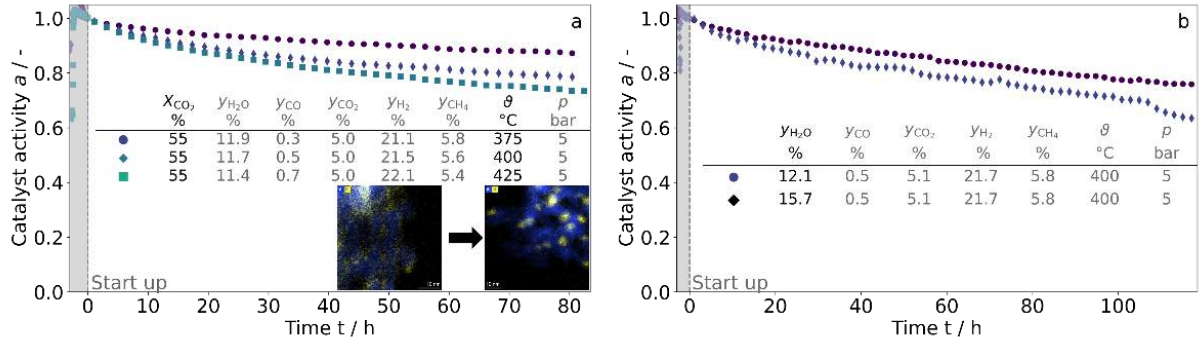

Figure 1: Effect of temperature (a) and partial pressure of water (b) on catalyst activity profiles in a CCRR. Post-mortem observation using EDS (a) reveals sintering of Ni particles.

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2026 / SEOUL, KOREA

MKF0278

The Role of Ni and Ru Sites in Thermo-Catalytic Ammonia Decomposition over Ni-BCZY cermet

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Keywords: ammonia decomposition; hydrogen generation; Protonic Ceramic Cell; microkinetic modeling

Introduction. Ammonia is a carbon-free hydrogen carrier, and its efficient decomposition is key for the operation of protonic ceramic cells. Ru-based catalysts are active but costly, motivating strategies to reduce Ru while maintaining performance. In this study, the effects of ruthenium and barium loading on nickel-based cermets support for ammonia decomposition were investigated. The most active catalyst formulation was selected for detailed microkinetic analysis of ammonia decomposition. Both experimental measurements and microkinetic modeling were performed to elucidate the influence of the support composition and metal–support interactions on the catalytic performance.[1]

Methods. Ammonia decomposition was investigated in a fixed-bed reactor using 1000 ppm NH_3 diluted in Ar over a temperature range of 473–873 K, with a GHSV of 50,000 h^{-1}. The catalysts were synthesized with varying loadings of Ru and Ba supported on YSZ, Ni-YSZ, and Ni-BCZY cermets. For the kinetic modeling, a dual-site surface microkinetic model was developed for Ru and Ni sites. Literature-based kinetic parameters were algorithmically optimized ensuring thermodynamic consistency using 1000 ppm NH_3 in the feed and validated against 500 and 3000 ppm NH_3 feed concentrations.[2,3]

Results and discussion. The experimental results confirmed that the bare Ni-BCZY cermet support is catalytically active for ammonia decomposition due to the presence of Ni. Therefore, a dual-site surface microkinetic model including both Ni and Ru active sites was developed for the best performing 0.5Ru/1Ba/Ni-BCZY catalyst. Figure 1 presents the results from the literature model and optimized model which accurately reproduced the experimental conversion trends over the temperature range tested.

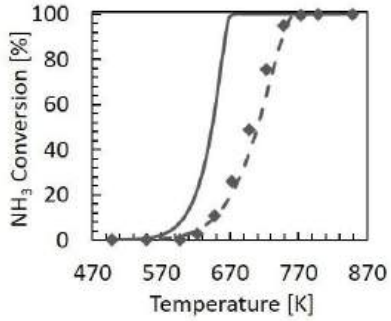

Fig. 1. Experimental (diamonds) and simulated NH_3 conversion using literature [3] (solid) and optimized[1] model (dashed). Cond: 3000 ppm NH_3; GHSV = 50,000 h^{-1}; ramp = 2 K min^{-1}; P = 1 bar.

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2026 / SEOUL, KOREA

MKF0317

Low Temperature Fast-SCR on Cu-SSZ-13 Catalysts: Evidence for Redox and Surface Nitrates Routes

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Fundamental

Keywords: Fast-SCR, Cu-SSZ-13, Transient Kinetic Analysis, Redox Mechanism

Abstract Body.

Introduction. Cu-SSZ-13 catalysts are widely employed for NO_x abatement via the NH_3 -SCR process. Their redox functionality and hydrothermal stability support a high DeNOx activity across a wide temperature range. The Fast-SCR reaction ($NO+NO2+2NH3 \rightarrow 2N2+3H2O$) is particularly important at low T (< 250 °C), where emissions control is most challenging. Understanding its mechanism is essential for predicting catalyst performance under realistic operating conditions. Previous studies describe copper nitrates [1], Brønsted acid sites [2], and redox [3] based mechanisms for Fast-SCR, yet quantitative models that reproduce transient behaviors remain limited. This work aims to construct a validated dynamic kinetic framework that captures the different interacting effects.

Methods. Two Cu-SSZ-13 samples, characterized by the same composition (2.6 % w/w Cu and SAR equal to 30), but with different hydrothermal aging levels (10 % v/v O2 and H2O in N2), were investigated. The degreened sample (DG) was treated at 550 °C for 4 h, while the aged one (AG) was treated at 650 °C for 50 h. Transient response methods are used to explore different operative conditions and are combined with transient kinetic analysis.

Results and discussion. On step feeding NO, NO2 and NH3 to a completely pre-oxidized catalyst, the transient behavior of these species, N2 and N2O are monitored, until they reach a steady state after over 6000 s, see square symbols in Fig. 1a. By assuming literature reaction mechanisms just based on nitrates as Fast SCR intermediates [1-3], the reactor model is not able to accurately simulate these transients. On the contrary, combining the redox features of Cu species with the surface nitrates chemistry [1] (Fig. 1c), the model provides a successful fit as shown by solid lines in Fig. 1a. Different operating conditions (catalyst pre-treatment, presence of O2, presence of H2O, NO/NO2 ratio, temperature) and catalyst aging provided further validation of this model.

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MKF0433

Composition and Reaction Modeling of Lignins during Hydroconversion

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Fundamental

Keywords: Lignin; Composition modeling; Molecular reconstruction; Kinetic Modeling; Stochastic Simulation Algorithm.

Abstract Body.

Introduction

The conversion of lignocellulosic biomass into liquid fuels and chemicals involves a wide range of processes. A major challenge in modeling these processes lies in the intrinsic structural complexity of lignin, which limits both its analytical characterization and the mechanistic understanding of its conversion pathways and kinetics. In this work, a molecule-based methodology is developed to model lignin hydroconversion by combining a probabilistic structural representation with kinetic Monte Carlo simulations.

Methods

Due to the heterogeneous and irregular nature of lignin, its molecular structure cannot be directly obtained from experimental analyses. Instead, multiple complementary analytical techniques have to be used to infer average structural features. In this work, these multi-level analytical data are combined so as to represent lignin by a probability matrix describing the occurrence of different lignin-derived moieties and inter-unit linkages. Each row of the matrix concerns a specific type of aromatic unit, while each column represents a type of side chain or inter-unit linkage. Sampling this matrix yields a representative ensemble of molecules whose average properties match those of the experimental lignin.

This molecular ensemble was then used as input for a kinetic Monte Carlo model based on Gillespie's Stochastic Simulation Algorithm. Lignin conversion was simulated by tracking the evolution of a discrete population of molecules undergoing a set of elementary reactions. Reaction parameters were derived from literature data on structurally related model compounds, allowing the reaction network to be generated dynamically during the simulation without requiring a predefined kinetic scheme.

Results and discussion

The methodology was applied to a wheat straw soda lignin (Protobind 1000), characterized experimentally by means of elemental analysis, 1H-NMR, 13C-NMR, and gel permeation chromatography. After phosphitylation, a 31P-NMR analysis was also performed. This lignin had an average molecular weight of 4915 g/mol, while its elemental analysis showed that the lignin contained 65 wt% of carbon, 28 wt% of oxygen, 6 wt% of hydrogen and 1 wt% of nitrogen. From these analytical data, a matrix of occurrence probabilities was created. After resampling, the set of 1000 molecules accurately reproduced the experimental elemental composition,

molecular weight, polydispersity index, and NMR signatures. The kMC simulations successfully predicted the yields of gas, liquid, and solid products, as well as gas composition, bio-oil characteristics, and the molecular weight distribution of the residual lignin.

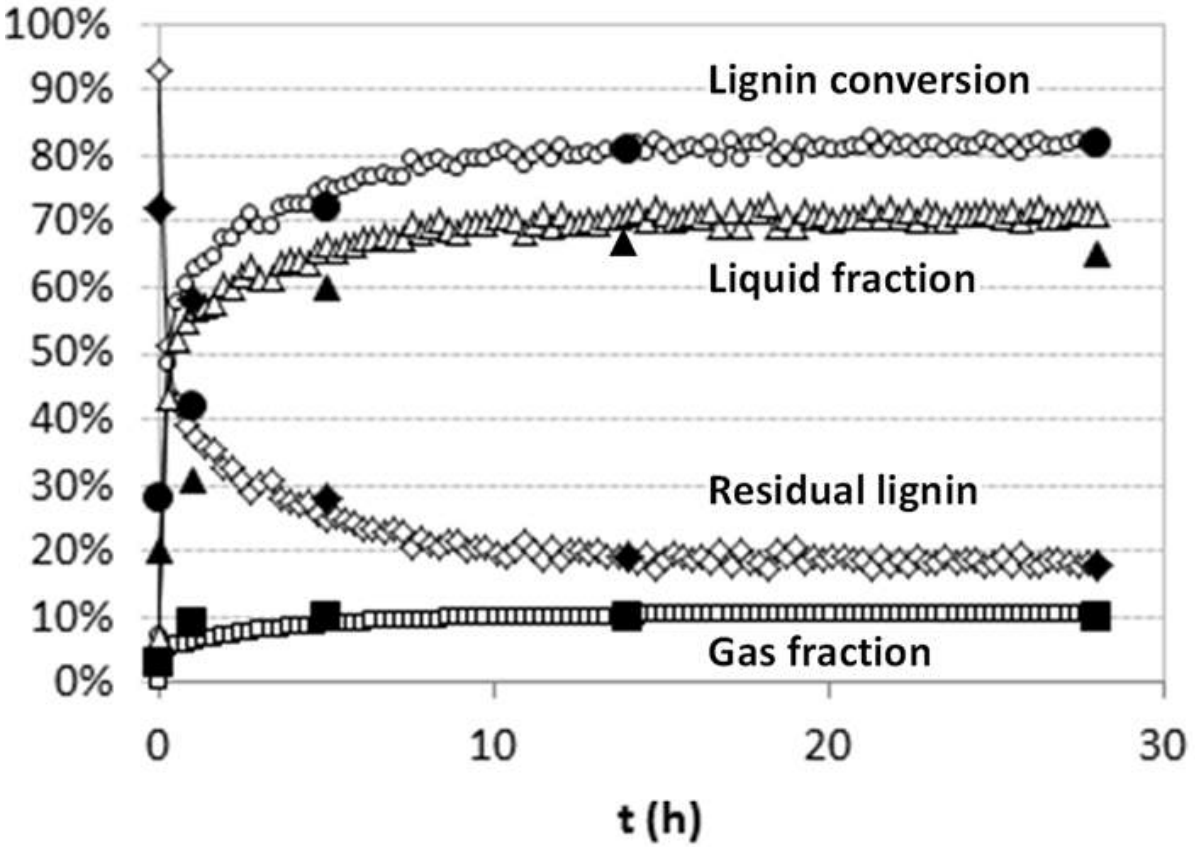

Figure 1. Reaction modeling: Evolution of the lignin conversion and the product fractions: experimental (closed symbols) vs. simulated (open symbols).

Conclusion

Overall, this stochastic framework provides a consistent and predictive tool for representing lignin structure and modeling its hydroconversion, offering new insights into biomass conversion mechanisms at the molecular level.

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MKF0636

Kinetic Study of Ethylene Hydroformylation over Rh supported SiO2 catalysts

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Fundamental

Keywords: Kinetic analysis: Reaction mechanism: Propionaldehyde

Abstract Body.

Introduction. Hydroformylation is an important reaction that converts alkenes, carbon monoxide, and hydrogen into aldehydes. Aldehydes are industrially valuable compounds, serving as key intermediates to produce alcohols and carboxylic acids. At present, Rh-based homogeneous catalysts are widely employed for industrial hydroformylation; however, they suffer from inherent drawbacks related to catalyst separation and recovery. To address these issues, heterogenization of hydroformylation catalysts by supporting them on rigid solid substrates has been proposed.[1] In this study, we first aimed to elucidate the reaction mechanism of hydroformylation over Rh species supported on silica-based materials, and subsequently investigated the effect of the support. Mesoporous silica MCM-41 and zeolite beta were further employed as model supports, and hydroformylation was examined to clarify the structure–performance relationship.

Methods. Rh was supported on the silica supports via an impregnation method. Catalytic reaction was performed using a home-made fixed-bed plug flow reactor. The fluent gas was analyzed by an in-line GC equipped with and an FID detector.

Results and discussion. First, we confirmed that the reaction was free from diffusion limitations under the standard reaction conditions by observing a constant reaction rate over parameters relevant to mass transfer. In addition to the target hydroformylation of ethylene, hydrogenation of ethylene to ethane proceeded as a side reaction. As reported previously, the hydrogenation reaction was faster than hydroformylation, and the ratio of reaction rates ($r_{Hydroformylation}/r_{Hydrogenation}$ denoted as ζ) was approximately 0.15.

The reaction rate dependence on the partial pressure of each reactant was examined. For hydroformylation, positive reaction orders of 0.44 and 1.0 were observed with respect to H_2 and ethylene, respectively, while a negative reaction order of −0.39 was observed for CO. These results suggested that CO strongly covers the active sites due to its preferential adsorption via electron donation, thereby inhibiting the adsorption of other reactants.
The rate-relevant step is therefore considered to involve adsorbed ethylene and dissociated hydrogen, assuming CO insertion step. Based on these kinetic analyses, a rate equation for ethylene hydroformylation was derived.

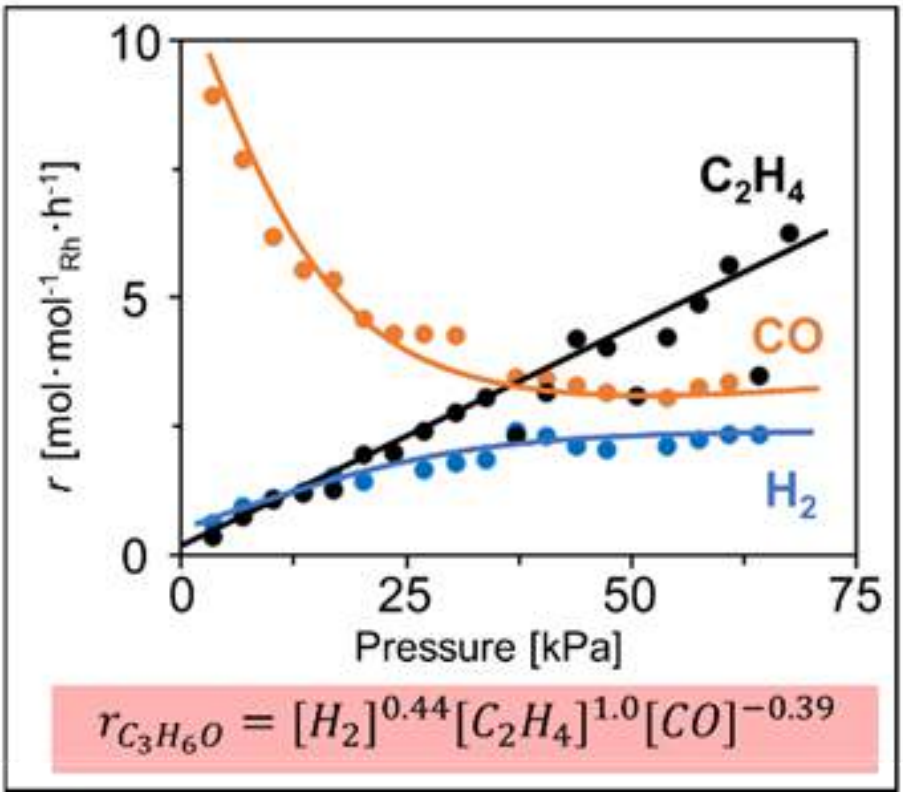

Figure 1. Rate dependence

Acknowledgments
This research was financially supported by JSPS KAKENHI Grant Number 25K08789. We acknowledge Prof. Wen-Yueh Yu and his group memberes (NTU) for H2 and CO adsorption measruements.

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ISCRE29 & APCRE11
2026 / SEOUL, KOREA

MKF0638

Impact of Fe-Fe3C-C phase evolution on methane pyrolysis kinetics: from catalyst structure to reactor scale

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Fundamental

Keywords: Low-C hydrogen, iron catalysis, methane pyrolysis, kinetic analysis, deactivation.

Abstract Body.

Introduction. Catalytic CH4 pyrolysis is a promising route for low-C hydrogen production. Iron catalysts are attractive due to their low cost and high activity. Pyrolysis is inherently dynamic as growth of carbon and evolution of solid phases (Fe-Fe3C-C) strongly affect catalyst activity and stability. These structural changes challenge kinetic analysis, hindering reactor design and scale-up. The nature of the active phase and the role of carburization is debated [1]. Here, we address this challenge with an integrated approach that combines operando synchrotron measurements to capture molecular-scale transformations at the particle scale, with packed-bed tests and modeling to derive kinetic expressions with mechanistic interpretation.

Methods. Fe-Al2O3 catalyst was obtained by fusion-decomposition using nitrate salts, with an equimolar Fe:Al ratio [2]. Operando X-ray absorption spectroscopy (XAS) and powder X-ray diffraction (PXRD) with online MS tests were carried out at ESRF synchrotron (BM23), with focus on H2-pretreatment and CH4-pyrolysis (1mgcat, 100% H2, then 2.5% CH4, 800°C), monitoring reduction, carburization, and C-growth. Complementary kinetic tests were performed in a packed bed reactor (PBR, 50-750 mgcat, 800°C, 2.5-95% CH4, 5-100 NL/h/gcat). Dynamic PBR modelling supports multiscale quantitative data analysis.

Results and discussion. Operando experiments in highly diluted streams and ultra-high space velocity showed that after CH4 injection, the fraction of a-Fe declined, while crystalline Fe_3C grew, simultaneously with the onset and dynamics of H2 formation (Fig.1a). At the PBR scale the same diluted feed experiments (Fig.1b) similarly revealed multiple kinetic stages: (1) rapid deactivation of metallic Fe sites due to C-blockage ($CH_4 \rightarrow CHX^* + H^* \rightarrow C^* + 2H_2$); (2) Fe_3C formation; (3) mitigated deactivation on Fe_3C and C-accumulation ($CH_4 \rightarrow CHX^* + H^* \rightarrow 1/n\ C_{n+2}\ H_2$). Thermodynamics and integral regime due to lower space velocity stretched the global dynamic response. At high CH4 concentrations and progressively increasing space velocity where quasi-differential regime established, the fingerprint of the particle dynamics turned into complex initial evolutions of the reactor performance, with a minimum-maximum trend in the conversion (circle in Fig.1c). The quantitative analysis of operando solid-phase and PBR data now opens to the development of comprehensive structure-activity-dependent kinetics.

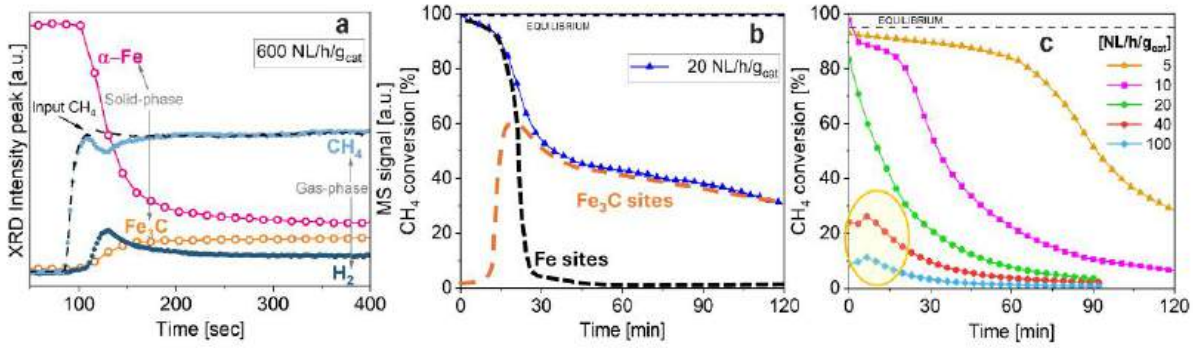

Fig.1: Pyrolysis tests: gas-phase with operando PXRD (a); PBR tests with 5% (b) and 40% CH4 (c).

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2026 / SEOUL, KOREA

MKC0536

Microkinetic modelling of Methane oxidation and NO_x reduction for stoichiometric CNG vehicles

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Keywords: CNG aftertreatment; microkinetic modelling; methane oxidation; NO_x reduction; DFT

Introduction

Aftertreatment of the stoichiometric natural gas vehicle exhaust is achieved using a three-way catalyst (TWC). Palladium-based catalysts are highly active for methane oxidation, while Rhodium promotes NO reduction. However, there are limited mechanistic studies on simultaneous CH_4 oxidation and NO reduction [1]. In this work, ab-initio calculations are performed to obtain the surface energetics and further develop a microkinetic model to study the combined methane oxidation and NO reduction over Pd and Rh catalysts.

Methods

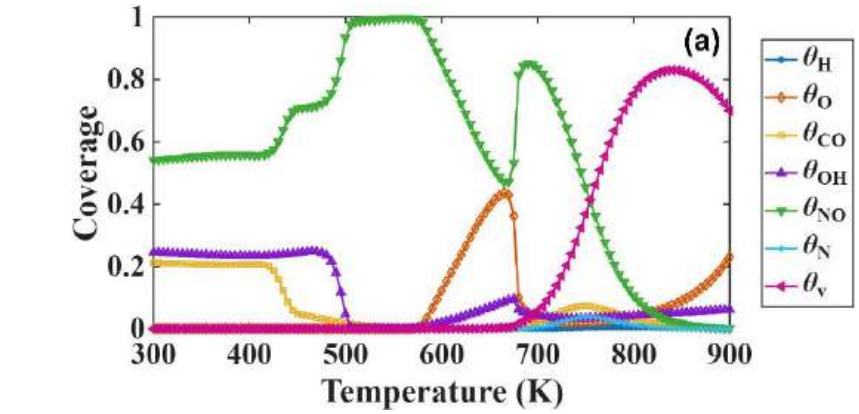
The mechanism for CH_4 oxidation and NO reduction over Pd(100) facet was proposed to consist of 19 elementary steps. The rate constants for these steps were determined using density functional theory (DFT) calculations with the transition state theory used as the basis [2]. The net rate of each step (r_k) was determined which was then used to compute the rate of change of surface coverage (θ) of the adsorbed species using Eq. 1.

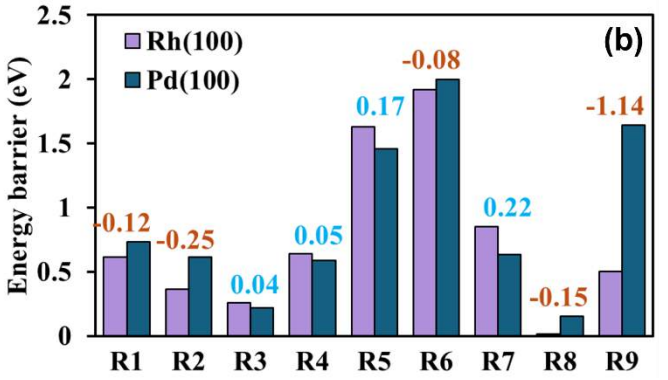
$$\frac{d\theta_i}{dt} = \sum_k r_k(\theta) n_{k,i} \quad (1)$$

The coverages were computed at 1 atm and in the range of 300 – 900 K for a representative gas mixture composition [1].

Results and discussion

The surface coverage profile of prominent surface species for varying temperatures is shown in Figure 1(a). Below 440 K, CO*, NO*, and OH* have significant coverages owing to their high adsorption energies**.** A negative correlation between NO* and CO*/OH* between 440 – 570 K is observed. NO* dissociates in the range 570 – 700 K, as shown by the inverse coverage relation of NO* and O*. The O* from NO* dissociation contributes to OH* formation in this range. With a further increase in temperature, most of the species desorb except for O* and OH*. Figure 1(b) depicts the comparison of energy barriers over Pd(100) and Rh(100). Pd shows a much higher barrier for NO dissociation, with comparable barriers for other reactions. Similar to Pd(100), the microkinetic model for Rh(100) is developed, and the results obtained by the integration of the two models will be discussed in the full manuscript.





R1	$CH_4^* + * \leftrightarrow CH_3^* + H^*$
R2	$CH_3^* + * \leftrightarrow CH_2^* + H^*$
R3	$CH_2^* + * \leftrightarrow CH^* + H^*$
R4	$CH^* + * \leftrightarrow C^* + H^*$
R5	$C^* + O^* \leftrightarrow CO^* + *$
R6	$N^* + N^* \leftrightarrow N_2^* + *$
R7	$O^* + H^* \leftrightarrow OH^* + *$
R8	$O_2^* + * \leftrightarrow 2O^*$
R9	$NO^* + * \leftrightarrow N^* + O^*$

Figure 1: (a) Surface coverage vs temperature, (b) Energy barriers for surface reactions over Pd(100) and Rh(100).

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ISCRE29 & APCRE11
2026 / SEOUL, KOREA

MKF0013

Simplifying Batch Reactor Models with Some Fast Equilibrium Reactions Using Extent of Reaction

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Fundamental

Keywords: extent of reaction, instantaneous equilibrium, dynamic modeling, parameter estimation, model simplification

Abstract Body.
A straightforward approach is proposed for formulating batch reactor models where some reactions are fast and can be assumed to be at instantaneous equilibrium, while slower reactions govern the process dynamics. A proposed new method uses extents of reaction (also known as reaction coordinates) to derive the model equations. Fast equilibrium reactions are described using algebraic equations, and slower reactions are described by ordinary differential equations (ODEs) for the corresponding extents of reaction. Algebraic material balances are used to track the behavior of individual species in terms of extents of reaction. The resulting differential-algebraic equation (DAE) models can be readily solved using standard DAE solvers. Compared to traditional species-based ODE models, the proposed DAE models involve fewer differential equations and contain fewer parameters that require estimation (or specification using engineering judgment). The methodology is demonstrated using a pharmaceutical saponification reaction network that includes two fast equilibrium reactions and four irreversible reactions. The resulting DAE model requires estimation of 4 kinetic parameters (instead of 6 in the traditional model) using experimental data. Estimation of the kinetic and equilibrium parameters, using data from five replicate batch experiments, results in parameter estimates that are statistically significant at the 95 % confidence level. The resulting DAE model provides a good fit to measured concentrations of methyl ester, butyl ester, and the sodium carboxylate product. By contrast, the corresponding traditional ODE model, which contains 6 kinetic parameters, results in estimability problems using the same dataset for parameter fitting. The proposed methodology provides a simple approach for modeling reaction systems where some reactions are in fast equilibriums, and other slower reactions determine the dynamic behavior of the batch reactor. The technique can readily be applied to reaction schemes involving a large number of reactions. Extensions are being developed to account for semi-batch and continuous reactor operation.

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MKC0090

Adaptation and Application of Dynamic Modeling for Gas Fermentation Under Cell Retention and Elevated Pressure Conditions

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Computational
Keywords: gas fermentation, kinetic model, acetogens, Clostridium ljungdahlii, pressure, process optimization

Abstract Body.

Introduction: CO2-containing emissions can serve as substrates for fermentation with acetogen bacteria to produce basic chemicals and fuels. However, due to the generally low product yields, the process design must be optimized for increased efficiency. For this optimization to be successful and for the development of advanced control strategies, a robust model is needed that can accurately predict system responses to varying process conditions. Only a few fermentation models have been developed for continuous cell retention or elevated pressure conditions [1,2], both of which are beneficial for integrating gas fermentation with CO2 separation technologies. Therefore, this study adapts a dynamic kinetic model from literature to simulate these conditions, enabling a model-supported process design with Clostridium ljungdahlii and similar organisms.

Methods: The literature model [1] was modified by adjusting key equations and re-estimating kinetic parameters derived from long-term fermentation experiments in a continuous stirred tank reactor. The prediction accuracy of the model was validated in long-term fermentation experiments. The validated model was then used to predict the impact of varying substrate gas compositions and flow rates on growth and maximum product yield.

Results and discussion: While the re-estimated base model could predict trends, it was challenged to represent the ethanol-to-acetate ratio under high gas flow, cell retention, and high-pressure conditions. The addition of a carbon dioxide dependency to the hydrogen uptake rate and the acetate-to-ethanol conversion rate improved the model's accuracy to predict biomass and product concentration trends under cell retention and moderately increased pressure conditions by up to 30% [3]. Predictions made with the validated models indicate an increase in product concentration at lower gas residence times, a change in optimal substrate gas composition for maximum product concentration, and a switch in main product depending on the substrate gas composition. Ethanol is the main product when the substrate gas mainly consists of H2 and CO, and is correlated with maximum biomass growth, while the maximum in acetate production is obtained when the substrate gas consists of 50% H2 in a mixture of CO and CO2 (Figure 1).

The advancements made to the model in this study allow conditions with high hydrogen substrate gas, cell retention, and moderate pressures to be described accurately. This enables an expanded application of the model as an optimization and prediction tool to screen feasible substrate gases, and can be a step toward using the model for process control [3].

ISCRE29 & APCRE11
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MKF0218

Morphology-Controlled Kinetics in the Catalytic Glycolysis of PET

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Fundamental
Keywords: Depolymerisation, Poly(ethylene terephthalate), Glycolysis, Kinetics

Abstract Body.

Introduction

The catalytic glycolysis of poly(ethylene terephthalate) (PET) is a promising strategy for enabling a closed-loop PET economy. To realise the recycling of varied real-word wastes it is important to understand how the recycling process operates with different forms of feedstock. While kinetic studies typically emphasise catalyst selection, loading, and temperature1,2, the influence of PET morphology is rarely quantified. This study examines how PET morphology impacts depolymerisation kinetics under $Zn(OAc)_2$ catalysis. By isolating morphological effects from catalytic ones, it aims to provide predictive insight for reactor design and industrial throughput.

Methods

$Zn(OAc)_2$ (0.48g), N-methylpyrrolidone (0.25mL) and ethylene glycol (30mL) were charged to a 100mL round-bottomed-flask and heated to 180°C under reflux. Addition of PET (5g) initiated the reaction. 1H qNMR was used to quantify PET conversion. Morphology was examined throughout the reaction using ^{1}H NMR, optical microscopy, differential scanning calorimetry (DSC), uniaxial compression testing, pycnometry, and particle size analysis.

Results

Under identical reaction conditions, depolymerisation was highly dependent on PET morphology (Figure 1A). Specifically, the kinetics and therefore environmental energy impact1 were dependant on the effective radius of the substrate (Figure 1B). A linear relationship between apparent rate constant and specific surface area enabled rate prediction across morphologies utilising shrinking-core kinetics. Morphology evolution was investigated throughout the depolymerisation. DSC showed early-stage annealing and lamellar thickening, followed by lamellar breakdown during depolymerisation. Microscopy revealed surface roughening and cracking that increased reactive area exponentially. Uniaxial compression testing indicated >95% loss of compressive strength by 20% conversion, consistent with mechanochemical weakening. End-group analysis showed a decrease in Mn correlating with embrittlement and fragmentation. Together, these observations support a mechanistic sequence of chain scission, annealing, surface cracking, and auto-acceleration via rising surface area. Applying mechanical grinding after early-stage weakening increased the apparent rate constant by a factor of 70 and reduced environmental energy impact by up to 33%.

Conclusion

PET morphology exerts a decisive influence on depolymerisation efficiency and reactor energy demand. Even with a robust catalyst such as $Zn(OAc)_2$, kinetics were constrained by substrate geometry, inline with a shrinking-core kinetic model. Integrating controlled grinding or mechanochemical mixing into glycolysis reactors could therefore deliver substantial gains in reaction rate, energy efficiency, and scalability for PET chemical recycling.

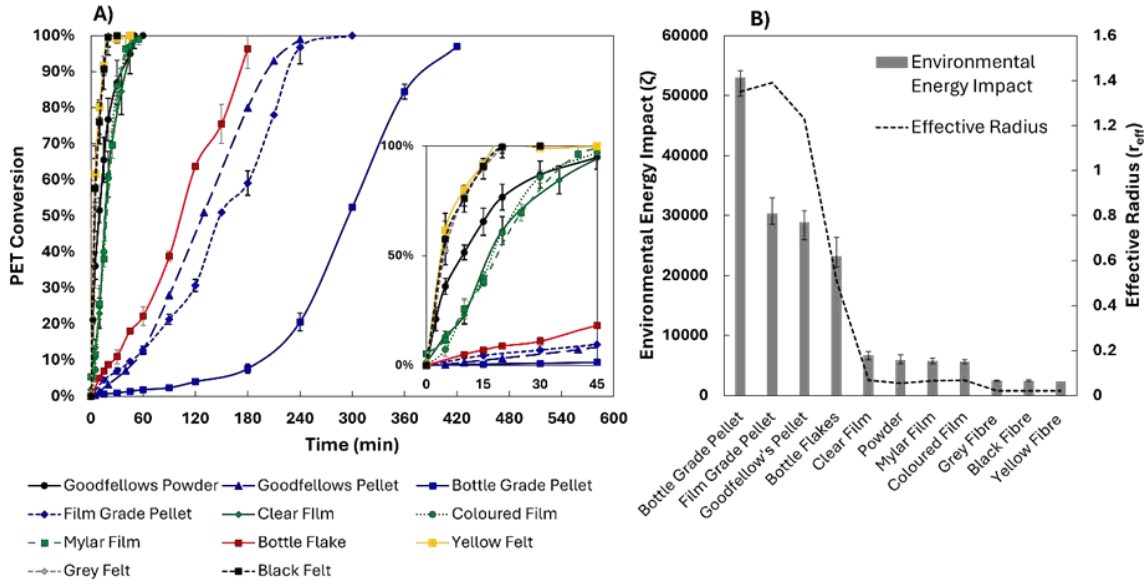

Figure 1A) PET conversion vs time for PET morphologies. B) Depolymerization environmental energy impact & effective radii for PET morphologies.

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ISCRE29 & APCRE11
2026 / SEOUL, KOREA

MKF0360

Unveiling Active Center of Ru3Sn7/ZnO Catalyst for Carboxylic Acids Hydrogenation: in situ DRIFTS Study

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Fundamental

Keywords: Hydrogenation, Carboxylic acids, Ru3Sn7 alloy, in situ DRIFTS

Abstract Body.

Introduction. The catalytic hydrogenation of carboxylic acids to alcohol is one of the promising techniques to upgrade the bio-derived carboxylic acids. In particular, bimetallic Ru-Sn catalysts have shown exceptional efficiency in selective production of alcohol. Additionally, many efforts have been made to investigate the active center of bimetallic Ru-Sn system. Especially, recent studies reported that the formation Ru3Sn7 alloy played crucial role of main active center in selective production of alcohol [1]. However, the precise role of Ru3Sn7 alloy in catalytic hydrogenation of carboxylic acids remains unclear.

This study aimed to clarify the active centers and reaction pathway on Ru-Sn bimetallic catalyst system during catalytic hydrogenation of carboxylic acids by employing in situ DRIFTS measurement.

Methods. The interaction of carboxylic acids with catalysts was analyzed by in situ DRIFT spectroscopy with an iS50 instrument (Thermo Fisher SCIENTIFIC) equipped with a Praying Mantis diffuse reflectance accessory. Acetic acid was selected as the probe molecule. After reduction step, the adsorption of acetic acid on catalysts was analyzed before the temperature programmed desorption and surface reaction under Ar and H2 flow, respectively.

Results and discussion. The acetic acid TPD results showed that the adsorbed acetic acid intermediates such as acetate and acetyl groups desorbed at higher temperature on Ru than Ru3Sn7 catalyst. The result was contradictory to the previous descriptions [1,2]. The optimized moderate adsorption energy on Ru3Sn7 might contribute to the lowered activation energy in RDS, resulting in fast alcohol formation.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

MKF0585

Development of thermodynamically consistent microkinetic model of a Pd-based three-way catalyst for natural gas vehicles

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Keywords: Three-way catalyst; Microkinetic modelling; Thermodynamic consistency.

Introduction

Natural gas vehicles are promising alternatives to diesel and gasoline vehicles considering abundant availability of natural gas reserves, lower price and lower emissions. Microkinetic models (MKMs) for three-way catalysts in gasoline vehicles do not consider a detailed CH_4 oxidation chemistry and hence are not applicable for natural gas vehicle exhaust. To the best of our knowledge, a comprehensive microkinetic model for a Pd-based three-way catalyst for natural gas vehicles involving CH_4 oxidation and NO reduction simultaneously is not available in the literature, which serves as a motivation for the study.

Methods

A detailed reaction scheme involving both CH_4 oxidation and NO reduction is considered, which consists of 42 elementary steps, 10 gaseous species and 21 surface species. Thermodynamic consistency of the microkinetic model is ensured by comparing the enthalpy change (ΔH) and entropy change (ΔS) of an overall global reaction with the summation of ΔH and ΔS of the corresponding elementary steps. A 1D+1D single channel isothermal monolith reactor model is employed to predict the spatio-temporal concentration profiles.

Results and discussion

The model results were compared against experimental data for a commercial Pd-based three-way monolith catalyst [1]. The model is able to capture all the major trends observed in the experimental data (Fig. 1). Based on sensitivity analysis, it is found that CH_4 dissociation is the rate determining step for CH_4 conversion whereas the combination of adsorbed CO and O to form CO_2 is a key step that governs CO conversion under rich, stoichiometric, as well as lean conditions. H-assisted NO dissociation is the rate determining step for NO conversion under rich conditions whereas the oxidation of adsorbed H greatly hinders NO conversion under lean conditions. Dissociative adsorption of H_2 is the rate determining step for H_2 conversion under lean conditions. Under rich and stoichiometric conditions, H_2 conversion is primarily influenced by the competitive oxidation of adsorbed H and CO. The role of H_2, CO, and CH_4 in NO reduction was investigated and it was observed that H_2 plays a dominant role in NO reduction.

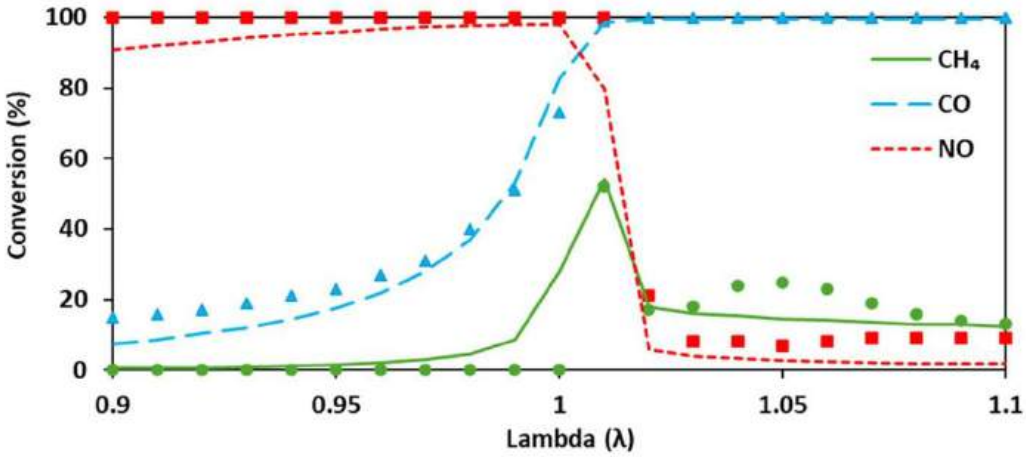

Fig. 1. Model-predicted (markers) and experimental (curves) conversions of CH_4, CO, and NO.

Conclusions

A thermodynamically consistent MKM is developed which is able to predict experimental data over a wide range of λ. Rate-determining steps are determined using sensitivity analysis. Reaction pathway analysis is performed to find the dominant pathways for CH_4, CO, and NO conversion. H_2 is identified as the primary reductant for NO.

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2026 / SEOUL, KOREA

MKF0630

Apparent Kinetic Parameters of Friedel–Crafts Alkylation over Hierarchical Beta Zeolites Derived from Pseudo-First-Order Modeling

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Fundamental

Keywords: Friedel–Crafts alkylation; Nanosponge Beta Zeolite; Pseudo-first-order kinetics

Abstract Body.
Friedel–Crafts alkylation is a representative acid-catalyzed reaction commonly used to probe the catalytic behavior of zeolitic materials. Although Beta zeolite possesses a three-dimensional pore network and strong Brønsted acidity, conventional forms often suffer from intracrystalline diffusion limitations that hinder effective active-site utilization and obscure intrinsic kinetic behavior. Hierarchical Beta zeolites with introduced mesoporosity offer a promising route to mitigate such diffusion constraints; however, quantitative kinetic comparisons based on turnover-normalized metrics remain limited. Simplified kinetic modeling that enables direct extraction of apparent rate constants and activation energies is therefore required to establish clear structure–kinetics correlations. In this study, the Friedel–Crafts (FC) alkylation of benzene with benzyl alcohol was employed as a model reaction to compare mesoporous and bulk zeolites using turnover-based analysis combined with pseudo-first-order kinetics and Arrhenius evaluation.
The FC alkylation of benzene with benzyl alcohol was conducted over Beta zeolites under identical liquid-phase conditions. Benzyl alcohol was treated as the limiting reactant, and reaction rates were evaluated by varying its amount. Catalytic performance was quantified using turnover number (TON) and turnover frequency (TOF), normalized by accessible acid sites. Assuming pseudo-first-order kinetics with respect to the limiting reactant, apparent rate constants were extracted from conversion data. Temperature-dependent experiments were performed and apparent activation energies were determined via Arrhenius analysis.
At low limiting reactant amounts, mesoporous and bulk Beta zeolites exhibited comparable TON values, indicating similar intrinsic activity under conditions where diffusion limitations are minimal. As the reactant amount increased, however, a clear divergence emerged: the mesoporous Beta zeolite showed substantially higher TON and TOF values, whereas the bulk catalyst exhibited only modest improvement, reflecting progressive loss of active-site utilization. Pseudo-first-order kinetic analysis revealed that apparent rate constants increased with reactant amount for both catalysts, but the increase was significantly more pronounced for the mesoporous Beta zeolite, leading to an amplified difference at higher loadings. Temperature-dependent studies further highlighted contrasting kinetic behavior. The reaction rate over mesoporous Beta zeolite exhibited strong temperature sensitivity, whereas the bulk catalyst showed only limited enhancement. Arrhenius analysis yielded a lower apparent

activation energy for the mesoporous catalyst, indicating facilitated reaction pathways. These results demonstrate that hierarchical pore architecture fundamentally alters the apparent kinetics of Friedel–Crafts alkylation by improving active-site accessibility and reducing diffusional resistance, rather than merely increasing surface area.

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2026 / SEOUL, KOREA

MKF0632

O2 co-feed as Diagnostic Tool to Investigate H-Poisoning on NH3 Decomposition over Ru-Based Catalysts

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Fundamental

Keywords: NH3 decomposition; Ru; hydrogen

Abstract Body.
Purpose. Ammonia decomposition for hydrogen production is attracting increasing attention; however, a deep understanding of the kinetics and reaction mechanism is essential for optimal catalyst and reactor design. Ruthenium is widely recognized as the most active metal for this reaction1, but our previous studies indicate that the strength of Ru-H* interaction is the primary bottleneck in NH_3 decomposition kinetics2. In this work, the potential of hydrogen removal from the catalyst surface was investigated through diagnostic O2 co-feeding experiments. A complete kinetic model was developed to fully characterize the NH3/O2 reacting system.
Methods. NH_3 decomposition, H2 oxidation, NH3 oxidation were investigated over $Ru/MgAl_2O_4$ catalyst in a fixed-bed reactor using diluted feeds, GHSV =20000 Nl/h/kgcat. 1-D reactor modelling was used to develop intrinsic kinetics of the various reactions.
Results. Figure 1 reports in symbols the results of experiments with 1% NH3 and 1%NH3+10%H2 feeds, that highlight the significant poisoning effect of H2 on NH3 decomposition. A simple rate expression with a negative (-1.5) order on H2 fully explains the observables2. In order to prove the potential benefit from H-scavenging, oxygen (O_2) co-feed was selected as the simplest diagnostic tool, as H_2 can react with O_2 via oxidation. Figure 1 also shows the results of an O2 co-feed experiment (1%NH3 + 0.25% O2), where at about 235°C a switch of the dominant reaction scheme occurred. At low temperatures, NH_3 oxidation was the main reaction ($4NH_3+3O_2 \rightarrow 2N_2+6H_2O$). Once O_2 concentration reached a characteristic threshold (estimated O-coverage=0.83), a rapid dynamic evolution was observed that gave rise to the onset of NH3 decomposition ($NH_3 \rightarrow 0.5N_2+1.5H_2$) with simultaneous H2 oxidation ($H_2+0.5O_2 \rightarrow H_2O$). Through the independent kinetic study of the single reactions (NH3 oxidation, NH3 decomposition, H2 oxidation) a full and very accurate prediction of the O2-cofeed experiment was obtained and revealed that the rate of NH3 decomposition is dramatically boosted by the H2 subtraction.

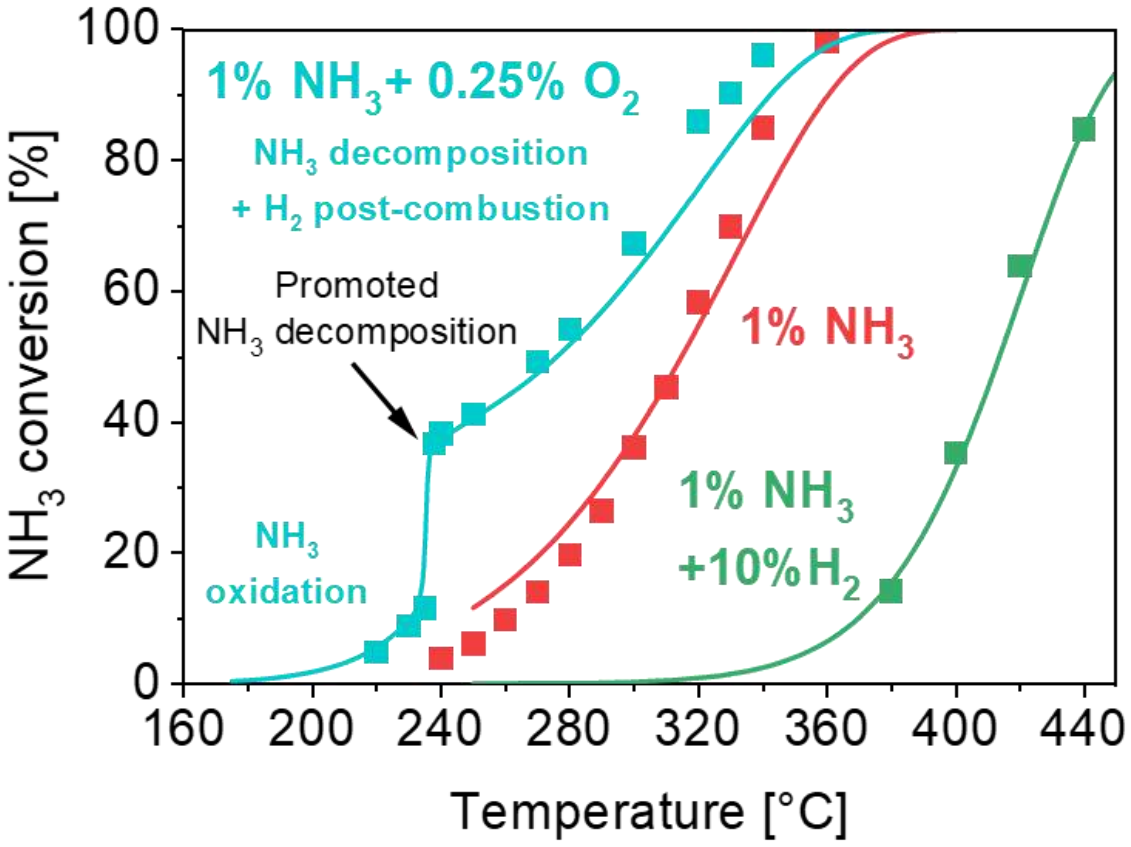

Figure 1. Experimental and modelling results of NH3 decomposition over Ru/MgAl2O4

Conclusions. H-poisoning was confirmed to be the main kinetic limitation of NH_3 decomposition. O2 co-feeding experiments clearly demonstrated the potential of H-scavenging from the Ru surface. Conservative H-scavenging strategies involve the catalyst formulation and the reactor design and operation and are currently explored.

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ISCRE29 & APCRE11
2026 / SEOUL, KOREA

MKF0006

Towards the upgrading of plastic pyrolysis oil: Understanding of the recombination reaction between olefin and hydrochloric acid

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Fundamental

Keywords: plastic pyrolysis oil, recycling, olefin, hydrochloric acid, recombination, hydrodechlorination

Abstract Body.

Hydrodechlorination using hydrotreating catalyst is one of the most efficient solutions for the chlorine removal from plastic-derived pyrolysis oils, prior to the upgrading into valuable monomers. During the hydrodechlorination, a problematic phenomenon is the possible recombination of olefins with hydrochloric acid (HCl), generated during hydrodechlorination, leading to the formation of organochlorine compounds and thus limiting the overall dechlorination efficiency.

This work aims to elucidate the effects of operating conditions and olefin chain length on the olefin-HCl recombination. Experimental tests were carried out in a 500 mL autoclave under hydrogen atmosphere, using a commercial sulfided NiMo/γ-Al_2O_3 catalyst. Model solutions composed of olefin (hexene-1, octene-1 or decene-1) and 1-chlorobutane dissolved in n-heptane were subjected to various temperatures (180-240°C) and pressures (1-3 MPa). The evolution of chemical species and chlorine distribution were analyzed by gas chromatography (GC-FID and GC-ICP-MS/MS).

Experimental results confirm that HCl, generated from the hydrodechlorination of 1-chlorobutane, combined with olefins to produce organochlorine compounds (chlorohexane, chlorooctane and chlorodecane). Raising the temperature from 180°C to 210°C enhanced the yield of 1-, 2-, and 3-chlorohexane thanks to the increase of HCl pressure obtained from chlorobutane dechlorination. However, at 240°C, the yield of chlorohexane isomers declines in the later stages of reaction. This behavior is consistent with the exothermic nature of the addition reaction, whose equilibrium is shifted back toward reactants at higher temperatures. The distribution of chlorohexane isomers follows the one of hexene olefin isomers. Increasing the total pressure enhanced the yield of chlorohexane due to the increase of partial pressure of olefins and HCl. Between the three olefins, there is no clear effect of olefin chain length on the recombination.

The experimental results underscore the need to select appropriate operating conditions to limit the recombination. Next studies would focus on the modeling of kinetic and thermodynamic aspects of the hydrodechlorination and the recombination.

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2026 / SEOUL, KOREA

MKF0056

Kinetic investigation of acid gas valorisation on NaX zeolite

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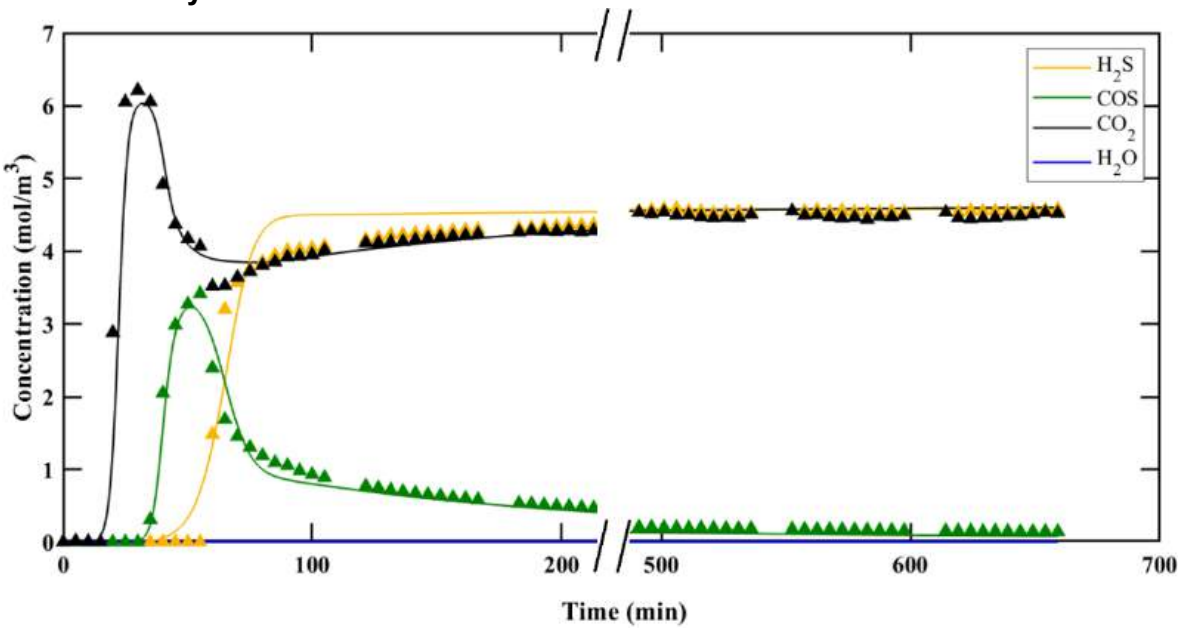
Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Fundamental

Keywords: Acid gas valorisation, CO2 utilization, Zeolites, Kinetic modelling, Catalysis, Adsorption

Abstract Body.



Rising CO_2 emissions make the development of practical CO_2 utilization routes increasingly important. Many technologies require highly pure CO_2 streams, limiting their applicability to industrial gases with minor impurities. In this context, the e-CODUCT project explores the conversion of acid waste gases, containing non-negligible amounts of CO_2 and H_2S, into carbonyl sulfide (COS) and water, with the former serving as an intermediate for CO and elemental sulfur production. Although COS formation is thermodynamically constrained, the use of zeolites, which simultaneously function as catalysts and adsorbents, allows for mitigating these equilibrium limitations. By selectively adsorbing water and removing it from the reaction environment, zeolites open a pathway for direct utilization of acid gases. In this work, COS formation experiments were carried out in a packed-bed reactor loaded with NaX zeolite at near-atmospheric pressure and 100 ºC. An elementary-step kinetic model based on the Langmuir–Hinshelwood–Hougen–Watson (LHHW) mechanism was developed. The

model and its estimated parameters are statistically significant and successfully reproduce the transient dynamics of the experimental trends. The predicted breakthrough order of components, with CO_2 appearing first and H_2S last, reflects the difference in their affinity for being retained on the zeolite. The model accounts for the roll-up of CO_2 and COS resulting from their competitive displacement by the more strongly bound H_2S. The model further reveals that a decline in COS formation occurs due to an accumulation of water on the zeolite's active sites, leaving limited room for reacting molecules, especially CO_2. Furthermore, the developed model was validated against experiments across various feed compositions and flow configurations. The simulated results were in good agreement with the experimental ones. Altogether, the model provides a reliable mechanistic description of COS formation by capturing the observed experimental behaviour arising from the interplay of competitive adsorption, reaction and water accumulation. Its agreement with experiments under diverse conditions confirms its robustness and demonstrates its potential to advance future reactor design and process optimization.

ISCRE29 & APCRE11
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MKF0070

Dual-Function Ligands Regulate the Nucleation Growth and Suppress the Ripening of Perovskite Quantum Dots

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Fundamental

Keywords: CsPbBr3 perovskite quantum dots, Dual-function ligands, Crystallization regulation, Suppression of Ostwald Ripening

Abstract Body.
Perovskite quantum dots (PQDs) are being studied as promising luminescent materials for optoelectronic devices owing to their tunable emission wavelengths, high photoluminescence quantum yield (PLQY), narrow full width at half maximum (FWHM), excellent charge transport properties, and superior solution processability. However, their industrialization is severely hindered by the formidable challenge of crystallization control, which originates from their high ionicity and thermodynamic instability.
This work investigates the regulatory mechanism of ligands on the crystallization and growth kinetics of CsPbBr3 PQDs. Traditional monofunctional ligands suffer from single-sided functionality, failing to simultaneously address the issues of uncontrolled nucleation/growth and inevitable Ostwald ripening. To overcome this bottleneck, we designed and screened a dual-function ligand, and synthesized CsPbBr3 PQDs via a room-temperature solution method. We conducted systematic characterizations including in-situ photoluminescence (in-situ PL), steady-state PL, X-ray diffraction (XRD), and scanning transmission electron microscopy (STEM).
Results demonstrate that the dual-function ligand effectively retards the crystallization and growth of PQDs, extending the crystallization reaction window from several seconds (in traditional systems) to over 1 hour while ensuring uniform particle size growth and long-term suppression of excessive ripening. In-situ PL measurements reveal that the CsPbBr3 PQDs have not yet achieved complete growth even after 1 hour of reaction. Steady-state PL tests indicate that the FWHM of CsPbBr3 PQDs is stably maintained at ~18 nm throughout the growth process, with the emission wavelength persistently centered at ~520 nm, reflecting excellent optical uniformity. STEM characterizations confirm that the average particle size of CsPbBr3 PQDs is 5.25 nm at 10 minutes of reaction, and remains stable at 8.05 nm after 24 hours of aging without noticeable Ostwald ripening.
This work achieves simultaneous regulation of PQD nucleation/growth and suppression of ripening, solving the long-standing bottlenecks in the synthesis and stability of PQDs. The outstanding size uniformity and long-term stability of dual-function ligand-modified PQDs lay a robust foundation for their large-scale preparation and practical deployment in high-performance luminescent devices.

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MKF0146

Reaction mechanism and kinetics of $CaCO_3$ hydrogenation

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Keywords: $CaCO_3$; hydrogenation; mechanism; kinetics; model

Introduction. High-temperature calcination of calcite minerals in energy-intensive industries represents a major source of global CO_2 emissions. Transforming abundant calcite minerals through hydrogenation offers a promising route to reduce these otherwise unavoidable emissions by producing value-added products.[1] however, advancement in this area has been constrained by an insufficient understanding of the underlying processes.[2] Herein, we for the first time elucidate the reaction mechanism of $CaCO_3$ hydrogenation and develop a reliable kinetic model. This kinetic model accurately describes the hydrogenation behavior of different types of calcite, demonstrating significant potential for reactor design and optimization of operating conditions.

Methods. The reaction mechanism was clarified using experimental data obtained from the hydrogenation of nano-sized $CaCO_3$ under deliberately designed conditions, including controlled temperature and CO_2 and H_2 partial pressures. Next, kinetic data were collected by varying temperature (600–700 °C) and H_2 partial pressure (0.2–1.0 bar) for three types of calcite (nano-sized $CaCO_3$, micro-sized $CaCO_3$, and calcite mineral) and used to estimate the kinetic parameters of the model. Finally, the developed model was applied to predict the hydrogenation behavior of large particles of these three $CaCO_3$, with intraparticle diffusion taken into account.

Results and discussion. For nano-sized $CaCO_3$ (average particle size160 nm) at 650 °C in 10% CO_2 (balance N_2), the CO_2 concentration remains constant (Fig. 1a), indicating no $CaCO_3$ decomposition occurs, as it far exceeds the equilibrium CO_2 concentration of $CaCO_3$ at 650 °C (1.1%). However, when H_2 is co-fed with CO_2 (still 10%), CO is produced and the CO_2 concentration decreases, revealing the direct hydrogenation of $CaCO_3$ ($CaCO_3 + H_2 = CaO + CO + H_2O$). Additional experiments on $CaCO_3$ hydrogenation without CO_2 in the feed show both $CaCO_3$ decomposition ($CaCO_3 = CaO + CO_2$) and reverse water-gas shift ($CO_2 + H_2 = CO + H_2O$) take place. Based on these observations, a reaction network comprising these three reactions is proposed, and a corresponding kinetic model is developed. The model fits the experimental data well (Fig. 1b) and can accurately predict the hydrogenation process of large particles (0.6 mm) composed of nano $CaCO_3$ (Fig. 1c). Moreover, the kinetic model is applicable to other types of calcite, demonstrating its broad utility.

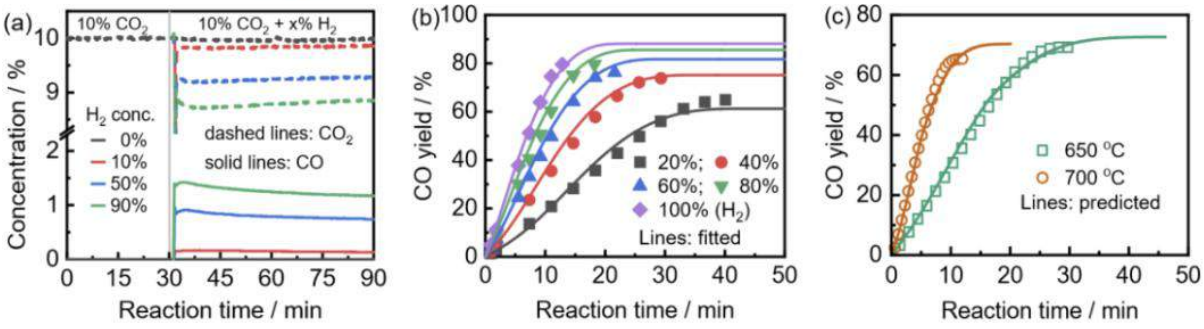

Fig. 1 (a) Concentration profiles of CO and CO_2 and (b) CO yield using nano-sized $CaCO_3$ (160 nm), and (c) CO yield using large $CaCO_3$ (0.6 mm).

Acknowledgments

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MKF0435

Kinetic studies on the catalytic ammonia decomposition over Nickel catalysts

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Abstract Category: Hydrogen - Hydrogen Storage (LOHC, NH3, MeOH etc)

Keywords: Ammonia decomposition, dynamic measurements, nickel catalysts

Abstract Body.
To reach greenhouse gas neutrality, the share of renewable energy must increase, but its intermittency creates a strong need for power-to-gas technologies for long-term chemical energy storage, such as hydrogen. To facilitate transport and handling, hydrogen can be converted to ammonia, stored and transported, and decomposed on demand on site [1]. The design of efficient ammonia decomposition reactors requires a detailed understanding of the reaction mechanism and catalyst-dependent kinetics. This study contributes to this issue by conducting stationary and dynamic experiments in differential fixed-bed reactors using various Nickel catalysts.
The first Nickel catalyst (10 wt%) was produced by incipient wet impregnation (IWI) on Al2O3 spheres. In addition, 10 wt% nanostructured Ni/Al2O3 catalysts were synthesized via spray-drying (SD) [2]. Furthermore, Nickel metal-organic-frameworks (MOFs) were also synthesized. For this purpose, Nickel(II) nitrate hexahydrate was dissolved in aqueous ammonium chloride/dimethylformamide with 1,3,5-tricarboxybenzene (BTC) and afterwards synthesized in an autoclave (20 mL) for 72 h at 120 °C [3]. The catalysts were thoroughly characterized by BET, TPR, XRD and chemisorption. Kinetic investigations were performed in a catalyst analyzer (BELCAT II, MicrotracBEL Corp.) while the gas composition was resolved via mass spectroscopy (GAM 200, InProcess Instruments). Next to temperatureprogrammed measurements, dynamic step measurements by switching between feed and inert gas were performed at varying temperatures.

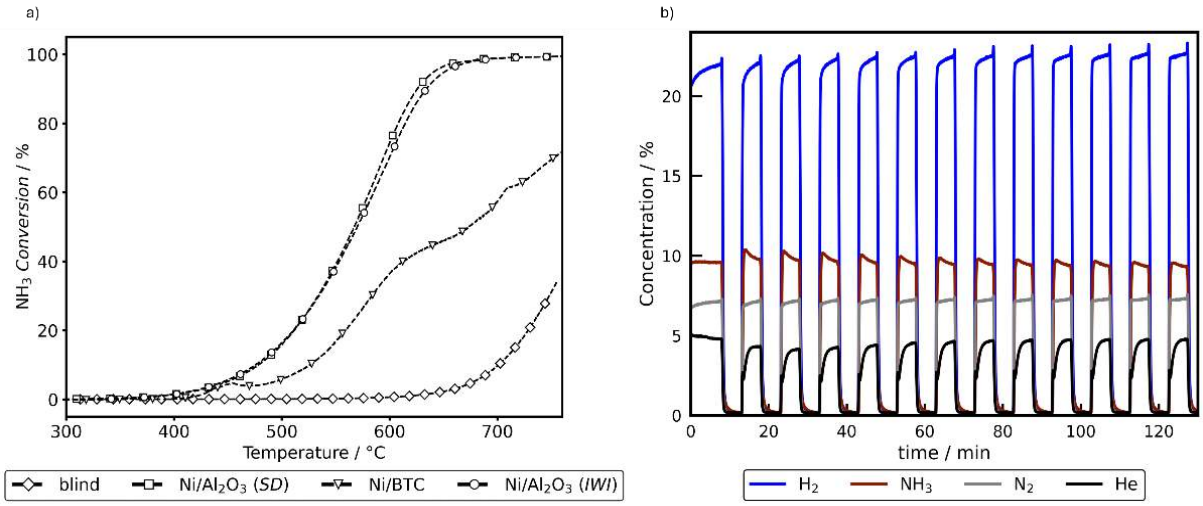

Figure 1: a) In temperature-programmed experiments, the conversion rates were measured with different nickel catalysts. b) Dynamic measurement with switching between 5 min reactive feed and 5 min flushing with Ar for 120 min at 550 °C, on Ni/Al2O3 produced via spray drying. Conditions: 30 mg catalyst, 30 % NH3 in Ar, p=1 bar.

In Figure 1a) the results of temperature-programmed measurements on different Nickel catalysts are depicted. Ni/Al2O3 (SD, IWI) achieve full conversion at 700 °C. For the dynamic measurements (Figure 1b)) the Ni/Al2O3 catalyst via spray-drying was used. During the dosing of the feed, the hydrogen concentration increases continuously with each step. In upcoming studies, additional dynamic measurements with different cycle times and novel catalysts will be conducted to further investigate the dynamic kinetics of ammonia decomposition.

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Mechanistic Insights into Heterolytic C-H Bond Activation over Boron Modified Ga2O3 Catalysts

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Fundamental

Keywords: Propane dehydrogenation; Heterolytic cleavage; Gallium oxide; Boron

Abstract Body.
Ga-based catalysts mediate propane dehydrogenation (PDH, C3H8 → C3H6 + H2) via heterolytic C–H bond cleavage across a Lewis acidic Ga3+ center and an adjacent basic O site [1]. This initial C–H scission is widely regarded as the rate-determining step. However, effectively lowering the intrinsic kinetic barrier of this heterolytic activation remains a challenging task. This study aims to elucidate how boron (B) incorporation modifies heterolytic C–H bond activation on Ga2O3.
Pristine and B-modified Ga-based catalysts supported on Al2O3 were synthesized via wet impregnation. The geometric and electronic structures of the catalysts were characterized by in situ XAS. The reaction mechanism and activation energy barriers were investigated using in situ DRIFTS, kinetic analysis, and DFT calculations.
EXAFS analysis revealed that B incorporation reduces Ga–Ga coordination, indicating a modification of the local Ga2O3 framework. This structural alteration led to a 13-fold increase in the propylene formation rate compared to pristine Ga/Al_2O_3. DFT calculations showed that B substitution significantly lowers the free energy barrier of the C–H bond cleavage by stabilizing the dissociated H species on neighboring oxygen sites. In situ DRIFTS provided spectroscopic evidence for the preferential formation of B–OH species during propane activation, confirming enhanced stabilization of heterolytically generated hydrogen.
This study demonstrates that B-modified Ga-based catalysts enhance propane dehydrogenation performance. Structural and spectroscopic analyses confirmed that B modifies the Ga–O framework and stabilizes surface hydrogen, thereby reducing the activation energy barrier for C–H bond cleavage. These findings highlight B incorporation as an effective strategy for designing efficient heterolytic C–H bond activation catalysts.

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MKP0567

Particle Dynamics and Microstructural Evolution in Polydisperse Suspension Coating and Drying

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Keywords: Particle dynamics; Lattice Boltzmann method; Coating and drying; Brush layer model; Hydrodynamic interaction

Introduction. Film coating processes are widely used in various industries, including lithiumion battery manufacturing, and are typically based on wet processing using particle suspensions, commonly referred to as slurries. These slurries consist of solid particles dispersed in solvents with polymeric binders and exhibit complex rheological behavior due to multicomponent interactions. Therefore, understanding the mechanisms governing particle migration, distribution, and microstructural evolution in multicomponent suspensions during coating and drying processes is of critical importance for controlling coating quality and final film properties.

Methods. Particle-based mesoscale simulations were employed to elucidate complex particle dynamics in suspension coating and drying processes. In particular, a lattice Boltzmann (LB) method was applied to explicitly capture hydrodynamic interactions among suspended particles and between particles and the surrounding fluid. For coating flow simulations under Couette and Poiseuille flow conditions, a novel dynamic model was developed to more realistically represent particle–binder interactions. In addition, LB-based strategies were investigated to suppress binder migration during film drying and to control stratification behavior in bidisperse particle systems during droplet drying.

Results and discussion. The effects of the Mason number on particle concentration and velocity distributions in coating flow fields are first discussed. The results reveal that hydrodynamic interactions play a key role in governing particle migration and spatial organization under different flow conditions [1]. Furthermore, the influence of hydrodynamic interactions on particle distribution and microstructural evolution during both film and droplet drying processes is examined, highlighting their critical role in stratification phenomena and drying-induced heterogeneity [2].

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KN0291

Computational Simulations and Artificial Intelligence for Heterogeneous Catalyst Discovery and Optimization

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Abstract Category: Invited Lecture - Keynote Lecture
Keywords: CO2 hydrogenation; Alcohols synthesis; Density functional theory (DFT) calculations; Catalyst design; Machine learning algorithms

Abstract Body.

Introduction. Methanol, central to the methanol economy, can be obtained from CO2 hydrogenation. Despite the great advances, there remains significant interest in designing highly active and selective catalysts for this reaction. Furthermore, ethanol and heavier alcohols are also important target molecules for catalyst development. Our recent works demonstrate the great potential of first principles simulations and machine learning algorithms in catalyst discovery and performance optimization [1-3]. Methods. DFT simulations were usually performed using the Bayesian error estimation functional with van der Waals correlation (BEEF-vdW) and the projector augmented wave (PAW) potentials, followed by mean-field microkinetic simulations. Decision tree-based machine learning algorithms were often employed with proper feature engineering for better interpretability. Performance of the designed catalysts can be further iteratively optimized. Results and discussion. In2O3-based catalysts have been shown to be effective for CO2 hydrogenation to methanol, although little is known about the structureperformance relationship. We performed extensive DFT calculations and microkinetic simulations to demonstrate the strong effects of its crystalline phase and surface termination [1], the coordination environment, formation energy, and coverage of the oxygen vacancy active site [4,5], and the identity and placement of the transition metal dopant on the catalytic activity and methanol selectivity [2,6]. These mechanistic investigations lead to the rational design of a hexagonal In2O3 catalyst [1] and single atom catalysts (SACs) with embedded transition metal dopants [2,6] with simultaneously high CO2 activity and methanol selectivity, promising for industrial applications. Our recent experimental and computational studies also established ZnFe2O4 in the spinel phase as an effective methanol synthesis catalyst for CO2 hydrogenation [3,7]. Interestingly, by tuning the crystalline phase and the pretreatment conditions, the product selectivity can be changed to mainly produce methanol, higher alcohols (for instance C3+-OH), or alkanes. Furthermore, machine learning algorithms can be further applied to iteratively optimize the productivity of target products such as methanol or higher alcohols for these multi-element catalysts. The adoption of an AI Agent-ExperimentSimulation closed loop brings unprecedented opportunities for the rapid development of advanced catalysts.

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MKC0020

Accounting for Input Uncertainty when Estimating Parameters in Reactor Models and Selecting Conditions for New Experiments

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Computational
Keywords: model-based design of experiments, A-optimal MBDoE, error-in-variables model, input uncertainty, parameter estimation, kinetic models

Abstract Body.
Traditional methods for parameter estimation and model-based design of experiments (MBDoE) assume that process inputs are perfectly known and that all variability occurs in measured process responses. Sometimes, however, chemical reactors have inputs with uncertainties that are as important as the variability in process outputs. Error-in-variables model (EVM) approaches are used to estimate uncertain inputs along with model parameters. Unfortunately, parameter estimation becomes more difficult when there is insufficient data to reliably estimate all uncertain inputs and parameters. In this situation, modelers may opt to estimate a subset of parameters or may decide to perform additional experiments. We developed an EVM-based subset-selection methodology that accounts for uncertain inputs. This method produced improved parameter estimates for a batch pharmaceutical-production model where there is substantial uncertainty in the initial concentration of a gaseous reactant, trimethylamine (TMA). Our research group has also developed an EVM-based MBDoE method that accounts for uncertain reactor inputs. The method is demonstrated using the pharmaceutical case study with uncertain TMA concentrations at the start of batch-reactor experiments. Information from two old batchreactor runs was used, along with the model equations and the proposed MBDoE algorithm, to design one or multiple new runs. When one new run is designed, the proposed method reduces uncertainty in the model parameters by 15 %, on average, compared to runs obtained using traditional MBDoE methods that ignore input uncertainty. Simulated data are used to show that the relative performance of the new MBDoE method is even better when larger input uncertainties are encountered. The proposed subset selection and MBDoE methods are straightforward to implement for multi-response chemical reactor models where some inputs are perfectly known and others are uncertain.

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MKC0387

Kinetic modeling of the pyrolysis of impure polyethylene

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Keywords: Chemical recycling; pyrolysis; kinetic modeling; polyethylene; cellulose; kinetic Monte Carlo

Introduction. Mankind is currently facing a massive environmental catastrophe caused by solid plastic waste (SPW). Developing efficient recycling processes that can handle the full complexity of this SPW is the only way to deal with this impending catastrophe. Current mechanical recycling techniques can for example not handle mixed plastic waste, which still contains impurities. The most common impurities are PET and paper [1]. The latter mostly consists of cellulose [2]. Ergo, chemical recycling processes like pyrolysis are being studied as a promising alternative. Pyrolysis decomposes thermally (above 450 °C) the SPW into pyrolysis oil, gas, and char. Pyrolysis oils can be steam cracked back into renewable base chemicals. However, the yield and composition of those oils is highly sensitive to impurities in the SPW. As such, pyrolysis processes can only be optimized if the underlying reactions are understood. Detailed kinetic models are the only tools that can provide the required insights.

Methods. This work develops a detailed kinetic model for the copyrolysis of HDPE and cellulose as a model system, as shown in Figure 1. A two-stage strategy is applied, combining experimental and modeling work. First, a broad dataset is measured using a micropyrolyzer operating under intrinsic kinetic conditions. The micropyrolyzer combines two-dimensional gas chromatography with FID and ToF-MS detectors to optimize the data's accuracy. Second, a detailed kinetic model for this system is constructed. The model uses a tree-based kinetic Monte Carlo (*k*MC) framework to describe the pyrolysis of HDPE, cellulose, and their interactions. The model can capture both the influence of these on the final product yields and the residence time distribution.

Results. The constructed kinetic model is validated against the obtained high-quality dataset and literature data. This combination ensures that the developed kinetic model is a versatile and adequate tool for simulating the binary pyrolysis of HDPE and cellulose, one of the most common impurities in SPW [1]. To conclude, our model boosts the fundamental understanding of pyrolysis processes for mixed SPW and enables the optimization and design of industrialscale processes, aiding in solving the universal SPW crisis.

Acknowledgments
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2026 / SEOUL, KOREA

MKC0426

Mechanisms and Predictive Modeling of Gas-Liquid Mass Transfer in Microchannel Taylor Flows

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Computational
Keywords: Microchannel reactor; Gas-liquid Taylor flow; Mass transfer; CO2 absorption

Abstract Body.

Keywords: Microchannel reactor; Gas-liquid Taylor flow; Mass transfer; CO2 absorption Introduction. Microchannel reactors offer significant advantages for gas-liquid mass transfer, which is further enhanced in Taylor flow by periodic interfaces and internal circulation within liquid slugs. [1] This study investigates the mass transfer behavior in microchannel with emphasis on liquid film evolution, and resulting mass transfer characteristics.

Methods. Three-dimensional simulations were performed using the volume-of-fluid (VOF) method to capture gas-liquid interfaces, with interfacial mass transfer modeled by the continuous-continuum surface transfer (C-CST) approach through a volumetric source term.

Results and discussion. The simulations reveal distinct flow regimes in the microchannel, including slug-bubbly, stable Taylor flow, and slug-annular flow, depending on the gas and liquid inlet velocities. Among these regimes, stable slug flow provides well-defined and periodic gas-liquid interfaces, enabling reliable characterization of interfacial mass transfer. Continuous CO2 dissolution leads to progressive bubble shrinkage along the channel, while the liquid film rapidly develops near the bubble front and remains nearly constant over most of the bubble body, indicating that axial variations in mass transfer are dominated by changes in bubble length and interfacial area rather than film thickness. [2] The instantaneous volumetric mass transfer coefficient kLa exhibits a clear axial dependence and decreases monotonically with increasing distance from the inlet. This behavior is primarily attributed to the progressive saturation of the liquid slugs and the continuous reduction in interfacial area caused by bubble shrinkage. Liquid inlet velocity plays a dominant role in regulating instantaneous mass transfer. The influence of diffusion transport is examined through variations in the Schmidt number. Decreasing the Schmidt number, corresponding to higher liquid-phase diffusivity, accelerates bubble shrinkage and enhances axial mass transfer performance. Finally, a predictive correlation based on overall gas-liquid mass transfer is proposed to quantify the volumetric mass transfer coefficient as a function of operating conditions and fluid properties.

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MKC0487

Decomposition of Nitrogenated Impurities in Plastic Waste Pyrolysis Oil: A Combined Experimental and Modeling Study

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Computational
Keywords: Automatic model generation, Pyrolysis, Plastic waste pyrolysis oil, Kinetic group additivity

Abstract Body.

Nitrogen-containing impurities in steam cracker feedstocks are a long-standing industrial concern, as they can lead to explosive gum formation and the production of hazardous species such as hydrogen cyanide (HCN). The growing use of plastic waste pyrolysis oils as alternative feedstocks intensifies this challenge, since these oils may contain significant amounts of nitrogenated hydrocarbons. Despite this, a detailed kinetic understanding of the behavior of nitrogen-containing impurities under steam cracking conditions remains limited. One of the main limiting factors is the computational effort required to calculate all the relevant kinetic and thermodynamic parameters ab initio.

In this work, a comprehensive kinetic model for the pyrolysis of nitrile impurities in plastic pyrolysis oils is developed using the PRIM-X modeling framework. Model generation is based on the β/μ-hypothesis and the pseudo-steady-state approximation for large radical decompositions, enabling the automatic generation of single-event based lumped reactions and significantly reducing computational cost. Thermodynamic parameters are assigned using the Genesys platform, relying on ab initio data and group additivity, while kinetic parameters are obtained via kinetic group additivity schemes [1] that were extended to allow fast estimation for the key β-scission and hydrogen abstraction reaction families. Experimental validation is performed using a steam cracking pilot plant. The feedstock consists of a polypropylene-derived plastic pyrolysis oil containing nitrogenated impurities.

The newly developed kinetic group additivity scheme predicts reaction rate coefficients within a factor of three at 1000 K, enabling accurate automatic model generation. The resulting kinetic model successfully captures the decomposition of the main nitrogenated impurities and predicts the formation of industrially relevant and potentially hazardous species such as HCN and acetonitrile, as can be seen in Figure 1.

This work provides a validated fundamental kinetic model for nitrogenated hydrocarbon pyrolysis that enables reliable modeling of nitrogen-containing plastic pyrolysis oils using updated kinetic group additivity schemes. The model is applicable as a valuable tool for assessing impurity behavior and safety risks in steam cracking of nitrogen-containing

feedstocks, while the updated kinetic group additivity schemes have applications in additional fields such as combustion of nitrogenated hydrocarbons.

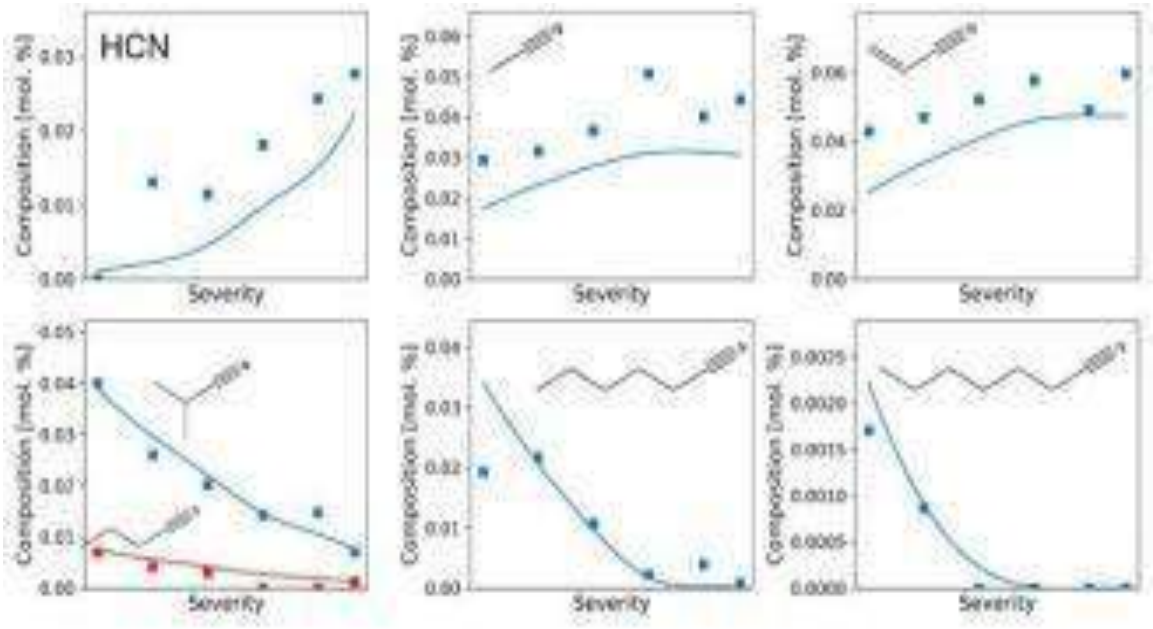

Figure 1. Comparison of experimental results (symbols) to model simulations (lines) for the steam cracking of a nitrogen-containing pyrolysis oil as a function of cracking severity. Pressure is set to 2.0 bar; the mass flow rate is 1.4583 g/s and the steam dilution is 0.5 kgH2O/kgHC.

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MKC0537

Bridging kinetic model extraction and multi-scale simulations by efficient neural-network-based kinetics

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Keywords: Machine learning, Neural ordinary differential equations, Surrogate modelling
Introduction. The design and application of catalytic systems rely on a detailed understanding of chemical processes occurring on the catalyst surface [1]. Since catalysis is inherently a kinetic phenomenon, accurate and predictive descriptions of reaction kinetics are essential for catalyst and reactor design. Such kinetics are commonly described using detailed physicsbased models. However, their development is time-intensive, requires substantial systemspecific expertise, and their evaluation is computationally expensive [2]. Recent advances in neural-network–based kinetic modeling address these limitations by providing efficient representations of detailed reaction kinetics. These neural-network-based kinetics can be efficiently trained in a data-driven manner, while preserving physical consistency. One example is the Global Reaction Neural Network (GRNN) shown in Figure 1, which embeds textbook chemical engineering design principles, including thermodynamic and stoichiometric consistency, to represent complex reaction kinetics [3]. By coupling such neural-networkbased kinetics with differentiable reactor models, in the context of neural ordinary differential equations, they can be trained directly on laboratory reactor measurements [3,4,5]. Beyond kinetic model extraction, they can also serve as surrogate models for established detailed microkinetic models. This enables computationally efficient multiscale simulations of industrial catalytic reactors that are otherwise infeasible [6]. In this contribution, we provide an overview of recent advances in the application of neural networks as efficient representations of detailed kinetics, spanning use-cases in kinetic model development and surrogate modelling for multiscale simulations.

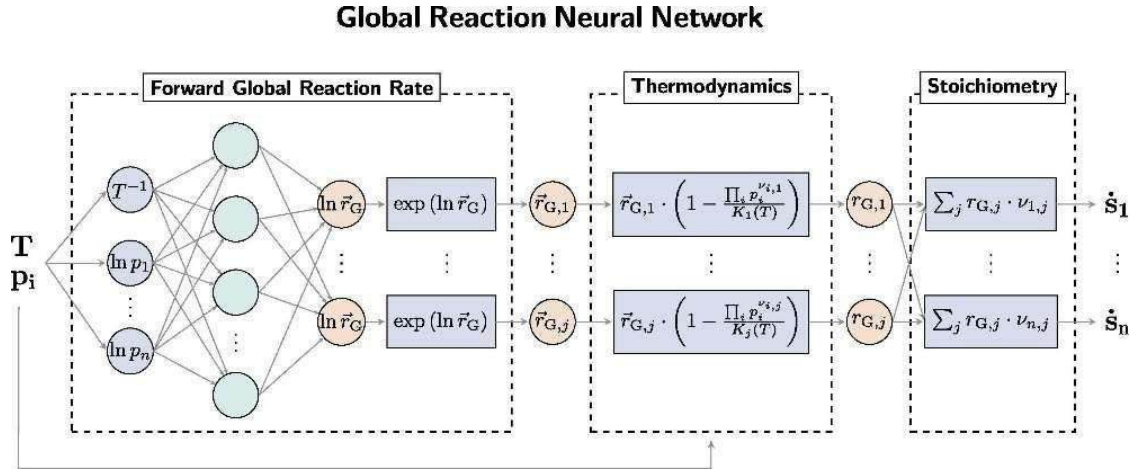

Figure 1: Global reaction neural network, embedding thermodynamic and stoichiometric information, which provides an efficient and physically consistent representation of detailed kinetics [3].

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MKC0026

Density functional theory and pair distribution function to understand catalytic graphitization of biocarbon from biomass

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Computational

Keywords: Biomass pyrolysis, Biocarbon, Catalytic graphitization, Pair distribution function, Density functional theory, Metal-carbon interaction

Abstract Body.

The recycling and preparation of carbon materials with well-organized graphitic structures from various feedstocks have long been an active area, as the produced graphitic carbon has a broad variety of applications including energy storage fields, electronics, environmental protection and composite materials due to its excellent conductivity, large specific surface area, high mechanical strength and outstanding chemical stability. Unlike the coal and other fossil fuel resources, the biomass like cellulose is renewable, eco-friendly and biodegradable, thereby being used as sustainable precursors for producing graphitic carbon materials. Pyrolysis is a widely adopted approach for the preparation of graphitic carbon from biomass, typically requiring the addition of metal catalysts to reduce the pyrolysis temperature and to promote the formation of well-ordered graphitic structures. In this work, at both the nanoscale and atomic scale, the advanced experimental analysis techniques like pair distribution function were employed to characterize the graphitic carbon structures formed after biomass pyrolysis. In addition, a modern materials computation method, firstprinciples calculation (DFT calculation) was used to investigate the interactions between catalytic metal and graphene-like structures. We found that, compared to non-impregnated cellulose and raw cellulose, metal-impregnated sample presents much more short-range, medium-range and long-range ordering carbon structures, which suggests the metal plays a crucial role in the graphitization process. On the other hand, the DFT-based energetics and electronic structure calculations reveal that a strong interaction, charge transfer and orbital hybridization appear on the metal-graphene interlayer. Our findings also explain the formation mechanism of graphitic structures observed in previous studies during metalcatalyzed graphitization. We believe the insights provided here would be helpful for those who would like to better understand the metallic catalytic graphitization process of biocarbon and the therein metal-carbon correlations.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

MKC0111

Multi-scale Modelling-Supported Catalytic Conversion Reactions towards Bio-based Chemicals

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Computational

Keywords: Biomass utilization, Kinetic modelling, Glucaric acid, Adipic acid

Abstract Body.

Purpose. Lignocellulosic biomass can be utilized to produce several valuable bio-based monomers. One route we developed targets the production of adipic acid, a key monomer for several widely used polymers. The process begins with the selective oxidation of glucose to glucaric acid, carried out over an AuPt/ZrO_2 catalyst. In a subsequent step, glucaric acid is converted into adipic acid using a Re/C catalyst. Similar catalytic principles have been used for other waste streams, such as oil waste. Glyceric acid, formed during biodiesel production, was successfully transformed into acrylic acid over the same Re/C system, demonstrating the broader potential of these catalysts in biomass valorization. Based on the results obtained, a microkinetic model was developed to study the complex reaction pathway in detail and to unravel the rate-limiting steps of the process itself for the whole reaction pathway.

Methods. The catalytic oxidation and dehydroxylation experiments were carried out in highpressure, high-temperature autoclave batch reactors. Several parameters (e.g., catalyst type/amount, temperature and pressure, reactions with intermediates) were varied to obtain reliable experimental data. All of this was used to build predictive kinetic models of oxidation and deoxydehydration reactions.

Results. After initial catalyst screening and DFT study of monometallic Au/ZrO2 and bimetallic AuCu/ZrO2 and AuPt/ZrO2, where the latter showed promising GA yields (30%). The optimized Au:Pt molar ratio was found to be 67:331,2. This ratio was used to develop a kinetic model with 700 experimentally determined concentrations. The kinetic model itself accounted for different oxygen species on the catalyst surface, which are responsible for different surface reaction rates of reactants and intermediates. Experiments also revealed the highest reported yield (77%) of GA, when the starting reactant is glucuronic acid in base free conditions3. Figure 1 shows the predicted yield of GA, based on time, temperature and partial pressure of O2.

To produce bio-based adipic acid, various catalyst supports, pretreatment methods, and reaction conditions were systematically evaluated4. The optimal system consisted of Re supported on carbon in methanol as the solvent, operated under 5 bar of H_2, achieving adipic acid yields of up to 95%5,6. When this Re/C catalyst was applied to the deoxydehydrogenation of the C_3 acid, glyceric acid, to acrylic acid, a combined yield of acrylic acid and methyl acrylate of up to 65% was obtained at 150 °C after 72 h under an inert N_2 atmosphere.

Conclusions. Moreover, conducting the reaction under 5 bar of H_2 at an elevated temperature of 180 °C enhanced DODH.

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MKC0128

Accounting for entropy in first-principles atomistic models – a marginal effect or a crucial consideration?

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Computational

Keywords: entropy, ethylene epoxidation, multiscale model, density functional theory, microkinetic modelling, packed-bed reactor

Abstract Body.

Introduction. Ethylene epoxidation is an important industrial selective oxidation process, widely used for the large-scale production of ethylene oxide, yielding several million tonnes annually. Silver has long been established as the most effective catalyst and has remained unsurpassed despite extensive research to identify superior alternatives [1]. First-principles modelling has provided deeper insights into the epoxidation reaction mechanism [2]. The contribution of entropy is generally overlooked, either completely neglected or described only by the conventional harmonic approximation (HA). In this study, however, the entropic effects for epoxidation on silver were evaluated using different density functional theory (DFT) approaches: HA, free translator (FT), hindered translator (HT), and complete potential energy sampling (CPES) [3].

Methods. Ab initio methods have been used to describe the process at the atomic scale. The results were then incorporated into a mesoscale description of the reaction mechanism using the mean-field microkinetic approach. The microkinetic framework was ultimately embedded within a comprehensive reactor-level process simulation. A continuous-flow packed bed reactor model was employed, accounting for axial dispersion effects [4]. Sensitivity analysis was also performed to identify critical kinetic steps in the system, namely the ratedetermining (RDS) and selectivity-determining steps (SDS) [5].

Results and discussion. Small differences in entropic contributions arising from different DFT approaches lead to substantially altered reactor-level performance, demonstrating that entropy has a significant impact. This is due to the exponential relationship between rate constants and the corresponding activation entropies. Notably, conventional HA showed the poorest performance, significantly overestimating entropy. However, we found that not all entropies require the same level of accuracy. In particular, the computationally expensive CPES is needed only for the barriers corresponding to the critical kinetic steps. The remaining barriers can be determined using simpler DFT approaches, such as FT, as these approximate values are sufficient and do not noticeably affect the predicted reactor-level performance.

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MKC0176

On-line optimization for integrated carbon capture and conversion process through a combined DFT-microkineticmodeling workflow

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Computational

Keywords: Dry Reforming, CCUS, Catalyst Screening

Abstract Body.

The Integrated Carbon Capture and Conversion (ICCC) is a promising catalytic process for producing syngas from CO2 and CH4 using a combined separation and reactor unit. Besides, its performance can fluctuate due to inconsistent feed ratios caused by the flue gas unit. Herein, the Ratings concept workflow based on density functional theory (DFT) is applied to overcome these problems in a two-step protocol: (i) catalyst identification, which designates the catalyst characteristics and predicts performance based on reactivity (RT-R) and stability (RT-S) ratings calculated based on activation energies obtained either from experiments or DFT, and (ii) catalyst optimization that optimized a catalyst's performance via the determination of new operating condition accounted for its deactivation over time. Moreover, temperature and feed ratio sensitivity were investigated, revealing that most catalysts are more sensitive to temperature change than to the feed ratio. This work applied the Ratings concept to optimize the integrated carbon capture and conversion process (ICCC), where the concept is divided into two parts: (1) catalyst identification, which is used to screen high-performance catalysts for the DRM reactor, and (2) catalyst optimization, where the concept constructs the database for the on-line optimization component to determine the optimal operating conditions setpoint that sustained the catalytic activity when catalyst deactivation occurs. First, a catalyst's stability ratings (RT-S) and reactivity ratings (RT-R) are calculated and used as coordinates to predict the desired reaction rate. The calculation of this coordinate links activation energies between a catalyst candidate and the reference catalyst, which can be obtained either from experiments or from DFT calculations. The optimization can be performed in two ways: by tuning the temperature and the feed ratio. The temperature adjustment is performed when the sensor detects a decrease in syngas production rate, before transmitting the signal to the reactor to set a new temperature setpoint, while for feed ratio tuning, the transmitter sends the signal to the makeup gas lines to adjust the feed ratio. The sensitivity analysis from the Ratings concept indicates that adjusting the temperature parameter is necessary to optimize the process. The on-line or real-time optimization component concerning the changing catalyst performance over time is integrated for faster and more accurate setpoint determination during the feedback or feedforward control loop calculations.

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MKC0452

REGULATION OF MICRO-ENVIRONMENTS BY MULTIMETAL PROMOTERS: A THEORETICAL STUDY ON CO_2 ACTIVATION OVER IRON CARBIDE CATALYSTS

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Computational

Keywords: Micro-environment, Multi-metal promoters, CO2 activation, Iron carbide Catalysts

Abstract Body.

Essentially developing and regulating the unique electronic property of iron carbide catalysts involving multi-metal promoters to understand the structure-activity relationship of the CO2 activation process is still a great challenge. Here, metals and transition metals were introduced as strategies for electronic structure regulation to theoretically understand the underlying nature of CO2 adsorption and activation behaviors over Fe3C catalysts. there exists a distance effect by the doped multi-metals. When the doped metals are closer and adjacent to each other, it will be more beneficial for CO2 dissociation, and when they are far away from each other on the catalyst surface, the effect of a single metal near CO2 becomes more pronounced and it facilitated CO2 adsorption but hindered dissociation. Many experimental results have also proven that smaller atomic radii are more conducive to enhancing catalytic activity [1-2], but our calculations had found that Mn atom was a good choice for forming dual-atom catalysts, which could significantly increase the adsorption stability of CO2 and facilitate the direct dissociation of CO2.

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MKC0627

Catalytic Roles of Reactive Hydrogen in CO2 activation via Reverse Water-Gas Shift on Rh and Pt Surfaces

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Computational

Keywords: CO2 activation, Reverse Water-Gas Shift, Microkinetic Modeling, Density Functional Theory, Rhodium-based catalyst, Platinum-based catalyst

Abstract Body.

Introduction. The Reverse Water-Gas Shift (r-WGS) reaction is a strategic route for upgrading CO2 into CO. However, the reaction mechanism remains insufficiently understood.

In particular, the activation of CO2 depends on the oxygen affinity of the catalyst material [1]. In this study, we investigated how surface oxygen affinity governs the initial CO2 activation and, in turn, the overall reaction mechanism. To this end, two catalyst materials with distinct oxyphilic characteristics -Rh and Pt- were employed and examined combining experimental and theoretical methodologies to elucidate the full r-WGS catalytic cycle.

Methods. Kinetic tests were performed in a quartz U-tube PFR under differential conditions, adopting highly diluted 4 wt.% Pt/aAl2O3 and Rh/aAl2O3 catalysts, under a wide range of operating conditions. Density Functional Theory coupled with the Wulff–Kaishew construction was used to describe catalyst dynamics under reaction conditions, adopting the methodology proposed by Cheula et al. [2], accounting for 100, 110, 111, 211, 311, 331 facets.

Results and discussion. As shown in Fig.1a, the r-WGS turnover frequency increases with CO2 partial pressure on both Rh and Pt, exhibiting similar apparent reaction orders across the entire temperature range investigated (from 350 to 650 °C). The data reported in Fig.1 illustrate the representative case at 550 °C. In contrast, the H2 dependence differs markedly (Fig.1b), with Pt showing a moderate positive order (~0.35) and Rh a much weaker one (~0.15). To rationalize these trends, we carried out a DFT-based, structure-dependent microkinetic analysis. Once the model was shown to accurately reproduce the experimental results, we performed a reaction path analysis to shed light on the partial equilibrium of the elementary steps. On Pt, hydrogen actively participates in the rate-determining step, where CO2* reacts with H* to form a COOH* intermediate. In contrast, on Rh, CO2* activation proceeds via direct dissociation into CO* and O*, with H* successively reacting with O* to form OH* and, ultimately, H2O*. Based on these mechanistic insights, we proposed distinct rate expressions for Pt and Rh, which successfully reconciled the experimental measurements. Moreover, Pt and Rh were found to exhibit different dominant active sites, i.e., Pt(111) and Rh(100), thus leading towards effective catalyst design and optimization.

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MKF0294

Aromatization Mechanisms and Kinetics of n-Heptane over Ga/ZSM-5 Zeolites

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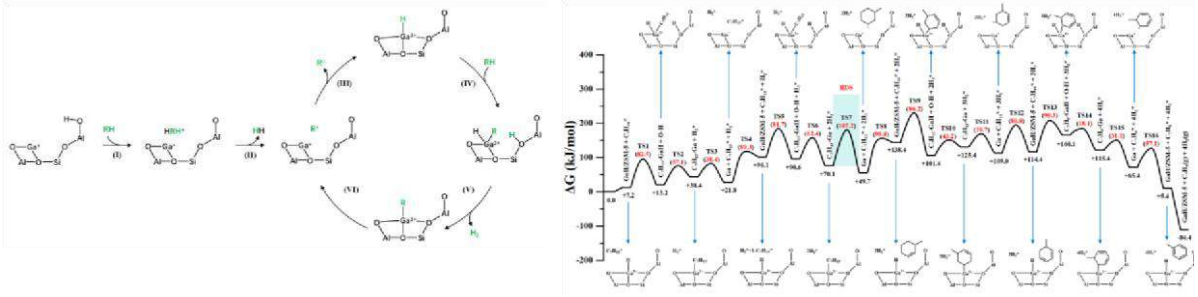
Keywords: *alkane; aromatization; zeolite; DFT; mechanism; kinetics*

Introduction. Zeolite-based catalysts such as H-ZSM-5 have gained widespread acceptance as a viable option for the aromatization of alkanes. However, unmodified H-ZSM-5 catalysts exhibit limited aromatization selectivity and are often dominated by cracking and isomerization reactions [1], leading to a high content of unwanted C1 and C2 in the product. To address this issue, the addition of transition metals such as zinc- and gallium has proven effective in facilitating dehydrogenation activity and suppressing cracking. In this work, we investigated the mechanism for the formation and restoration of the $[GaH]^{2+}$ active site at Lewis-Brønsted acid site pairs in the presence of n-heptane reactant using density functional theory (DFT) calculations. We also comprehensively explored the entire reaction pathways involved in the dehydrocyclization of n-heptane to toluene over the active $[GaH]^{2+}$ site [2].

Methods. Periodic DFT calculations were carried out using a mixed Gaussian and plane wave basis sets within the CP2K code. The Gibbs free energy was then computed using classical statistical mechanics, taking into account the zero-point energy and the vibrational entropy.

Results and discussion. While it is generally believed that the $[GaH]^{2+}$ active site is created through a two-step proton migration process from the BAS to the Ga^+ site, DFT calculations revealed that proton migration from the framework oxygen atom to the Ga^+ site is highly unfavorable from a kinetic standpoint. Instead, we identified the three-coordinated carbenium ion as a pivotal intermediate in the formation of the $[GaH]^{2+}$ active site. Notably, the generation and restoration of the $[GaH]^{2+}$ active site become kinetically unimpeded when the carbenium ion acts as a bridge. Furthermore, it has been found that the $[GaH]^{2+}$ active site significantly reduces the activation barrier for the C-H bond cleavage compared to BAS. Bader charge analysis and COHP results confirmed that $[GaH]^{2+}$ facilitates the activation of the C-H bond of n-heptane while inhibiting C-C bond cleavage.



(a) (b)

Figure 1 (a) Schematic illustration of generation and regeneration of $[GaH]^{2+}$ in the catalytic cycle of alkane dehydrogenation; (b)The Gibbs free energy profiles for the aromatization of n-heptane to toluene over Ga/H-ZSM-5 zeolite.

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Oral Presentation

Reactor Modeling and Design

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

DFN0641

Radial Heat Transfer in Industrial-Sized Fixed-Bed Reactors under Steady-State and Dynamic Conditions

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fundamental

Keywords: radial heat transport, non-isothermal fixed-bed reactors, dynamic modeling, CO2 methanation

Abstract Body.

Polytropic, wall-cooled fixed-bed reactors are widely applied for strongly exothermic reactions and are of particular interest for Power-to-X (PtX) applications such as ammonia synthesis and CO2 methanation due to their suitability for load-flexible operation. Under such dynamic operating conditions, reliable prediction of radial temperature profiles and axial hot-spot formation is essential for reactor design and operation. The radial heat transport in fixed-bed reactors is commonly described using either the αW-model or the more computationally demanding λR-approach, with the latter reported to be more suitable for reactive systems. However, calibration may improve the accuracy of the αW-model while retaining its advantages in terms of model simplicity. Thus, this work compares a calibrated αW-model with the λR-approach to evaluate their suitability for describing temperature profiles in industrial-sized polytropic fixed-bed reactors under high-load conditions.

Steady-state and dynamic CO2 methanation experiments were performed in a PtX lab pilot plant using an industrial-sized, wall-cooled fixed-bed reactor loaded with a Ni@Al2O3 catalyst. The experiments were conducted under industrially relevant operating conditions, including pressures of up to 25 bar(g) and feed flow rates of up to 250 LN min-1. The reactor is equipped with a distributed temperature sensing system to resolve axial temperature profiles along the reactor centerline as well as along the inner reactor wall with high spatial (~ 0.65 mm) and temporal (~ 20 Hz) resolution. To describe the thermal behavior of the reactor, a two-dimensional dynamic pseudo-homogeneous model is applied. Within the model, radial heat transfer is represented by either the αW- or λR-approach. The αW-model is calibrated by using non-reactive heat transfer experiments to determine correction factors for thermal transport parameters (ucool, αW, λbed,conv, λbed,cond) independently of reaction effects. Subsequently, both modeling approaches are applied to CO2 methanation experiments.

Figure 1 shows representative temperature profiles revealing pronounced axial and radial gradients, including distinct hot-spot formation during CO2 methanation under high-load conditions. Calibration of the αW-model using non-reactive experiments results in good agreement with experimental data and enables a consistent description of temperature profiles under reactive operating conditions. Ongoing research focuses on evaluating the ability of the λR-approach to reproduce the measured temperature profiles, as well as on

assessing both modeling approaches under dynamic reactor operation. Overall, the results indicate that the αW-model can be used to accurately describe temperature profiles in industrial-sized fixed-bed reactors operated under high-load conditions, given that appropriate calibration is applied.

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DFN0685

A NEW MASS-CONSERVING TWO-PHASE MODEL FOR A BUBBLING FLUIDIZED-BED GASIFIER

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fundamental

Keywords: Gasification, syngas, fluidized bed, mathematical modeling

Abstract Body.

Introduction. Two-phase models based on the Kuuni-Levenspiel formulation have been widely used to predict the performance of fluidized bed gasifiers. However, in most studies, the model formulation originally developed for isothermal systems is used to model the nonisothermal system, leading to a violation of conservation principles. In addition, a sophisticated screening procedure is required to choose kinetic models which are valid over a wide range of operating conditions. A mass-conserving two-phase model is developed in the present study to overcome the limitations of the previous studies.

Methodology. The gasifier is divided into two parts: fluidized bed and freeboard. The fluidized bed is assumed to comprise gaseous coalescing bubbles rising through an emulsion of gas and solids. Steady-state species and energy balances are written for the system, wherein the conventional models used to calculate the bubble fraction and expanded bed height are modified to satisfy mass conservation. Furthermore, a detailed kinetic model discrimination exercise is performed by comparing the performance of various combinations of global kinetic models to that of a free-radical kinetic mechanism. The model performance is validated against data obtained from a pilot-scale gasifier. The effect of oxygen, steam flow rates, and the rate of heat loss on the gasifier performance is analysed.

Results and discussion. Fig. 1 (a) shows the comparison of the predicted syngas composition with the measured data. The model predicts the composition of the syngas exiting the gasifier with an accuracy greater than 80%, considering the system complexity and uncertainty. Analysis of reaction rates shows that char combustion is the only dominant reaction in the oxygen-rich region near the distributor plate. As oxygen is depleted along the gasifier height, water-gas reaction dominates, while the Boudouard reaction proceeds at low rates. Among the various sensitivity analyses performed, Fig. 1 (b) shows the effect of steam flow rate on the cold gas efficiency and the molar flow rates of major syngas components at the gasifier outlet. It is shown that altering the steam flow rates is an effective strategy to increase the H2/CO ratio without significantly affecting the cold gas efficiency. Other insights obtained from the analyses of reaction rates and effects of operating conditions will be presented in the full manuscript.

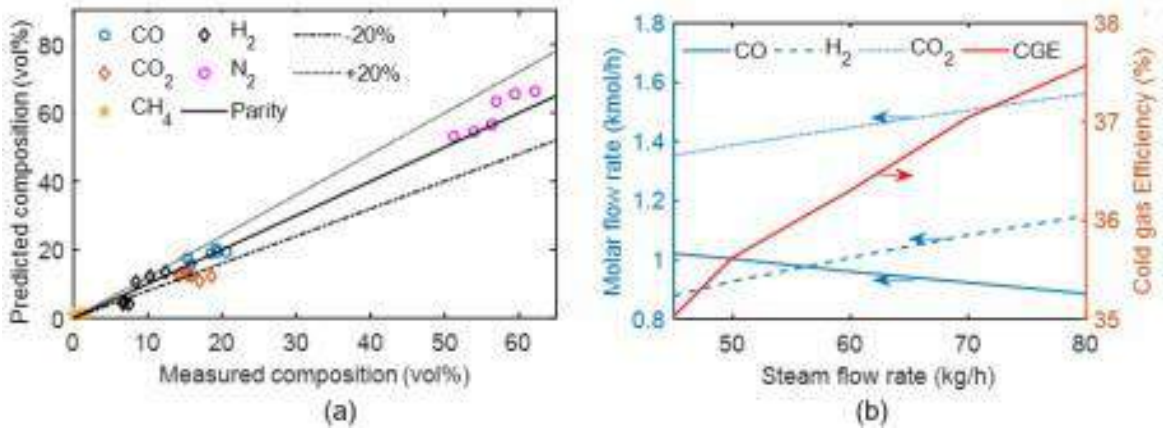

Fig. 1. (a) Comparison between model predictions and measured data, (b) Effect of steam flow rate.

Conclusions. A new mass-conserving model for a fluidized-bed gasifier is developed.

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KN0175

Reaction engineering of non-oxidative methane conversion via coupled surface and gas-phase radical pathways

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Abstract Category: Invited Lecture - Keynote Lecture

Keywords: Nonoxidative methane conversion, Methane pyrolysis, Ethylene, Aromatics

Abstract Body.
Direct non-oxidative methane conversion enables the production of olefins and aromatics along with hydrogen formation, but coke formation and low carbon utilization efficiency limit practical operation. Methane to olefins, aromatics, and hydrogen (MTOAH) represents a catalytic pyrolysis pathway, where both catalytic surface kinetics and gas-phase radical reactions govern overall performance. Selective ethylene production therefore requires reaction engineering approaches that explicitly control the relative rates of surface-mediated C-H bond activation and gas-phase-mediated C-C bond coupling.
In this work, we investigate a catalytic reactor designed to enable such control under nonoxidative conditions by promoting rapid methane activation on catalytic surfaces, followed by downstream C-C bond coupling in a gas-phase reaction zone via the MTOAH pathway. A series of Fe-based catalysts are investigated to determine the role of surface Fe species in facilitating C-H bond activation while suppressing coke formation. Hydrogen co-feeding is applied to regulate radical concentrations. The relative contributions of surface- and gasphase reactions were quantified to identify dominant kinetic regimes. In parallel, a machine learning-assisted reaction engineering framework is employed to optimize operating conditions and extract descriptors governing transitions between surface- and gas-phaselimited regimes. A resistively heated reactor is also implemented to increase energy efficiency under high-temperature operation.
Highly dispersed surface Fe species preferentially promoted methyl radical formation with minimal coke formation. Methane conversion proceeded through a coupled reaction network that limits the attainable conversion under non-equilibrium conditions. The rate of methane activation on the catalyst surface exceeded that of gas-phase reactions, indicating that overall performance was governed by reactor-level residence time and radical transport rather than intrinsic surface kinetics alone. Optimizing of reactor operating parameters significantly enhanced C2 hydrocarbon formation. Co-feeding methane with hydrogen at 1230 °C achieved an ethylene yield of 21%. Compared to an adiabatic reactor, the resistively heated reactor achieved comparable C2 productivity with approximately fivefold lower electrical power consumption, enabling stable operation at the kilogram-per-day scale. This work establishes that optimizing MTOAH requires reactor-level control rather than further enhancement of intrinsic catalyst activity. From a chemical reaction engineering perspective, coordinated

design of catalyst properties, reactor architecture, and operating conditions is essential to regulate residence time, radical transport, and energy delivery. Resistive heating provides an effective strategy to supply thermal energy locally and efficiently under high-temperature conditions while maintaining favorable reaction regimes. The proposed reactor concept offers a scalable engineering framework for methane conversion and provides practical guidelines for improving carbon utilization efficiency.

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DFN0698

Thermodynamic Modeling and Optimization of Light Naphtha Hydroisomerization: Implications for EnergyEfficient Refinery Operation

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fundamental
Keywords: Hydroisomerization; Thermodynamic equilibrium; Reaction engineering; Process optimization

Abstract Body.
Light naphtha hydroisomerization is a key refinery process for upgrading low-octane linear paraffins into branched isomers with higher octane number, which are suitable components for gasoline blending. In modern refineries, the hydroisomerization of n-pentane and nhexane represents an attractive alternative to aromatics formation, allowing the production of high-quality gasoline while complying with increasingly strict environmental regulations. However, due to the reversible and mildly exothermic nature of the isomerization reactions, process performance is inherently limited by thermodynamic equilibrium, which establishes the maximum achievable yield of isoparaffins under given operating conditions. Operating beyond these limits often leads to unnecessary severity and increased hydrogen consumption, highlighting the need for equilibrium-based reaction engineering analysis.

In this work, the thermodynamic equilibrium of light naphtha hydroisomerization reactions was analyzed in detail to determine the optimal operating conditions for maximum isomerate production and octane enhancement. The reaction network of the process was constructed based on a bifunctional reaction mechanism, considering metal-catalyzed dehydrogenation–hydrogenation steps and acid-catalyzed skeletal isomerization, with olefins treated as reaction intermediates. A total of 72 molecular reactions involving 33 hydrocarbon species in the C_5–C_6 range were included in the model.

Thermodynamic equilibrium calculations were carried out using the Peng–Robinson equation in an equilibrium reactor (REquil) implemented in ASPEN Plus®. The responses analyzed were the overall isomerate yield, defined as the combined yield of i-C_5 and i-C_6, and the research octane number (RON) of the isomerized gasoline. The selection of operating conditions was based on industrial practice, considering temperature, pressure, and hydrogen-to-hydrocarbon molar ratio as the main variables influencing reactor performance. The combined effect of the operating variables was evaluated using a Taguchi L16 design, and the resulting data were analyzed using response surface methodology to identify optimal operating regions and variable interactions. The RON was calculated from the product composition using a standard blending correlation.

The results showed that isomerate yield was favored at relatively low temperatures, while pressure and hydrogen availability played an important role in stabilizing reaction

intermediates and avoiding undesirable side reactions. Within the operating range studied, a maximum equilibrium isomerate yield of up to 91.6 wt.% with a RON of 86.35 was obtained.

The results confirmed that hydroisomerization performance was strongly constrained by thermodynamic equilibrium and that further increases in severity did not necessarily translate into improved product quality. The equilibrium-based approach provided a quantitative benchmark for reactor operation and identified operating windows that reduced unnecessary severity and hydrogen overuse while preserving yield and octane.

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DFN0705

Model-Based Fault Diagnosis and Fault Tolerant Control in Closed-loop Safety-Critical Chemical Reactors: An Experimental Study

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fundamental

Keywords: semibatch, reactor safety, fault detection

Abstract Body.

In recent years, the heightened emphasis on process safety has spurred significant advancements in fault detection and isolation methodologies within the chemical reactors. We have previously experimentally demonstrated fault diagnosis in both open-loop and closed-loop Continuous Stirred Tank Reactor (CSTR) systems, specifically applied to the alkylpyridine N-oxidation process1,2. Various control strategies, including adjustments to coolant flow rate and inlet coolant temperature, were investigated to maintain reactor temperature stability under rapid and frequent setpoint changes and varying fault conditions. We experimentally validated closed-loop feedback control systems capable of detecting and estimating faults through the analysis of residual signals, thereby enhancing operational safety and reliability.

Based on these works, we then advance to achieve fault-tolerant control (FTC). Active FTC integrates fault detection (FD), a reconfiguration scheme, and an adaptable controller3,4. FD is critical to active FTC, enabling adaptive reconfiguration of the controller to accommodate new operating conditions by detecting, isolating, and estimating faults. To rigorously evaluate system states and outputs against safety thresholds, the concept of the maximal admissible set (MAS) is employed5. This set defines the permissible boundaries for states, guiding reconfiguration decisions by indicating safe operating conditions and necessary intervention points. In this work, we develop a DSS-based FTC strategy for a CSTR model, addressing the challenge of maintaining safety under both minor and major faults. The results show that the nominal controller effectively manages minor faults, maintaining the system within the DSS without further intervention. However, major faults exceed the capability of the nominal controller alone. To counteract this, we introduce a "Plan B" intervention strategy involving a controlled injection of cold solvent to expand the DSS and restore safety margins. Two practical criteria for activating Plan B, based on fault estimates and DSM thresholds, ensure precise and timely fault responses. Thus, accurate DSS computation facilitates effective FTC actions, significantly enhancing system resilience and safety under demanding operational conditions.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

DFN0578

Design of Dynamic Operation for NH3 Synthesis from Exhaust NO gas over Pt/TiO2 Catalyst

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fundamental

Keywords: Ammonia, Kinetic Modelling, Operation Design, Optimization

Abstract Body.

Introduction.

Recently, the catalytic reaction process of nitrogen oxides in exhaust gas to ammonia (NOx to Ammonia, NTA) has attracted attention as an innovative nitrogen cycle system1. While the NTA process employing CO and H2O as reductants has been carried out in prior works2, the effective utilization of H2 remains an important issue. Moreover, the optimal design and effectiveness of reductant feeding operations for maximizing NH3 yield under fluctuating feed concentrations have not been sufficiently investigated. Herein, we develop the dynamic operation of NO-CO-H2O-H2 reaction process utilizing syngas derived from various methane reforming for NH3 production. Furthermore, the overall evaluation of NTA process was carried out by means of time-dependent one-dimensional dynamic simulation and experiment incorporating the surface coverage analysis.

Methods.

A fixed-bed flow reactor with 1 wt% Pt/TiO2 (Rutile) catalyst was utilized to acquire dataset for the kinetic modeling. The model based on the Langmuir-Hinshelwood mechanism was developed to demonstrate the kinetics of the reaction mechanism. The surface coverage calculation was performed using an ODE solver within a plug flow reactor model combined with the derived reaction rate equation. Then, an integrated simulator combining NOx adsorber and NTA process was designed to dynamically evaluate reductant feed operations in response to change in flow rate of feed of NO.

Results and discussion.

The derived reaction rate model which assumes NH3 formation as the rate-determining step showed high accuracy with the experimental data (R2 = 0.99). Subsequently, two different reductant feeding methods, dynamic operation and steady-state operation, were evaluated with varying H2/CO molar ratios and temperatures. Notably, the developed multi-stepwise operation can optimally control surface coverage θi of key reaction intermediates which contributes to enhanced NH3 production. As an example of simulation results, Fig. 1 shows that multi-stepwise consistently sustained a higher surface coverage of θCOOH* along the axial direction of the reactor, contributing to θH* enhancement for NHx synthesis. In the simulation and experiments for dynamic operation, the NH3 concentration at the reactor outlet

was significantly increased by applying the multi-stepwise method. Hence, we have demonstrated optimal design of dynamic operation for reductant feeding to maximize NH3 production throughout operation time, by using the reactor simulation that could provide the spatiotemporal data for behavior of abundant surface intermediates (ASI).

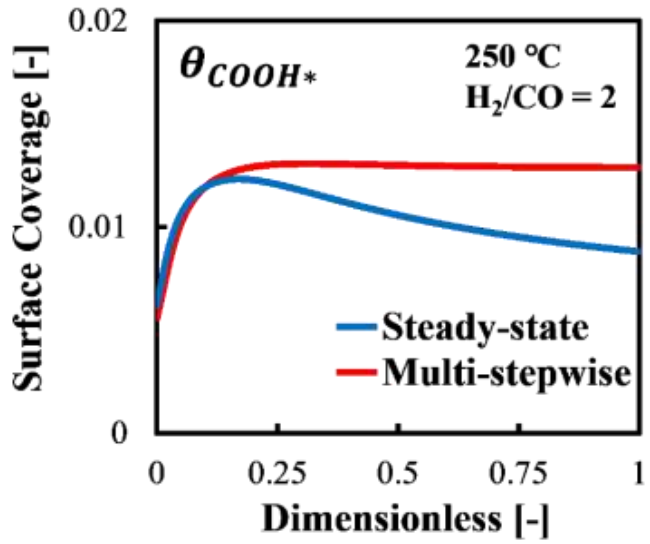

Fig. 1 Surface coverage results in the NO-CO-H2O-H2 reaction

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DFN0431

Creating Digital Twins of Gamma-Alumina Supports by means of 3D Pore Network Models

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fundamental

Keywords: Nitrogen sorption; Mercury porosimetry; Pore network models; Gamma alumina supports

Abstract Body.

Introduction

Porous materials are widely used as catalyst supports in the chemical industry, with γalumina being the most commonly used due to its low cost and ease of fabrication. The architecture of the porous network strongly influences catalyst performance through its impact on surface area, mass transfer, and mechanical strength. Industrial catalyst particles are typically large to limit pressure drop, thereby making internal mass-transfer limitations critical when using active phases with substantial intrinsic activities. In this context, a detailed understanding of both the textural properties and the topology of catalyst supports is essential to further improve catalyst performance. In this work, pore network models were developed to represent γ-alumina supports.

Results and discussion

Five γ-alumina samples, obtained from boehmite precipitation and subsequent shaping into pellets, were characterized experimentally by nitrogen adsorption and helium pycnometry [1]. Pore networks were generated using a stochastic discrete reconstruction algorithm in which pores are represented as cylindrical elements connecting nodes arranged on unstructured lattices [2]. Structural heterogeneity and network topology were controlled through model input parameters.

Nitrogen adsorption–desorption isotherms and scanning curves were simulated using the Kelvin equation to describe capillary condensation, combined with the Harkins–Jura equation to account for adsorbed film thickness prior to condensation. The textural properties of the digital pore network were calculated both geometrically and by processing the network through computer-equivalent characterization techniques. An invasion percolation approach with a dynamic priority list was employed to capture phase transition and percolation phenomena constrained by the topology of the network. The simulated isotherms reproduced the characteristic hysteresis observed experimentally for alumina catalyst supports. By iteratively adjusting the network parameters, good agreement was obtained between the textural

properties of the digital twins and those measured experimentally. Tracer diffusion was subsequently simulated within the reconstructed pore networks using a Fickian diffusion framework. The resulting back-calculated tortuosity factors agreed with experimental values within approximately 20%.

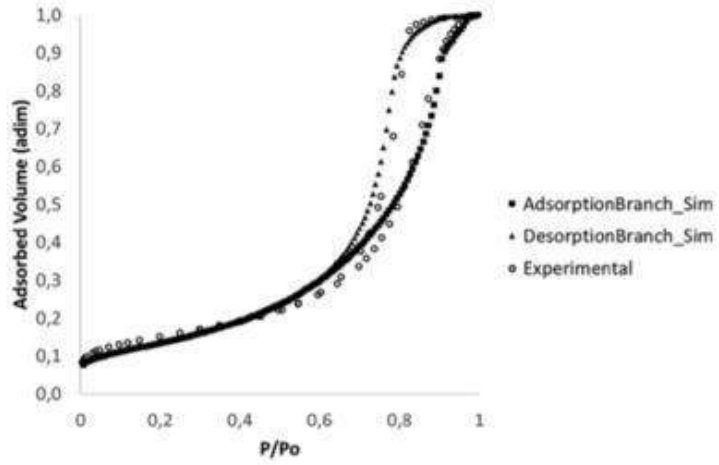

Figure 1. Nitrogen sorption: experimental (open symbols) vs. simulated (closed symbols).

Conclusions

Overall, the proposed pore network–based digital twin approach provides a consistent framework to link the synthesis-dependent pore architecture and the transport properties of γ-alumina supports. Currently, diffusion–reaction simulations are being performed for the selective hydrogenation of butadiene to quantify the influence of pore network properties on the catalyst effectiveness factor.

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DFN0602

Dynamic simulation and scenario study of washcoated electrified reverse water gas shift reactor

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fundamental
Keywords: Electrification, washcoat catalyst, reverse water gas shift, zero washcoat thickness model

Abstract Body.

The electrification of chemical processes has emerged as a promising pathway for substantially reducing global carbon dioxide emissions. In particular, conventional combustion-based reactors, which inherently emit large quantities of CO_2 to reach and maintain chemical equilibrium, stand to benefit significantly from electrification. In parallel, the utilisation of CO_2 emitted from industrial and energy sectors enables the sustainable production of carbon-based chemicals. One key route is the reverse water–gas shift (RWGS) reaction, in which CO_2 reacts with hydrogen to produce synthesis gas.

In this study, a computationally efficient dynamic simulation framework is developed for an electrified RWGS reactor, with validation against experimental data. The present work focuses on transient reactor behaviour, which is essential for understanding start-up, load changes, and process control under electrified operation. The reactor employs a washcoat catalyst, enabling relatively uniform catalyst temperatures and thereby reducing the risk of carbon deposition. However, the associated mass-transfer limitations necessitate careful system-level optimisation.

To address the computational burden associated with conventional computational fluid dynamics (CFD), a reduced-order modelling strategy is adopted. The framework couples two-dimensional (2D) transient mass and energy balances in the gas phase with a onedimensional (1D) kinetic model applied at the reactor wall, where the catalyst is assumed to be located. A zero washcoat thickness (ZWT) assumption is employed, allowing catalytic reactions to be implemented as source terms in the governing equations. This approach avoids explicit resolution of the catalyst domain while retaining sufficient physical fidelity, reducing the computational domains from three to two.

The energy balance is validated using dynamic furnace temperature responses, while the kinetic model is validated against concentration profiles. The model successfully reproduces

both the temporal evolution of axial temperature profiles and the dynamic response of reactant and product concentrations, while reducing computational loads.

Crucially, the dynamic framework enables the investigation of electrical power modulation and control strategies. Scenarios involving step changes, ramping, and periodic variation of electrical input are analysed to assess reactor stability, thermal inertia, and conversion efficiency. The results demonstrate that electrified RWGS reactors can achieve performance comparable to conventional systems, while offering enhanced stability and significantly reduced indirect CO_2 emissions. Moreover, dynamic simulation provides a powerful tool for identifying optimal operating policies that minimise energy consumption while maximising CO_2 utilisation under realistic, time-varying conditions.

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DFN0500

Strategies for industrial-scale methanol synthesis via CO2 hydrogenation under load-flexible conditions

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fundamental
Keywords: methanol synthesis, carbon dioxide hydrogenation, reactor modelling, part-load operation

Abstract Body.

The transition towards renewable energies requires efficient solutions for energy storage and transportation. For long-distance importation of renewable energy, hydrogen and its derivatives are particularly suitable [1]. One often proposed hydrogen carrier with a high potential is methanol, as it is one of the most important bulk chemicals being used in many chemical production processes and therefore, infrastructure is available [2]. Furthermore, it can easily be integrated in the energy sector as well. However, fluctuating availability of renewable energy for hydrogen production led to new research challenges in the field of catalyst, process and reactor design. In the overall process, either a sufficiently large buffer storage facility must be provided, or the methanol plant has to be operated flexibly. Flexible operation down to 10-20 % load significantly reduces levelized cost of methanol [3]. Research is therefore being conducted to determine how existing technologies can be used for load-flexible operation.

As part of this work, we conducted a detailed analysis of the part-load behavior of a largescale methanol reactor. Here, a one-dimensional pseudo-homogeneous reactor model of a steam-cooled industrial-scale methanol synthesis reactor has been developed. This reactor model was built in AVEVA™ Process Simulation and relies on common sub-models for heat transfer, powder kinetics and diffusion. Finally, this reactor model was combined with a process simulation of the methanol synthesis loop to determine flexibility measures and to evaluate various part-load strategies.

Cooled reactors are sensitive to load changes in make-up gas (MUG) flow rate, resulting in the formation of hot spots. As expected, results show that a reduction in MUG flow rate leads to an increase in temperature and a shift in the hot spot position. Stability can be improved by using various flexibility measures, such as MUG pressure and cooling temperature, in order to optimize operation in each load condition. Reducing the pressure or increasing the temperature leads to lower reactor conversion, resulting in a higher recycle ratio and thus a lower demand for make-up gas flow enabling part-load operation of the system. Regardless of which flexibilization measure is applied, reactor extinction and overheating as well as catalyst deactivation must be avoided.

We have demonstrated that part-load operation of an industrial methanol reactor down to

10 % load is possible while maintaining the hotspot temperature of the full load case. The related flexibility measures and part-load strategies will be presented.

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2026 / SEOUL, KOREA

DFN0556

Physically consistent neural network surrogates of catalytic reactors with detailed surface kinetics

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fundamental
Keywords: Physics-informed neural networks, Catalysis, Hard-constraints, Surrogate modelling, Chemical kinetics, Atom conservation

Abstract Body.
Introduction. Motivated by their potential to unlock real-time control of catalytic devices and model-based process design under full mechanistic detail, we develop physics-informed neural networks (PINNs) of catalytic reactors [1]. For the first time, we inform the PINNs about detailed surface kinetics, which is done by coupling with an auxiliary neural network surrogate [2] of the steady state surface reaction rates. In contrast to numerical solutions, the kinetic surrogate is fully compatible with automatic differentiation and up to 105 times faster to evaluate, accelerating model training accordingly. This allows quick and meshless predictions of composition profiles. Further, we propose a dedicated neural network layer that imposes atom conservation as a hard constraint based on a completion approach. This guarantees the physical consistency of predicted reactor compositions and thus reduces the amount of data required for model training, in our case, by a factor of ten.

Methods. For our PINN framework we use a feed forward neural network, then add exponential output activation to guarantee positivity and append the proposed atom conservation layer [1]. For training, we simulate 160 pairs of inlet-outlet compositions of an isothermal Nickel-catalyzed 1D-pseudohomogeneous methanation reactor under steadystate. Additionally, 8000 collocation points are sampled within the reactor to adjust the slope of the predicted profiles according to a kinetic surrogate [2] which mimics a microkinetic mechanism [3] with a relative error below 0.25%.

Results and discussion. Despite being trained only with inlet/outlet data, our new framework provides accurate concentration profiles as exemplary shown for a catalytic CO2 methanation reactor in Fig. 1 (left). Generally, predicted conditions are accurate within 4.5 % relative error over a wide range of feed compositions and temperatures (4 % CO2, 5.310.6 % H2 in N2 at 500-900 K) as shown in Fig. 1 (right). This accuracy is only possible by the combination of PINNs with the atom conservation layer, which simultaneously closes the atom balance and preserves the positivity of the concentrations. As a result, despite the model simplicity, predictions are more than 1000 times faster than ODE integration with Cantera (21 µs vs 28 ms). Overall, our approach is straightforward to implement and can be readily integrated into existing reactor modeling workflows, enabling rapid adoption within the catalysis and reaction engineering community.

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DFN0560

Understanding unsteady operation of washcoated monolith reactors for emission-control

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fundamental

Keywords: Simulation, CFD, Multiscale Modeling, Microkinetics

Abstract Body.

Introduction. Catalytic reactor systems for emission-control are subjected to time-varying feeds and boundary conditions. Beyond adapting to dynamic operating conditions, deliberately imposed dynamic operation has emerged as a promising strategy to enhance reactor performance [1]. In this context, recent experimental studies employing short reducing pulses (SRPs) in monolithic reactors have demonstrated significant potential [2].

The strong coupling between phenomena and scales in catalytic reactor systems poses substantial challenges for numerical modeling. Computational fluid dynamics (CFD) combined with transient microkinetic models enables a detailed description of both the flow field and the evolving local surface chemistry. To date, only few studies simulated the macroporous structure of washcoated catalytic reactors using a CFD–microkinetic framework.

Methods. To address these challenges, a three-dimensional CFD framework is developed, that resolves fluid dynamics and heat transfer while incorporating detailed surface chemistry through transient microkinetic models. The framework combines OpenFOAM for solving the Navier–Stokes–Fourier equations with Cantera for heterogeneous reaction kinetics. Catalytic washcoats are modeled using a pseudo-continuum porous medium approach, with effective parameters directly derived from simulations of representative macroporous structures, as depicted in Figure 1. Computationally efficient integration of the microkinetic model is ensured by employing the operator splitting approach.

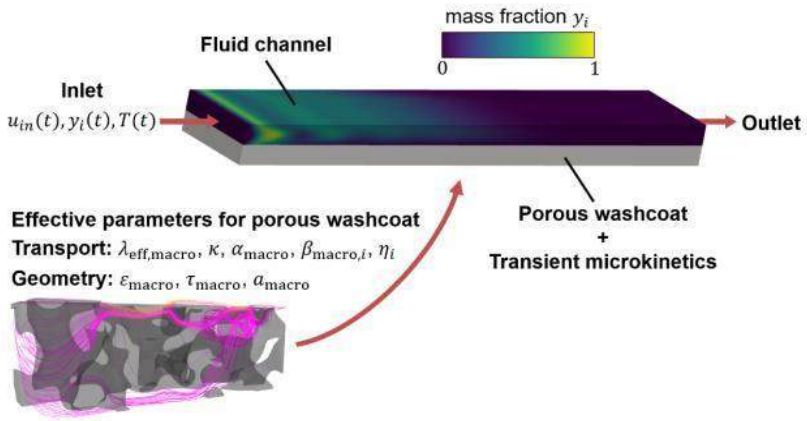

Figure 1: Schematic illustration of the multiscale concept.

Results and discussion. As a demonstration, the reactive flow over a porous catalytic plate is simulated and compared against experimental two-dimensional planar laser-induced fluorescence (2D-PLIF) measurements, in a configuration similar to that reported by Wan et al. [3]. While the full microkinetic framework is still under development, preliminary simulations based on a simplified adsorption–desorption model already reveal pronounced spatial and temporal variations in surface coverage under transient operation. These results illustrate the strong coupling between local flow structures, mass transport, and surface state dynamics, emphasizing the necessity of resolving local surface conditions when analyzing transient reactor behavior.

Outlook. The proposed framework provides a platform for studying dynamically operated catalytic reactors under realistic conditions. Future work will focus on predicting the transient performance of monolithic reactors under flexible feed loads. Furthermore, the detailed spatial resolution of surface reactions enables the systematic optimization of washcoat morphology with respect to transport limitations.

Acknowledgments
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ISCRE29 & APCRE11
2026 / SEOUL, KOREA

DFN0600

Multiscale Modelling of Transport Phenomena in Tubular Fixed-Bed Reactors

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fundamental
Keywords: Computational fluid dynamics, packed-bed reactor, transport phenomena

Abstract Body.

Tubular fixed-bed catalytic reactors are widely employed in the chemical industries due to their operational simplicity, robustness, and suitability for a broad range of heterogeneous catalytic reactions. Despite these advantages, reactor performance is strongly governed by transport phenomena within the packed bed, including pressure drop, heat transfer from the reactor wall toward the bed centre, and mass transfer between the fluid and catalyst surface. Accurate characterisation of these coupled phenomena is essential for reducing operating costs, limiting energy consumption, and improving product yield and selectivity.

In this study, a multiscale simulation framework was developed to systematically investigate the effects of catalyst pellet size on hydrodynamic, thermal, and mass transfer behaviour in a tubular fixed-bed reactor. A physics engine was first employed to generate realistic random packings of cylindrical catalyst pellets within a reactor of fixed diameter and length, capturing particle-scale heterogeneity such as contact points, void distribution, and near-wall packing structures.

The generated packing geometries were subsequently imported into a three-dimensional computational fluid dynamics (CFD) model to resolve fluid flow, heat transfer, and species transport under constant wall temperature. Inlet temperature and superficial velocity were varied to assess their combined influence on pressure drop, thermal fields, and mass transfer characteristics. Performance indicators included bed voidage, pressure drop per unit reactor length, axial and radial temperature profiles, species concentration distributions, and transient thermal response.

The results reveal a strong dependence of bed characteristics on catalyst pellet size. Decreasing pellet diameter leads to reduced bed voidage due to denser packing, particularly near the reactor wall, resulting in a pronounced increase in pressure drop, consistent with classical packed-bed flow correlations. Higher inlet velocities further amplify pressure losses due to increased frictional resistance. From a thermal perspective, smaller pellets enhance radial heat transfer by shortening characteristic diffusion lengths and increasing solid–fluid interfacial area, although this benefit is accompanied by higher pressure penalties. Similarly, improved mass transfer performance is observed for smaller pellets due to reduced diffusion resistance within the packed bed.

Based on the CFD results, effective transport properties, including pressure drop correlations, effective thermal conductivity, and effective mass diffusivity, were quantified and incorporated into a two-dimensional mathematical model. This coupling enables computationally efficient reactor-scale simulations while retaining particle-scale physical fidelity. Overall, the proposed

multiscale framework provides a robust pathway for linking particle geometry to macroscopic reactor performance and supports the optimisation of catalyst design and operating conditions in fixed-bed reactors.

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DFN0551

Maximizing Cu/ZnO/Al2O3 Catalyst Performance by Unlocking Intrinsic Methanol Selectivity with In-Situ Water Removal

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fundamental

Keywords: Methanol, CO2 Utilization, Dynamic Modelling, Adsorption

Abstract Body.

Introduction.

Manufacturing methanol from CO2+H2 has been frequently researched for its promise as a greener alternative to the typical synthesis route from syngas. However, unlike the syngas route, using CO2 produces water, which inhibits methanol yields and selectivities [1]. By co-loading a zeolite sorbent alongside a Cu/ZnO/Al2O3 (CZA) catalyst, water can be removed in-situ, temporarily enhancing methanol rates. This work aims to model the performance of these sorption-enhanced (SE) reactors and maximize CZA performance by accessing high selectivities, unavailable under steady-state operation, in water's absence.

Methods.

A plug-flow, isobaric, isothermal, packed-bed reactor model was developed to predict the performance of SE reactors. The kinetic model developed by Vanden Bussche & Froment for CO2 hydrogenation was used [1]. To model mass transfer of water into the zeolite sorbent, a linear driving force model was used, where isotherm effects were accounted for. A Langmuir-type isotherm expression for water in Molsieve 3A was used.

Results and discussion.

Simulations show enhanced methanol and CO formation when water is removed from the reactor, in line with literature observations [2]. Removing water from the reactor significantly affects the catalyst performance, but the enhancement is both thermodynamic and kinetic in nature. By tuning the catalyst loading, the thermodynamic and kinetic benefits can be separated and compared. Tuning the sorbent loading allows for adjustment of the degree of water removal. Figure 1 shows that the benefit of water removal is greater under kinetic control, and that there is also a significant selectivity advantage when compared to the thermodynamically controlled regime. In fact, similar integral methanol yields are attained in both regimes.

$$\varepsilon\frac{\partial C_i}{\partial t} = -\frac{\partial\left(u_g C_i\right)}{\partial z} + (1-\varepsilon)\varphi_{cat}\rho_{cat}\sum_j v_{ij}r_j - (1-\varepsilon)\varphi_{ads}\rho_{ads}\frac{\partial q_i}{\partial t}$$

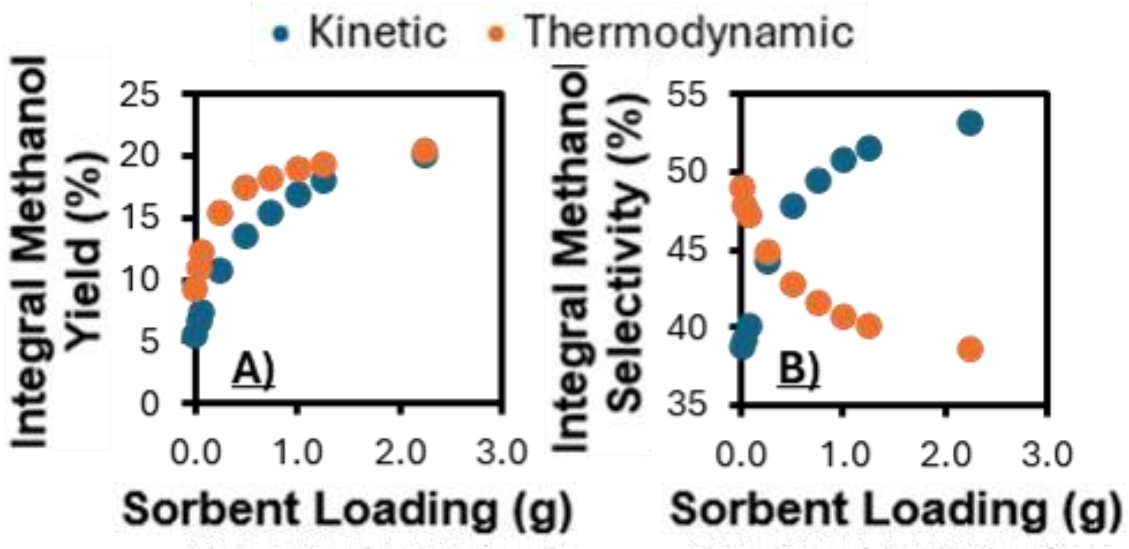

Figure 1: Reactor Species Balance and A) Integrated methanol yields and B) selectivities in SE reactors across the transient period. Kinetic catalyst loading = 37.5 mg CZA; Thermodynamic catalyst loading = 750 mg CZA. Temperature = 225°C; Total Pressure = 40 bar.

Conclusions

This work demonstrates the utility of SE reactors for enhancing CZA performance for CO2 hydrogenation, compared with typical steady-state operation in packed-bed reactors. Methanol formation suffers from kinetic and thermodynamic limitations that are alleviated when water is removed. This work highlights SE's ability to unlock the innate methanol selectivity of CZA catalysts, which is inaccessible under steady-state operation due to water's presence. However, it requires low catalyst loadings to guarantee kinetic control. This selectivity boost in the kinetic-controlled regime even produces methanol yields comparable to those of SE reactors loaded with an order of magnitude more catalyst.

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DFN0073

Shallow-bed Reactor Design for the Conversion of Natural Gas to Ethylene by Oxidative Coupling

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fundamental

Keywords: Natural gas conversion, Oxidative coupling of methane, Oxidative dehydrogenation of ethane, Autothermal reactor, Particle ignition

Abstract Body.

Introduction

Natural gas is being converted to useful chemicals such as ammonia, hydrogen, and methanol which involves syngas production at the first step. Among the alternative direct processes, oxidative coupling of methane (OCM) is seen as an attractive option to produce C2 products especially ethylene bypassing syngas route. Extensive research has focused on developing stable, active catalysts that selectively convert methane to ethylene while minimizing CO and CO2 byproducts; however, the process is still limited to commercialization due to heat management concerns. In this work, we demonstrate the feasibility of carrying out OCM with natural gas feed autothermally in a shallow packed-bed reactor through comprehensive ignition-extinction analysis.

Methods

We utilize experimentally validated 10-step global kinetic model over La2O3/CaO proposed by Stansch et al. [1] to investigate bifurcation features of the OCM process. A cell model that accounts for inter-phase heat and mass transfer resistances along with intra-particle diffusional resistance is employed to capture particle level ignition, which arises from solid-fluid inter-phase temperature and concentration gradients and is distinct from that of reactor scale heat and mass dispersion [2]. Bifurcation diagrams are computed using the pseudo-arc length continuation method.

Results and discussion

We show that there exists a minimum amount of oxygen in the feed to convert methane-ethane mixtures with reasonable conversion and improved ethylene selectivity. Eggshell type catalyst particles are advocated to avoid the pore diffusion limitation that not only decreases the region of autothermal operation but also reduces ethylene selectivity. For the specific kinetics considered, high hydrocarbon to oxygen ratio at the catalyst surface favors ethylene formation that enhances ethylene selectivity by operating under external mass-transfer controlled regime (Fig.1). However, exit conversions are poor due to mass transfer limitations; therefore, multi-layered bed with a few layers of catalyst particles is proposed to achieve complete conversion of oxygen. Moreover, feasibility of high-pressure operation is demonstrated with improved productivity and ethylene yield. Our computations show the possibility of obtaining 75-85% ethylene selectivity at 20-25% methane and nearly 40% ethane conversion per pass.

Comparing to the base case of pure methane feed, close to 30% enhancement in the ethylene selectivity is observed, demonstrating the promotional effect of ethane cofeed and enabling direct natural gas conversion without separating C1 and C2 hydrocarbons.

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ISCRE29 & APCRE11
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DFL0540

Experimental Thermal and Hydrodynamic Characterization of a 2D Electrothermal Fluidized bed Reactor for CFD-Based Design

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fluidization/Multiphase Flow Reactors

Keywords: Electrothermal fluidized bed, Joule heating, 2D lab-scale prototype, Thermal characterization, Hydrodynamics, CFD modeling.

Abstract Body.
Electrothermal Fluidized Bed reactors (ETFB) offer a disruptive approach to high temperature processing (~ 1100 °C) by combining particle-scale Joule heating with rapid pulsed operation. Heating and quenching cycles on millisecond-to-second timescales selectively favour reactions with high activation energies while suppressing undesired side reactions during lower-temperature intervals. Despite this potential, thermal and hydrodynamic design of electrothermal fluidized beds remains poorly understood, limiting their rational scale-up and optimization.
This work presents an experimental thermal and hydrodynamic characterization of a ETFB in a two-dimensional prototype, with the objective of generating high-quality data to support and inform a Eulerian-Eulerian CFD modeling framework. The reactor consists of stacked alumina and quartz plates (3 mm), with a bed diameter of 50 mm, a height of 70 mm, and an internal thickness of 17 mm (Figure 1). Synthetic graphite particles with a size distribution of 150 – 250 µm were used as the electrically conductive bed material. Heating was achieved using a rectangular central graphite electrode (20 mm) surrounded by two rectangular graphite electrodes (70 mm height), powered by a SM70-CP-450 DC power supply (70 V – 450 A). A 3 mm quartz window enabled mid-wavelength infrared (IR) thermal imaging for spatially resolved temperature measurements, while particle voidage was quantified through image analysis using ImageJ.
A parametric experimental study was conducted by varying volumetric gas flow, central electrode position, and applied voltage. Transient temperature evolution and effective electrical current through the bed were monitored to capture coupled thermal – hydrodynamic – electrical behavior. Experimental results demonstrate that electrode position has a strong influence on reactor thermal performance. For instance, increasing the distance between the electrode and gas distributor from 10 mm to 20 mm reduced the steady-state temperature from 210 °C to 89 °C. In addition, a decrease in effective current is observed as the bed transitions from transient to steady-state operation, associated with increasing gas velocity

and temperature. The magnitude of this current drop depends on electrode position, ranging from approximately 35 % at zero electrode-distributor distance to about 20 % at larger separation.

The collected experimental data was used to develop a CFD model in OpenFOAM, providing a basis for identifying optimal operating and design conditions. This combined experimental-numerical approach supports the development of physics-based design strategies for electrothermal fluidized bed reactors. Future work will focus on extending this framework toward scalable, energy-efficient reactor configurations.

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2026 / SEOUL, KOREA

DFN0439

Accelerating Catalytic Reactor Design Space Exploration Using Surrogate Modeling Techniques

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fundamental

Keywords: Catalytic Reactor Design; Surrogate Modeling; Design Space Exploration; gPROMS Process

Abstract Body.

Introduction. R&D departments in the process industry are increasingly focused on sustainability and circularity, driving innovation in chemical processes. These efforts introduce new catalytic reactor design challenges, where rapid innovation is essential, but decisions often must be made with incomplete information, introducing risks that must be quantified and mitigated to ensure successful industrial-scale implementation. Advanced process modeling (APM) of catalytic reactor systems is vital for managing technological risks and accelerating innovation, particularly through rapid design space exploration and reactor optimization [1]. However, predictive models that capture all relevant phenomena can be computationally demanding, limiting the ability to efficiently explore design space.

To address this, surrogate modeling techniques can be integrated into reactor models to improve computational efficiency without sacrificing accuracy. This paper demonstrates how surrogate modeling can be incorporated within a detailed first-principle model to accelerate design space exploration and optimization.

Methods. Rigorous modeling of complex reactor systems requires detailed consideration of kinetics, mass transfer, intrapore diffusion, and heat transfer. For systems with complex reaction kinetics, distributed pellet models are often used to represent catalyst pellets, but these are computationally expensive and impractical for large-scale design space exploration. To address this, the catalyst effectiveness factor is combined with lumped pellet representations, provided the effectiveness factor can be accurately calculated. Analytical solutions are feasible only for simple systems, while complex mechanisms require numerical approaches.

In this work, a single pellet model with distributed representation is used to efficiently generate effectiveness factor data across a wide operating envelope. A neural network-based surrogate model is then trained to capture the complex dependency of effectiveness factor on operating conditions. Once validated, this surrogate model is deployed within a lumped pellet-based full-scale reactor model, enabling efficient calculation of reaction rates and supporting rapid, reliable design space exploration. APM software like gPROMS Process is essential for efficient implementation of this methodology, offering robust tools and workflows for model development and deployment.

Results and discussion. Applying this methodology to CO_2 methanation reactor systems showed that neural network-based surrogate models can accurately predict effectiveness

factors as functions of operating conditions. Deploying these models within industrial-scale reactor simulations enabled rapid and efficient design space exploration, significantly reducing computational time and complexity.

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DFN0604

MultiCAT: a GUI-based AI-integrated platform for catalytic reactor modeling and kinetic parameter estimation

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fundamental

Keywords: Chemical Reaction Engineering, Reactor Modeling, Kinetic fitting, Fixed-bed reactors, Fluidized-bed reactors, Digital twins

Abstract Body.

Introduction.

Modern chemical reactor design and optimization increasingly demand tools capable of bridging rigorous multiscale scientific models with practical data-centric workflows. MultiCAT is a powerful computational platform that transforms how chemical reactions are analyzed, designed, and controlled by seamlessly combining advanced reactor modeling with data-driven analysis into a unified environment. The platform empowers users to simulate, interpret, and optimize chemical processes from the laboratory bench to full-scale industrial operation, all within an intuitive graphical interface accessible even to users without deep in-house expertise in catalysis or kinetics. Unlike traditional standalone simulation codes, MultiCAT integrates reactor physics, data analytics, and kinetic interpretation, enabling efficient exploration of complex reacting systems and digital twin creation for real-time prediction and control.

Methods.

MultiCAT combines first-principles reactor models with data-driven analysis to enable comprehensive simulation and diagnostic workflows for fixed- and fluidized-bed reactors. The platform includes a broad set of validated engineering correlations for effective transport properties, ensuring reliable reactor-scale simulations. Its GUI (see Fig. 1) allows easy definition of simulation scenarios and efficient post-processing of results, while supporting direct import of experimental kinetic data for automated parameter fitting. The modular structure of MultiCAT also enables rapid creation of reactor digital twins, which can be directly implemented into process simulators for plant-wide analysis, optimization, and control.

Results and discussion.

The MultiCAT platform has demonstrated strong capabilities for advanced reactor modeling through industrially relevant case studies. As a representative example, MultiCAT has been applied to a multitubular fixed-bed reactor for phthalic anhydride synthesis, enabling detailed 1D/2D(+1D) modeling of temperature, pressure, and concentration profiles, including intraparticle transport limitations. This allows accurate prediction of hot-spot formation and reactor performance under different operating conditions (see Fig. 1). In addition, MultiCAT supports kinetic data analysis from laboratory and pilot-plant experiments, with automated kinetic parameter fitting that accounts for transport phenomena and reactor non-idealities.

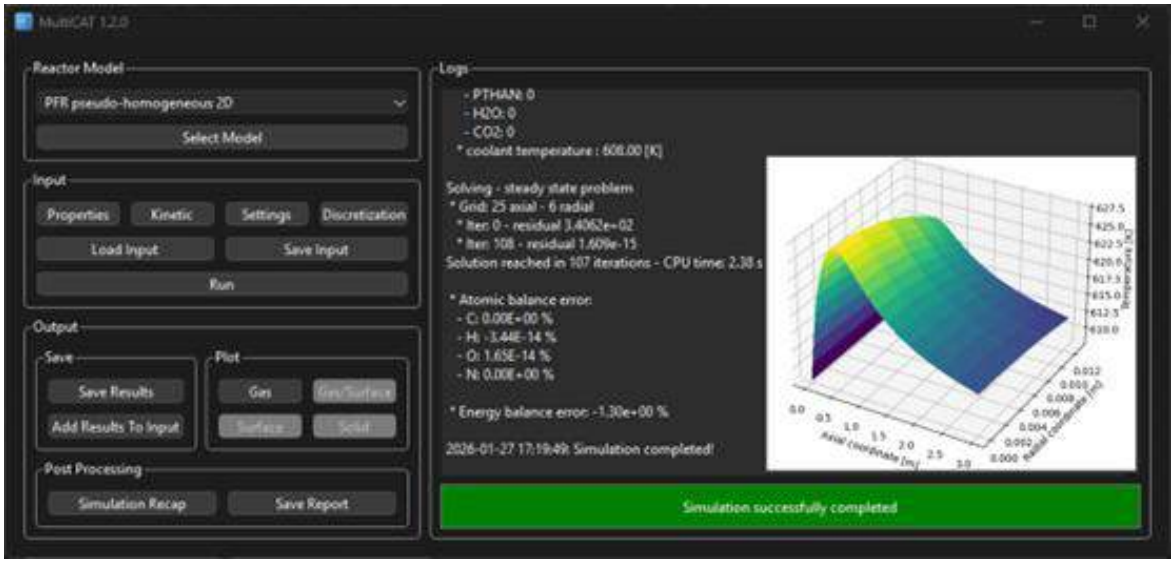

Fig 1. GUI-based MultiCAT window and reactor simulation temperature profiles

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DFN0645

Numerical Investigation of Heat Transfer–Pressure Drop Trade-Off in Periodic Open Cellular Structures for Intensified Catalytic Reactors

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fundamental

Keywords: Periodic open cellular structures (POCS), heat transfer–pressure drop trade-off, correlation-based numerical modeling

Abstract Body.
Efficient thermal management continues to be a major challenge in catalytic tubular reactors, particularly for strongly exothermic or endothermic processes. Traditional packed-bed reactors offer high catalyst inventory but suffer from limited radial heat transfer and high pressure drop, often necessitating high flow rates and long reactor lengths to prevent hot spots and thermal runaway. Periodic open cellular structures (POCS), enabled by additive manufacturing, present an alternative by combining high porosity, enhanced internal heat transfer, and low pressure drop. However, existing work often treats heat transfer and pressure drop separately and lacks a unified design-oriented modelling framework suitable for performance comparison and optimisation.

In this study, we develop a numerical framework to directly compare the heat-transfer and pressure-drop characteristics of packed beds, bare POCS, and packed POCS under identical operating conditions. Established literature correlations for effective radial thermal conductivity, wall heat transfer coefficient, and pressure drop are incorporated into a one-dimensional pseudo-homogeneous energy model (the αW-model). This enables systematic evaluation of geometric parameters, including porosity, strut diameter, and unit-cell type (cubic versus diamond), with respect to thermal performance and hydrodynamic behaviour. Parametric simulations demonstrate that diamond-based POCS exhibit substantially higher radial heat transfer than cubic POCS and conventional packed beds, while maintaining a significantly lower pressure drop. Hybrid packed POCS configurations show promise in balancing enhanced heat transfer with increased catalyst inventory, but their performance strongly depends on geometry and flow conditions. We introduce a performance metric that quantifies the heat transfer–pressure drop trade-off, enabling rapid design space exploration and identification of optimal regions where thermal gains incur minimal hydrodynamic penalties.

The novelty of this work lies in the unified, correlation-based numerical methodology that explicitly links structural geometry to both heat transfer and pressure drop without relying on costly experiments or full CFD simulations. This framework facilitates the model-based design and optimisation of structured reactor internals and provides practical insights for advancing catalytic reactor intensification.

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DFN0686

First principles-based predictive modeling of a tubular reactor for thermal methane pyrolysis

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fundamental

Keywords: Turquoise hydrogen, methane pyrolysis, reactor modeling

Abstract Body.
Introduction. Methane pyrolysis has emerged as a lower-CO2 alternative for co-generation of turquoise hydrogen and solid carbon. Predictive reactor models with reliable kinetics are lacking. To this end, a flow reactor model comprising reduced-order global kinetics is derived from detailed chemistry and tuned and validated with bench-scale data. The reactor model efficiently predicts the performance of a commercial-scale reactor.

Methods. A dynamic non-isothermal 1D model is developed for a tubular flow reactor for noncatalytic thermal methane pyrolysis (Fig. 1 (a)). The model equations combine mass, momentum, and energy balances for the gas and solid phases and a reduced-order reaction scheme (Fig. 1(a)). The scheme is developed through reaction pathway analysis using a benchmarked free-radical mechanism and literature experimental data [1]. The coupled PDEs are solved in MATLAB and the results are analyzed to assess the performance of a methane pyrolysis reactor over a wide range of operating conditions.

Results and discussion. Fig. 1 (b) compares the tuned reactor model-predicted CH4 conversion and the H2 yield with the temperature-controlled experiments reported by Lott et al. [1]. The model predictions show very good agreement with the data (accuracy > 95%). The model is applied to simulate an adiabatic reactor by varying the feed temperatures and the H2/CH4 ratio (τ = 3s), with the resulting yield of solid carbon shown in Fig. 1 (c). Feed temperatures higher than 1500°C are needed to obtain an appreciable carbon yield, while higher H2/CH4 ratios are found to be associated with higher carbon yield at a specific feed temperature. At H2/CH4 ratios ≤ 3, the carbon yield is found to be nearly proportionate to the H2 yield, as exemplified for H2/CH4 ratio of 2 in Fig. 1 (d). The difference between the two is attributed to the formation of C2 hydrocarbons. C2H2 concentration increases monotonically, while C2H4 concentration exhibits a maximum with respect to feed temperature (Fig. 1 (d)). The trends obtained for an adiabatic reactor and a reactor with heat losses (typical commercial reactor configuration) differ significantly from those for isothermal operation owing to endothermicity of CH4 decomposition. Further insights into the effect of design and operating conditions will be discussed in the full manuscript.

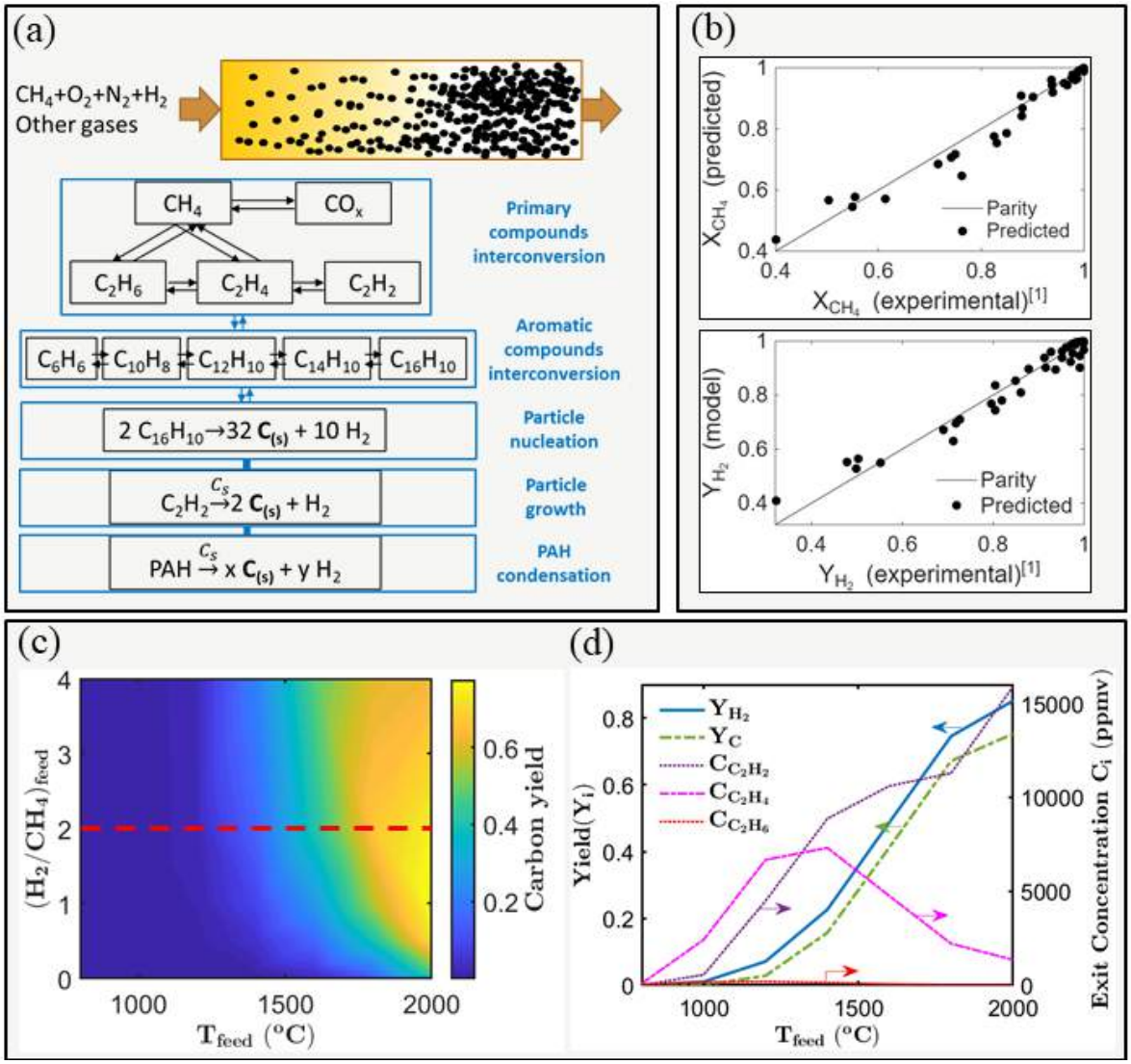

Fig. 1. (a) Reactor schematic and reaction pathways, (b) Parity plots, (c) Effect of feed conditions on carbon yield, (d) H2, C yields and C2 species concentrations at H2/CH4 ratio of 2

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DFL0640

Virtual Process Engineering: Building World Models for Process Industries

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fluidization/Multiphase Flow Reactors

Keywords: Digital twin; Artificial intelligence; Multiscale method; World model

Abstract Body.

Introduction. With wider and deeper application of artificial intelligence (AI) in chemical engineering and all process industries, building a world model for the training and testing of the AI models and agents becomes a must. It is preferably a digital twin of the real facilities and plants with multiscale details of the physical and chemical processes inside. However, this poses great challenges to the accuracy of the numerical methods and computational cost involved. Virtual process engineering[1] aims to provides a revolutionary engineering approach to industrial-scale modeling and simulation of the multi-scale reaction and transport processes using high performance computing.

Methods. For real chemical processes, the multi-scale coupling of reaction, adsorption/ desorption, diffusion and convection can be simulated efficiently in pseudo-particle modeling[2], which integrates the advantages of both soft- and step-potential molecular dynamics methods. At the reactor level, direct numerical simulation (DNS) is only affordable to lab-scale systems, while less costly continuum-based multi-fluid models suffer low accuracy. Coarse-grained methods and sub-grid-scale models have been proposed to address this dilemma, such as the EMMS-DPM[3,4].

Results and discussion. Quasi-real simulation of pilot circulating fluidized beds (CFBs) and full-loop simulation of industrial CFBs[5] has been achieved, a solid step towards real-time simulation of industrial systems. The PPM and EMMS-DPM can be coupled further to address trans-level problems, from reactions to reactors[6]. Furthermore, AI-based acceleration method[7] has shown new pathways to the final goal of VPE, building world models for process industries.

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DFL0643

Mapping of Gas-Liquid Flow Regimes and Bubble Dynamics in a Dual-Impeller Stirred Tank Using Non-Intrusive Measurement Techniques and Machine Learning

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fluidization/Multiphase Flow Reactors

Keywords: Gamma-ray Densitometry (GRD); Machine Learning (Mask R-CNN); High-Speed Imaging; Gas-Liquid Stirred Tank Reactor; Bubble Size Distribution; Gas Volume Fraction

Abstract Body.

Gas-liquid stirred tank reactors (STRs) are fundamental to chemical reaction engineering, particularly for processes involving gas-liquid reactions relevant to sustainable and carbon-neutral technologies such as CO2 utilization, hydrogenation, and aerobic oxidations. The hydrodynamic characteristics of these reactors, namely gas volume fraction, bubble size distribution (BSD), Sauter mean diameter (SMD) and flow regimes, play a role in governing interfacial area, mass and heat transfer rates, and overall reactor performance. Dual-impeller configurations are increasingly employed to improve gas dispersion and overall mixing efficiency in gas-liquid STRs. Despite their growing industrial relevance, comprehensive experimental data remain limited. In particular, clear relationships between operating conditions, including impeller speed (N) and superficial gas velocity (Vsg), and geometrical parameters such as impeller design, impeller spacing-to-diameter ratio (S/D), and liquid height-to-tank diameter ratio (H/T) are not yet well established. Moreover, the influence of these parameters on local gas-liquid dynamics, including BSD, SMD, and flow regime transitions, remains poorly understood. This limitation primarily arises from the challenges associated with non-intrusive measurements and the need for robust data analysis methodologies capable of delivering reliable hydrodynamic characterization for improved prediction and reactor design.

In the present study, an integrated experimental approach combining gamma-ray densitometry (GRD) and high-speed imaging is employed to systematically characterize the gas volume fraction, BSD, SMD, and flow regimes in a gas-liquid (compressed air-Millipore water) STR (T = 0.19 m) equipped with a novel Rushton+mixed (RT-6+MI) [1] dual-impeller configuration. Gamma-ray densitometry enables non-intrusive, chordal-averaged measurements of gas volume fraction under opaque and high-gas-loading conditions, while high-speed imaging provides detailed visualization of bubble dynamics. Bubble detection and size estimation are performed using a machine-learning-based (Mask R-CNN) image analysis

framework, enabling robust, automated extraction of bubble characteristics across a wide range of operating conditions (N = 300-500 rpm and Vsg = 2-6 mm/s). The combined use of these complementary diagnostics enables the construction of a flow-regime map that links gas volume fraction and bubble size to impeller speed and gas flow rate, thereby providing reaction-relevant hydrodynamic insights.

The integrated GRD and high-speed imaging measurements reveal a strong dependence of gas volume fraction and bubble size characteristics on impeller spacing (S/D) and operating conditions, as shown in Figure 1. Increasing S/D enhances gas dispersion uniformity, reduces bubble coalescence, and promotes smaller SMD, leading to distinct transitions between loading, flooding, and complete dispersion regimes. The resulting flow-regime map, supported by visual flow patterns, provides reaction-relevant hydrodynamic insights for optimized dual-impeller gas-liquid reactor design.

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DFL0646

Model-based assessment of heterogeneous secondary reactions and the relevance of char loading in fluidized bed pyrolysis of biomass

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fluidization/Multiphase Flow Reactors

Keywords: biomass, pyrolysis, fluidized bed, secondary reactions, modelling

Abstract Body.
Biomass fast pyrolysis can support decarbonization by substituting fossil fuels, enabling carbon-neutral energy and supplying hard-to-decarbonize sectors with renewable fuels and platform chemicals. During fast pyrolysis, biomass decomposes to biochar, bio-oil and gases through a complex network of series-parallel thermally activated chemical reactions. However, bio-oil is characterized by high viscosity, high water content, acidic pH and limited stability. These issues stimulate research investigations aimed at improving the design of pyrolytic converters and process conditions to maximize yield/selectivity toward valuable compounds.
Fluidized bed reactors represent a favourable environment for biomass fast pyrolysis. However, particle heating and time-temperature history, biomass and volatile/gas residence times, gas-solids contacting and mixing need to be carefully controlled to drive conversion along the prescribed chemical pathway. A specific concern regards the course of secondary reactions between depolymerization products and char, whose progress may alter the yield and composition of the bio-oil. The relevance of the heterogeneous vapor-char interaction to bio-oil production emphasizes the importance of proper control of char loading establishing during steady operation of a fluidized bed pyrolytic converter, that must be carefully controlled by proper reactor design and operation.
In the present study fluidized bed pyrolysis of biomass is assessed with a focus on operational modes that maximize the yield to depolymerization products: pyrolytic sugars, from decomposition of holocellulose; BTX and substituted monoaromatics, from decomposition of lignin. Accordingly, the reactor design and operating conditions are selected so as to minimize secondary interaction between primary pyrolytic vapours and biochar. A shallow fluidized bed with overbed feeding of relatively fine biomass particles is considered. A one-dimensional model including the key features of the fluidized bed pyrolytic converter is developed. The remarkable feature of the model is careful consideration of processes that control the establishment of a steady char loading in the bed, namely, entrainment, elutriation, attrition, and bed drain/regeneration. Primary pyrolytic decomposition of biomass and secondary reactions have been modeled using a semi-detailed reaction scheme. Different kinetic mechanisms are considered for the secondary reactions of the main macropolymers (cellulose,

hemicellulose and lignin), including sugars dehydration and fragmentation, demethoxylation and demethylation of guaiacyl-containing structures from lignin depolymerization, uptake and decomposition of aromatic structures on char surface. Model results elucidate the role of heterogeneous secondary reactions, the main composition of bio-oil and the proper management of char loading during fluidized bed pyrolysis, providing criteria for optimal reactor design and operation.

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DFL0110

Measured and modeled gas concentration profiles of a 180 kW pilot-scale methanation bubbling fluidized bed reactor

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fluidization/Multiphase Flow Reactors

Keywords: Bubbling Fluidized Bed, Concentration Profile Measurements, Two-Phase Model, X-Ray Tomography

Abstract Body.

Introduction

CO2 hydrogenation to methane provides a reliable way to store and transport energy from otherwise unusable renewable electricity (PV, wind, hydropower) through the existing natural gas grid. Catalytic bubbling fluidized bed reactors (BFB) offer great flexibility in accommodating a wide variety of feed gas compositions, including those from biogas plants, wood gasifiers, and other potential CO2 sources:

$CO2 + H2 \leftrightarrow CO + H2O$
$CO + 3\ H2 \leftrightarrow CH4 + H2O$

Methodes

A 180-kW nominal-output pilot-scale fluidized-bed reactor was used to measure gas concentration profiles at various heights within the bed, offering valuable insights into the reactor. Tested gas compositions comprise the conversion of gasifier product gas from allothermal and autothermal gasification with and without hydrogen addition as well as biogas hydrogenation (Power-to-Gas). Input varied from 50 kW to 410 kW; pressures varied from 3 bar to 9 bar.

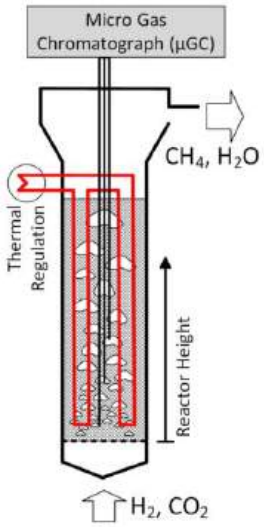
Vertical heat exchanger tubes inside the reactor provided effective cooling directly within the bed. However, internals such as heat exchanger tubes influence the formation of particle-free voids in the fluidized bed, often called bubbles, which greatly impact the mass transfer in the reactor.

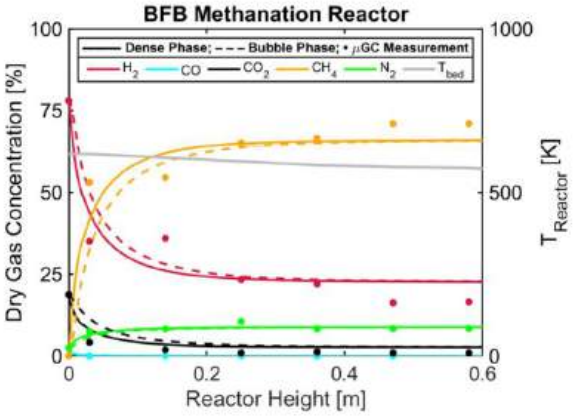
A two-phase numerical model was created to better understand the interaction of chemical reactions and heat/mass transfer in the reactor. The model uses the inlet gas composition and the measured temperature profile from the pilot-scale reactor as inputs and predicts the gas concentration profile. The model consists of two phases: the bubble phase, considered particle-free, and the dense phase, viewed as a homogeneous catalyst emulsion where the reaction occurs. Mass transfer between the two phases is included. The fluid-dynamic parameters of the fluidized bed model are based on cross-verified measurements obtained through X-ray tomography and optical probing under non-reactive conditions.

Results and discussion

The modeling results generally showed good agreement between measured and predicted concentration profiles. It turned out that the temperature distribution in the reactor needs to be considered carefully due to the temperature difference between the thermo-oil cooling and the catalyst-rich dense phase. This is especially relevant for feed gases with high CO2 concentrations, because CO2 conversion is represented in the model as Reverse Water Gas Shift reaction followed by CO methanation, where the RWGS is strongly temperature dependent.

The validated model provides a deeper understanding of the interaction between reactions and mass transfer in the reactor, supporting process optimization and risk-free scale-up of the technology.





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DFL0324

Effect of gas properties on transport disengaging height of iron ore in a fluidized bed

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fluidization/Multiphase Flow Reactors

Keywords: iron ore, entrainment, gas density, fluidized bed, transport disengaging height

Abstract Body.

Introduction.

Hydrogen-based fluidized-bed iron reduction has attracted considerable attention for carbon-neutral steelmaking. In this reactor, the transport disengaging height (TDH), defined as the height above which particle entrainment rates and solid holdup reach a constant value, serves as a critical design parameter [1]. However, TDH prediction under low-density hydrogen conditions remains challenging, as most existing correlations were developed using high-density gases such as air [2]. Furthermore, the TDH is strongly affected by the physical properties of the particles such as the fraction of particles below 45 ㎛ (F45) which affects formation of clusters [3]. In this study, the effects of gas density (ρg) and superficial gas velocity (Ug) on the TDH of iron ore particles were investigated.

Methods.

Experiments were conducted in a gas–solid fluidized bed (0.05 m I.D. × 5.0 m height) with iron ore particles (~2800 μm). The ρg (0.164–1.82 kg/m³) was controlled using helium, air, and their mixture. The Ug was varied from 0.60 to 2.02 m/s. The TDH was determined using a freeboard–entrainment model to identify an exponential-decay of ε_s in the dilute phase. Clustering behavior of particles in the freeboard was visualized using a He–Ne laser sheet

Results and discussion.

The TDH increased with increasing Ug and ρg due to the enhanced drag force, which promotes particle entrainment into the freeboard. The TDH further increased as the F45 increased, because the Sauter mean diameter decreased, leading to decrease of Ut. Observation of clustering behavior revealed that detached fines coexisted as both clusters and as individual particles in the freeboard. A TDH correlation for iron ore particles was developed by adopting the critical size (dcrit) [4] to account for the clustering of adhering fines. The proposed model successfully predicted the measured TDH values within the experimental range.

Acknowledgments

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DFL0634

Identification of Volatile Cloudy Zone in a Liquid-injecte d Fluidized Bed by CFD-DEM Simulation

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fluidization/Multiphase Flow Reactors

Keywords: Fluidized beds; CFD-DEM simulation; Liquid evaporation; Cloudy zone; Heat and mass transfer

Abstract Body.

Introduction.

In liquid-injected fluidized bed processes, such as ethylene polymerization, it is crucial to quantitatively identify the cloudy zone consisting of gas bubble, droplets and wet particles. While various experimental methods exist for measuring relevant parameters, a comprehensive understanding of the characteristics of the cloudy zone remains challenging.

Methods.

By applying digital image analysis on the bubble characteristics in a 2D wet-particle fluidized-bed, we study the evolution of bubble characteristics with increasing liquid content. Furthermore, the cloudy area in a fluidized bed for gas-phase ethylene polymerization process was simulated by CFD-DEM method. We then established a heat and mass transfer model of liquid injection, film coating and evaporation process to quantitate the droplets and wet particles, characterize the gas-liquid-solid cloudy zone.

Results and discussion.

Image analysis of simulation results reveals a horseshoe-shaped cloudy zone and elucidates the life cycle of wet particles, transitioning from dry to wet and back to dry. The investigation identifies five distinct stages characterized by changes in evaporation rate, temperature, and liquid mass during the core-annular flow of wet particles. Importantly, the temperature gap between dry and wet particles diminishes as thermal energy transfer during droplet-particle collisions weakens at higher liquid injection rates.

Acknowledgement

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ISCRE29 & APCRE11
2026 / SEOUL, KOREA

MKF0662

Complex Network Approaches for Flow Regime Recognition in Gas-Solid Fluidized Beds

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Keywords: gas-solid fluidized bed; flow regime recognition; complex network; pressure fluctuation; machine learning; nonlinear dynamics

Introduction. Gas-solid fluidized beds are pivotal in chemical and energy processes, where flow regime transitions significantly influence operational efficiency. Traditional methods for analyzing pressure fluctuation signals—time-domain, frequency-domain, and state-space approaches—are often limited in capturing the nonlinear and nonstationary dynamics inherent in fluidization systems. Recent advances in complex network theory offer a novel paradigm for characterizing flow regimes and fluid dynamics by mapping time-series data into network structures, enabling the extraction of topological features that reflect underlying hydrodynamics.

Methods. This study presents three distinct complex network frameworks for flow regime analysis, including Flow Regime Complex Network (FRCN), Directed Weighted Complex Network (DWCN), and Horizontal Visibility Graph (HVG).

Results and discussion. FRCN achieved 98.2% accuracy in identifying single-bubble, exploding bubble, and transport regimes.[1,2] DWCN analysis revealed that key fluctuation modes dominate specific regimes. Network statistics (node strength, clustering, centrality) showed strong agreement with Kolmogorov entropy, confirming their utility as dynamics descriptors.[1,3] HVG metrics demonstrated high sensitivity to the bubbling-to-turbulent transition. When used as input features in machine learning models, HVG-based attributes enabled >95% accuracy in discriminating bubbling, transition, and turbulent regimes.[4]

The integration of complex network theory provides a robust, multi-perspective framework for flow regime characterization in gas-solid fluidized beds. Each network construction method - FRCN, DWCN, and HVG - offers unique insights into flow dynamics, from regime identification to nonlinear feature extraction and machine learning compatibility. These approaches not only enhance the understanding of fluidization mechanisms but also pave the way for real-time monitoring and intelligent control of industrial fluidized bed systems.

Acknowledgments

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DFL0240

Design and Process Intensification of a Microbubble-Interfacial Reactor for Catalyst-Free Oxidative Degradation of Phenolic Compounds

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fluidization/Multiphase Flow Reactors

Keywords: Process Intensification; Microbubble; Degradation; Multiphase Flow

Abstract Body.
Introduction: This study aims to design and improve a novel reactor system that utilizes the unique gas-liquid interface of microbubbles to achieve efficient, catalyst-free oxidative degradation of recalcitrant organic pollutants in wastewater. The specific target was the degradation of phenolic compounds under mild conditions.
Methods: A continuous-flow microbubble-interfacial reactor was designed. In this system, an aqueous solution of phenol (initial concentration: 0.1 g/L) was treated at ambient temperature and pressure without adding any catalysts. The oxidative degradation was driven solely by the intrinsic properties of the microbubbles, such as their high interfacial area, localized high temperature upon collapse, and generation of strong electric fields. Subsequently, performance was evaluated by measuring phenol degradation efficiency after a 4-hour treatment cycle using HPLC. Furthermore, Computational Fluid Dynamics (CFD) modeling was employed to simulate multiphase flow, bubble dynamics, and mass transfer within the reactor. Ultimately, the model was used to optimize key design parameters to maximize interfacial area.
Results and discussion: The experimental results demonstrated that the optimized microbubble reactor achieved a degradation efficiency of 80% within 4 hours under catalyst-free and mild conditions. The CFD simulations provided insights into the hydrodynamic behavior, confirming that the optimized design significantly enhanced microbubble dispersion, bubble size distribution, and interfacial mass transfer, which are the factors governing the oxidative degradation performance. Overall, this work successfully demonstrates the feasibility and efficacy of a catalyst-free advanced oxidation process based on microbubble technology. The integration of experimental validation and CFD modeling proves to be a powerful approach for the rational design and process intensification of such reactors. The microbubble-interfacial reactor presents a promising, energy-efficient, and environmentally friendly alternative for wastewater treatment, eliminating the need for catalysts and their associated recovery challenges and secondary pollution.

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DFL0414

Ignition of hydrogen in a fluidised bed of silica during non-premixed operation

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Keywords: fluidisation; optical diagnostics; non-premixed; ignition; hydrogen combustion

Purpose. Combustion in fluidised beds attracts renewed attention for the thermochemical conversion of hydrogen (H_2)[1] and ammonia (NH_3)[2]. Solid particles, *e.g.* silica sand, dissipate heat from combustion, enabling lower operating temperatures and reduced nitrogen oxide formation. Non-premixed combustion with bubbles of H_2 traversing through a bed of particles fluidised by air, eliminates risks of flashback and is therefore attractive for reactor safety.

Methods. A two-dimensional quartz reactor, heated to 670°C, was used to house silica particles (d_p=212-300 μm), fluidised by mixtures of air and N_2 at the minimum fluidisation velocity (U_{mf}). Mixtures of H_2 and N_2 were injected separately above the sinter at a superficial velocity (U-U_{mf}) corresponding to U/U_{mf}=1.5-2.0. The O_2 content in the fluidising gas was varied between 11-62 vol.%, corresponding to global equivalence ratios between 1.33-0.33, respectively. Burning bubbles released OH* chemiluminescence, captured with an intensified CCD camera with a 307 nm band-pass filter. A high-speed camera imaged the bubbling flow.

Results. The intensity of OH* chemiluminescence, a marker of local heat release rate during ignition[3], was strongest near the bubble centre and diminished towards the bubble boundary. No diffusion flame was detected at the bubble boundary. Ignition occurred 20-80 mm above the gas distributor, corresponding to induction times of 100-400 ms, which were nearly an order of magnitude longer than the characteristic times of O_2 mass transfer between a bubble and emulsion gas[4] (8-34 ms for d_b=2-6 mm). While a flammable mixture formed before ignition was detected, ignition was likely delayed due to radical quenching.

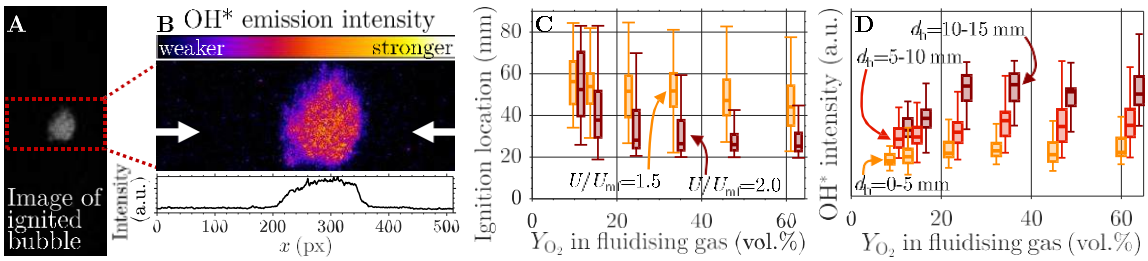

Figure 1: A) and B): OH* distribution in an ignited bubble. C) Position above distributor upon ignition as a function of U/U_{mf} and Y_{O_2} in the fluidising gas. D) Intensity of OH* emission in ignited bubbles, for a range of bubble diameters (d_b) and Y_{O_2} in the fluidising gas. In Figs. C and D, boxes span the interquartile range with a line marking the median; whiskers mark minimum and maximum values.

At U/U_{mf}=2.0, increasing O_2 concentration shifted ignition lower in the bed due to enhanced O_2 ingress. Ignition height at U/U_{mf}=1.5 was less sensitive to O_2 concentration, as ignition in small bubbles was likely limited by radical quenching rather than fuel-air mixing.

Counterintuitively, OH* emission was stronger under globally fuel-lean conditions, suggesting that enhanced ingress of O_2 enables bubbles to reach flammable conditions earlier, enabling ignition before significant H_2 loss to the emulsion phase driven by preferential diffusion.

Conclusions. Hydrogen bubbles in an air-fluidised bed ignited across the bubble volume instead of forming a diffusion flame at the bubble boundary. Ignition at low U/U_{mf} was hindered by radical quenching on solid surfaces, and at high U/U_{mf} by ingress of O_2.

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KN0049

Generation, accumulation, dissipation and monitoring of electrostatic charges in gas-solids fluidized beds

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Abstract Category: Invited Lecture - Keynote Lecture

Keywords: gas-solid, fluidized bed, electrostatics, generation, accumulation, dissipation, monitoring

Abstract Body.
The electrostatic charges of particles in the fluidized bed are a net result of charge generation from particle-particle and particle-wall collision and charge dissipation from contact with grounded surfaces and ionization of fluidizing gases. The charging behaviour depends on particle properties (e.g. glass beads or polyethylene), gas properties (e.g. nitrogen, argon, moist air) and the properties of reactor wall surface (e.g. stainless steel or acrylic, grounded or un-grounded). It was observed that particles gained less charges in argon gas than in nitrogen and air, which can be attributed to the charge relaxation, which predicts that the charge density of fluidized particles is limited by the gas breakdown field intensity of the fluidizing gas. Such a theory also predicts that the charge buildup process will be similar in fluidized bed of different fluidizing gases before the gas breakdown occurs. Such a hypothesis was validated from the measured dynamic charging behaviour of the fluidization of polyethylene particles. The effect of moisture content was found to depend on the wettability of bed particles, as the absorbed water layer modified the dielectric and conductive properties of the particles leading to changes in charge generation and dissipation during the particle-wall contacts. Bipolar charging between large and small particles during their contact may also contribute to the charge buildup in fluidized beds, especially at low level of charge density. The understanding of bipolar charging mechanisms requires further investigation in the future. Due to the dynamic nature of electrostatics in fluidized beds, online monitoring of particle charge density in fluidized beds remains a challenge and requires the development of hybrid sensors to extract charge density from intertwined particle dynamic signals and the transfer/introduced charge signals.

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DFL0443

High-throughput simulation and optimization of gas-solid fluidized bed for the clean coal utilization

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fluidization/Multiphase Flow Reactors

Keywords: Data training, CFD-DEM simulation, gas-solid flow, multi-component particles

Abstract Body.
Dry coal beneficiation using a gas-solid fluidized bed is an important technique for the clean coal utilization in the water-scarce western regions of China: however, the complex gas-solid interactions and bed structure characteristics restrict its industrial scale-up. To address this issue, a multiscale simulation model that has been validated on the pilot-scale equipment (Jia et al. Chemical Engineering Journal, 2025, 511: 161912) was further employed to investigate the effects of industrial scale-up and intensification strategies in this work. The high-throughput simulations on the super computer of CPU-GPU were conducted to classify more than 300 coal types with the aim of fitting different coal and reactor in the best performance. Besides, the effects of gas velocity, discharge speeds, bed density and particle density or size are taken into consideration in the AI algorithm to provide quantitative insights and engineering guidelines for the scale-up of fluidized beds in the coal beneficiation process, ultimately supporting the optimal design of efficient, large-scale separation devices.

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CDC0180

Functionalization of corn-cob-derived biochars as innovative bio-based CO2 adsorbents

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Capture

Keywords: Corn cob biochar, CO2 adsorption, Chemical activation, amino-modified biochar, metallized biochar

Abstract Body.
Introduction. The improper disposal of agricultural waste contributes to environmental and health risks. Among agricultural biomasses, corncob (CC) is an abundant byproduct deriving from corn production. The high organic carbon content (45-50%) in its layered structure makes it a promising candidate for biochar production through slow pyrolysis. Biochar is a promising carbon-based material for low-temperature CO2 capture from flue/fuel gases as an economically viable alternative to commercial activated carbon. Since the CO2 adsorption uptake can be enhanced through chemical activation, metal doping, and ammine functionalization, this study investigates the conversion of CC into biochar via slow pyrolysis and its functionalization with KOH, MgO, and ethylenediamine (EDA), evaluating CO2 adsorption performance and the corresponding adsorption mechanisms.
Methods. Biochar is produced via slow pyrolysis in a horizontal fixed-bed reactor at 500 °C, 800 °C, and 900 °C (BC500, BC800, and BC900, respectively), with a heating rate of 10 °C/min, a residence time of 1h, and a N2 flow rate of 4 ml/min. Chemical functionalization with KOH is performed on BC800 according to [1] with some modifications. Metal doping with MgO is performed on BC900 as described in [2]. EDA modification is performed according to[3] on BC500 and BC800. After the physicochemical characterizations, CO2 adsorption tests are conducted with a breakthrough setup on two lab scales. 200 mg of sample, placed in a U-shaped fixed bed quartz reactor (id=4mm), is first pre-treated with an N2 flow rate at 130 °C for 1h, and then CO2 adsorption tests are performed at 25 °C by sending a flow rate of 10ml/min, 20 % of CO2 (80% N2). The CO2 outlet concentration is measured using a gas chromatograph (GC, Inficon). The scale-up experiment is carried out following the same procedure with approximately 1 g of sample, thus increasing the hourly gas space velocity (GHSV). Granular active carbon (Norit RB4 W) is used as a reference. Optimization tests are performed by increasing the CO2 (20, 40, 80%v/v).
Results and discussion. Among all the samples investigated, BC800-KOH800 exhibited the highest microporous surface area (800 m2/g), high aromaticity and stability (H/C=0.011, O/C=0.11), high basicity (5267 mmol/g), and a CO2 removal efficiency of almost 90 % on a 1g scale, comparable to GAC.

ISCRE29 & APCRE11
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DFL0598

CFD-DEM study on the effect of drag, life and hydrodynamic torque in a dense -gas solid fluidized beds with non-spherical particles.

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fluidization/Multiphase Flow Reactors

Keywords: CFD-DEM, Fluidized beds, Non-spherical particles

Abstract Body.

Fluidized Gas-solids fluidized beds are used in many industrial applications because of their better heat and mass transfer rate. Most of the studies available in the literature used a spherical shape particle, however in real particle is of non-spherical shape. Importantly non-spherical particles experienced lift and torque together with drag forces. These forces significantly change the hydrodynamics of fluidized beds. Therefore in this work, we studied the effect of drag, lift, and torque on hydrodynamics of dense-gas solids 3D fluidized beds. We performed CFD-DEM simulations on 3D fluidized beds with dimensions similar to those of the experimental by Mema et. al.[1]. Hölzer, & Sommerfeld [2] drag correlation was used for the drag force and the lift and torque from Sanjeevi [3] and Zastawny [4]. Both have proposed correlations based on single particle (S-P) and multiparticle (M-P). We compared both their models and the comparison was made under different flow conditions and for different particle aspect ratios. The results are compared with the experimental data. The comparison is made on the basis of particle velocities, particle circulation, void fraction distribution, and particle orientation. At first instant it was observed that multi-particle correlations of lift and torque show better agreement with the experimental results, when compared for particle axial velocity and solid fraction distribution. S-P based correlations overpredict particle axial-velocities because these models do not take into account the effect of particle packing. The lift and torque correction from Sanjeevi shows better agreement compared to that of Zastawny. With drag only a higher particle bed height is predicted when compared to lift and torques. Including lift promotes lateral motion of the particles in a bed. In a dense regime, constant collisions cause particles to spin rapidly, making lift force a significant factor in particle dispersion. Including torques does not show any significant difference in particle velocity and distribution, however, particles circulations are better predicted when torque is incorporated together with drag and lift at all flow conditions. Therefore, it is suggested that the effect of hydrodynamic lift and torque should not be ignored dense gas-solid fluidized beds.

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KN0220

Light Oils Synthesized by Methane Homologation over a Novel Hierarchically Porous Titania Catalyst Designed for a Non-Thermal Plasma

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Abstract Category: Invited Lecture - Keynote Lecture

Keywords: methane conversion, non-thermal plasma catalysis, light oil synthesis, mesoporous materials, hierarchically porous materials

Abstract Body.

Light Oils Synthesized by Methane Homologation over a Novel Hierarchically Porous Titania Catalyst Designed for a Non-Thermal Plasma

Porous-architecture engineering offers a unified strategy to steer hydrocarbon chain growth across both electrified and conventional gas-to-liquids routes. Here, we integrate two complementary studies: non-thermal plasma–assisted direct methane homologation to fuel-range liquids and pore-length–controlled Fischer–Tropsch (FT) synthesis.

Hierarchically porous TiO2/SiO2 hybrid catalysts with tunable Ti/Si molar ratios were designed via controlled macro-/mesophase structuring to enhance plasma penetration, methane activation, and subsequent conversion of reactive intermediates, enabling one-step production of gasoline-/diesel-range light oils (C5–C16). Plasma-accessible macropores and diffusional mesopores facilitate interactions among radicals/ions and adsorbed species, while increasing Ti content suppresses consecutive dehydrogenation that drives coking. Density functional theory (DFT) links the superior coke resistance of TiO2 to a lower CH3 desorption energy and a higher barrier for CHx dehydrogenation, favoring methyl desorption and radical coupling (chain growth) over carbon deposition.

In parallel, ordered mesoporous supports with nearly identical pore diameters and cobalt crystallite sizes but systematically varied pore lengths were used to isolate residence-time effects in FT synthesis. Shorter pores increased CO conversion and the C2–C4 paraffin ratio while decreasing C5+ selectivity and producing a non–Anderson–Schulz–Flory distribution. A characteristic residence time ($t_{p,i} \propto L_p^2/D_{eff}$) rationalizes these trends by quantifying reduced in-pore residence time for shorter pores. In situ DRIFT further shows that short pores disfavor strong bridge-type CO relative to weak linear CO adsorption, consistent with reduced propagation probability and enhanced hydrogenation.

Collectively, the combined results highlight how coupling transport control, such as plasma accessibility or pore residence time with surface reaction energetics, provides a principled route to tune chain growth and mitigate deactivation in methane-to-liquids chemistry.

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DER0084

Explaining the High-Pressure Advantage in Reactive Carbon Capture Electrolysis: 1D Multiphysics Resolution of BPM/Cathode Interfacial CO_2 Generation

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Abstract Category: Reactor Modeling and Design - Reactor Design - Electrochemical Reactors

Keywords: Reactive carbon capture, bicarbonate electrolysis, bipolar membrane, membrane electrode assembly, COMSOL Multiphysics, high-pressure operation

Abstract Body.

▶ Purpose: Reactive Capture of CO2 (RCC) electrolysis enales direct conversion of bicarbonate-rich capture solutions without supplying purified gaseous CO_2. However, the mechanistic origin of performance enhancement under pressurized operation remains poorly unders tood because the decisive chemistry occurs in a highly localized region. Here, we target the cathode catalyst layer (CL)–bipolar membrane (BPM) interface, where BPM-generated protons can rapidly convert bicarbonate to transient CO_2 that dissolves and becomes the immediate reactant for CO_2 electroreduction.

▶ Methods: We develop a one-dimensional, steady-state, full-cell COMSOL Multiphysics model for a bicarbonate-fed MEA electrolyzer incorporating a hierarchical BPM (anion-exchange layer/water-dissociation junction/cation-exchange layer facing the cathode). The model couples ionic/electronic charge conservation with multicomponent Nernst–Planck transport through porous media, homogeneous carbonate chemistry ($HCO_3^-/CO_3^{2-}/H_2CO_3/CO_2$), BPM water dissociation and ion migration, and porous-electrode kinetics for CO_2RR and HER. Gas-phase CO_2 is treated using a pressure-dependent solubility constraint (Henry's law) together with interphase mass transfer to quantify CO_2(aq) availability and bubble accumulation.

▶ Results: Building on prior bicarbonate mass-transport modeling that reports strong interfacial gradients and appreciable carbonic acid adjacent to the membrane (0.1–1 mM), alongside very low steady-state CO_2 in the CL due to rapid consumption, we explicitly resolve the BPM-driven "CO_2-generation zone."

The model predicts that this zone is governed by the competition between BPM proton flux and alkaline neutralization by reaction products, and is highly sensitive to BPM water-dissociation kinetics, cation-exchange-layer ionic resistance, and CL transport (thickness/tortuosity). Increasing pressure elevates dissolved CO_2 and suppresses gas-phase accumulation, thereby reducing transport losses and increasing proton utilization for in situ CO_2 formation relative to neutralization.

Conclusions: This 1D full-cell framework provides a mechanistic basis for high-pressure RCC

enhancement by linking BPM water dissociation, interfacial speciation, and multiphase transport to local CO_2(aq) availability and selectivity. The model yields practical design/operation maps that prioritize BPM and CL parameters to maximize CO_2RR performance in bicarbonate-fed MEA electrolysis.

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2026 / SEOUL, KOREA

DER0233

Modeling Bipolar Membrane Electrodialysis for Isolation of Lactic Acid

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Abstract Category: Reactor Modeling and Design - Reactor Design - Electrochemical Reactors

Keywords: Bipolar membrane, Electrodialysis, Mathematical modeling

Abstract Body.

Purpose

Lactic acid (LA) is a versatile chemical intermediate and a precursor for poly-lactic acid (PLA), a sustainable alternative to PET. While industrial production relies primarily on glucose fermentation, the resulting lactate salts require complex downstream processing—including acidification and esterification—which accounts for approximately 50% of total operating costs. Bipolar Membrane Electrodialysis (BMED) offers a promising alternative for direct acid recovery. However, optimizing this process requires robust unit operation modeling to reduce energy consumption and cost. This study presents a mathematical 0D-transient BMED model designed to predict performance and elucidate the complex multi-physics dynamics governing the separation process.

Methods

A batch-mode BMED model was developed in MATLAB to simulate the recovery of LA. The model incorporates the Nernst-Planck equation to describe ion transport (diffusion, migration) and explicitly accounts for water transport mechanisms (osmosis, electro-osmosis) and acid-base equilibrium reactions. The governing equations were solved using the ode15s solver. To ensure model fidelity, parameter estimation was performed against experimental data to determine key ion exchange membrane properties, following rigorous mass balance adjustments of the raw experimental data.

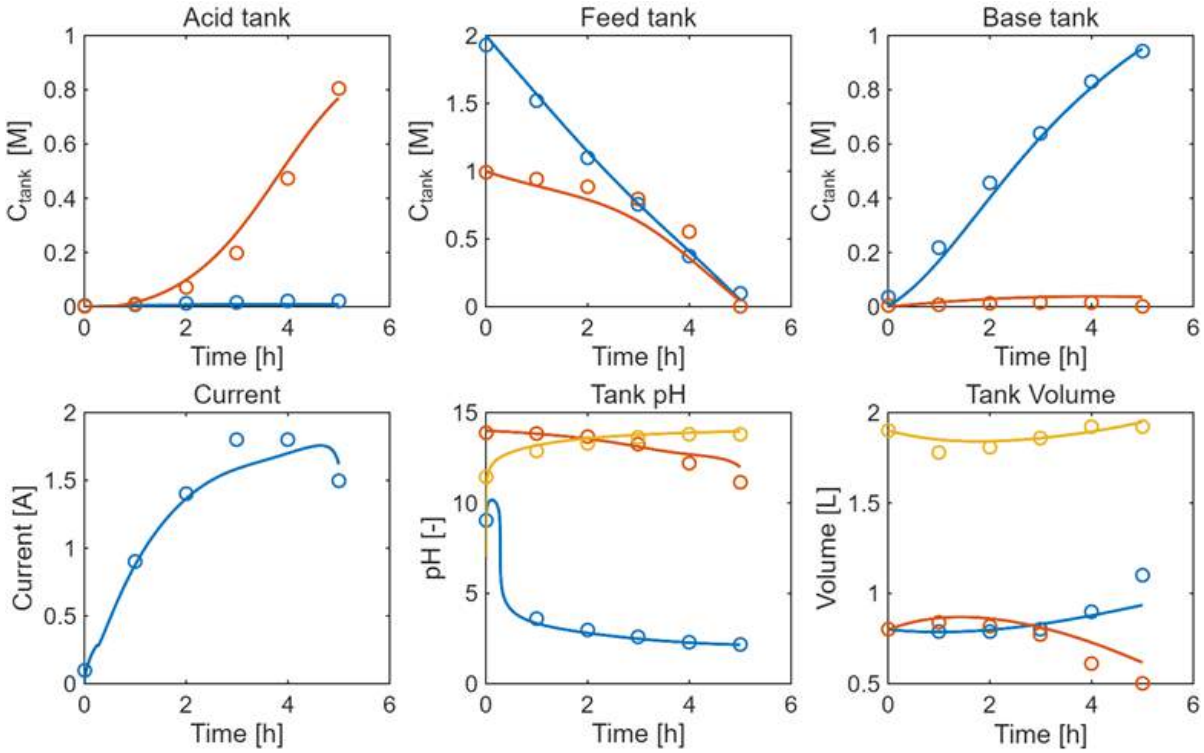

Fig. 1 Model validation was performed using experimental data. In the concentration plot, the orange and blue lines represent the lactic acid and potassium ion concentrations, respectively. For the tank pH and volume profiles, the orange, blue, and yellow lines correspond to the feed, acid, and base tanks.

Results

Fig. 1 illustrates the model validation against experimental data collected at 30 V with a feed composition of 1.0 M lactic acid and 2.0 M potassium lactate. The simulation demonstrated high accuracy, achieving a mean relative error of less than 20%. Parameter estimation revealed that ion exchange membrane water uptake increased at lower initial feed concentrations, a trend consistent with osmotic pressure effects reported in literature. Furthermore, the model successfully captured the dynamic current transition observed during experiments. Analysis indicates this transition is driven by the equilibrium voltage shift resulting from pH gradients across the bipolar membrane. Notably, this transition behavior was observed to diminish at high current densities.

Conclusion

This study successfully developed and validated a physics-based BMED model capable of capturing multi-physics behaviors in batch operations. The model provides a reliable tool for optimizing process conditions to minimize energy and production costs. Future work will extend this framework to continuous mode operation and employ global sensitivity analysis to quantify parameter uncertainty.

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DER0612

3D Multiphysics Modeling of PEM fuel cells: From Validation to Gas Channel Optimization

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Abstract Category: Reactor Modeling and Design - Reactor Design - Electrochemical Reactors
Keywords: PEMFC channel geometry, Multiphysics modelling, model validation

Abstract Body.

Introduction. Proton exchange membrane fuel cell (PEMFC) operation involves complex, coupled phenomena, including heat transfer, species and charge transport, multi-phase flows, and electrochemical reactions. Direct measurement of these internal processes is challenging and costly due to the compact, enclosed cell design. Multiphysics modeling provides detailed insights into these processes, enabling predictive analysis of cell performance.
Accurate validation against experimental data is essential to ensure reliability and applicability. Once validated, such models can be used to optimize design parameters, such as gas channel geometry, balancing reactant distribution, pressure drop, and electrical losses.
Methods. A single 5 cm2 PEMFC was designed and simulated using the ANSYS Fluent PEM Fuel Cell Module within a three-dimensional domain. The geometry included a membrane electrode assembly (MEA), serpentine flow channels, and current collectors.
The model incorporated coupled conservation equations for mass, momentum, species, charge, and energy, with specialized sub-models for multiphase flow, electrochemical reactions, and electric potential distribution, with Butler–Volmer equation for the electrochemical kinetics. Simplifying assumptions included laminar incompressible flow, ideal gas behavior, homogeneous isotropic porous properties, and steady-state operation. The model was first validated against experimental data in a single-serpentine cell by varying different critical parameters within physically meaningful ranges to fit the polarization curve across the kinetic, ohmic, and transport-limited regimes. Subsequently, advanced channel geometries were implemented to improve electrical contact and promote turbulence on the cathode side, using a triple-serpentine design with a trapezoidal cross-section and the previously validated MEA parameters.
Results and discussion. The baseline model, based on a single-serpentine channel design, was first validated and used to investigate distributions of key operating parameters, including liquid water saturation, temperature, and local current density, which are difficult to measure in situ. Through stepwise adjustment of kinetic, ohmic, and mass transport parameters, the methodology enabled effective calibration with minimal input modifications. This framework provides a general approach for systematic model validation. Its application supported the subsequent optimization of gas channel design, considering the validated MEA parametrization and implementing the optimized channel configuration. The results demonstrated increased maximum power output, owing to improved water management at high current densities, facilitated by the trapezoidal shape which optimizes water evacuation and pressure drop.

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DMB0011

Membrane-based reactive separation process intensification for H2 production

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Abstract Category: Reactor Modeling and Design - Reactor Design - Membrane reactor

Keywords: Membrane reactor, H2 production, C1 conversion, Biomass gasification, Plasma catalysis

Abstract Body.
C1 chemical conversion (e.g., CH3OH, biomass, etc.) enables the production of high-value-added chemicals and green fuels, serving as a critical pathway toward carbon neutrality and peak carbon emissions. However, C1 conversion processes commonly face shared challenges, including difficulties in catalytic activity modulation, harsh reaction conditions, thermodynamic equilibrium limitations, and overly complex process. In this talk, two distinct membrane reactor designs for intensifying H2 production will be presented: (I) Biomass gasification for syngas/H2 production faces efficiency challenges due to impurities like particulate matter (PM) and tars. We developed an integrated ceramic membrane reactor (Figure 1a) combining a SiC membrane for PM filtration and a Ni-catalyst for tar reforming. The system achieved synergistic intensification, removing ~97% PM and ~90% tars in situ, while demonstrating stable performance over five cycles at 800 °C. (II) Electrified methanol steam reforming (MSR) assisted by nonthermal plasma (NTP) is a pivotal enabler for clean hydrogen production at ambient conditions with several advantages. We optimize the NTP-assisted MSR by catalyst engineering, as well as membrane technology (via a 2D MXene nanosheet membrane reactor, Figure 1b). Our findings reveal that integrating a MXene membrane within a dielectric barrier discharge (DBD) NTP reactor enabled the reactive-separation process, improving methanol conversion (~87%), H2 formation rate (0.8 mmol/min) with higher purity (~97%), as well as showing a good stability in a ~40 h time-on-stream (ToS) operation.

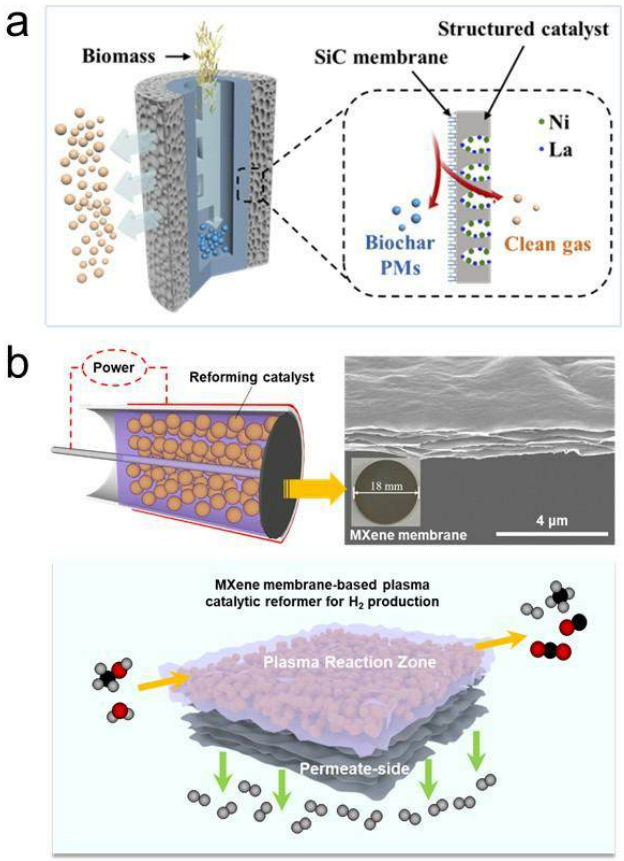

Figure 1 Membrane-based reactive separation process for H_2 production: (a) membrane reactor for biomass gasification and reforming to syngas production, and (b) plasma catalytic membrane reactor for intensifying MSR to H_2 production.

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DPL0681

Overcoming thermal degradation in continuous conversion of water into hydrogen peroxide in a flexible microwave plasma reactor

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Abstract Category: Reactor Modeling and Design - Reactor Design - Plasma

Keywords: hydrogen peroxide, microwave plasma, plasma–liquid reactor, renewable electricity

Abstract Body.

Introduction. Hydrogen peroxide is a key oxidant for environmentally benign oxidations and water treatment, but today it is produced almost exclusively by the anthraquinone process in large, centralized plants that are dependent on the constant supply of fossil resources. This makes on-site, flexible use difficult. Plasma-based routes can in principle generate H_2O_2 directly from water and electricity, yet current concepts struggle to combine continuous operation, commercially relevant concentrations, and acceptable energy yields.

Methods.

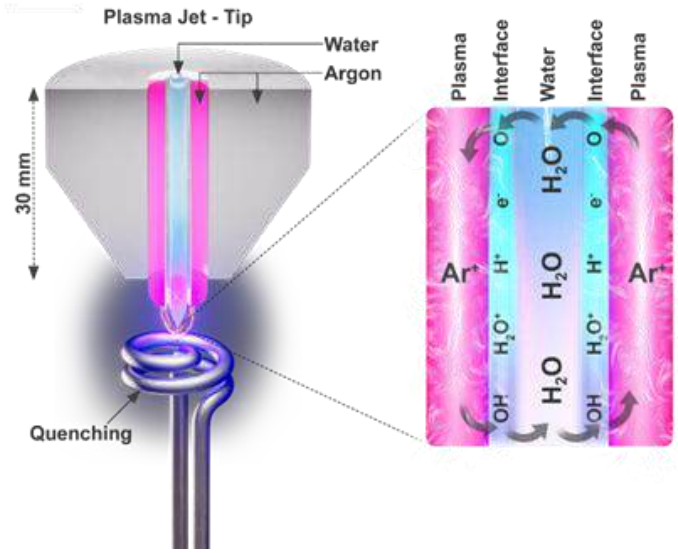

Fig. 1. Schematics of the plasma at the tip of the reactor and quenching system.

We developed a nanosecond-pulsed coaxial microwave plasma reactor that converts water directly into H_2O_2 using argon as plasma gas. A 2.45 GHz microwave torch is driven with pulses of 300–700 ns, while water is fed as a fine spray (0.2–2.5 mL·min^{-1}) into the afterglow. A compact cooling coil provides strong quenching of the post-discharge. H_2O_2 is quantified by titration/UV–vis. Gas-phase H_2 and O_2 are monitored online with a high-sensitivity gas analyzer, and time-resolved optical emission spectroscopy provides qualitative trends in

excitation and electron density. A simple plug-flow model is used to separate effective H_2O_2 formation and decomposition terms as a function of residence time and peak power.

Results and discussion. Under optimized pulsed conditions and with quenching, the reactor produces H_2O_2 continuously at concentrations up to 50–54 mM (0.17 wt%), i.e. in the range of commercial formulations, with energy yields up to 1.2 g·kWh^{-1} based on absorbed power. A systematic parametric study shows that duty cycle and pulse time control the balance between formation and thermal degradation, whereas the water flow (residence time) governs the achievable concentration. The PFR analysis indicates that the apparent formation rate is nearly independent of power, while the decomposition rate increases sharply at high peak power, consistent with thermally activated pathways. Long-term experiments demonstrate stable operation over several hours. We will discuss the resulting design rules for nanosecond-pulsed plasma–liquid reactors, implications for scale-up, and opportunities to integrate such electrified reactors as modular, on-site H_2O_2 sources in chemical and environmental processes.

Acknowledgments
EU GreenSWaP project (ID: 101161583)

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DMB0140

Equilibrium Shift in Oxidative Carbonylation via in-situ Water Removal Using a Recirculation Membrane Reactor with a Hydrophilic LTA Zeolite Membrane

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Abstract Category: Reactor Modeling and Design - Reactor Design - Membrane reactor

Keywords: Membrane reactor, Oxidative carbonylation, Water removal

Abstract Body.
The oxidative carbonylation of alcohols represents an attractive C1 transformation route for the synthesis of dialkyl carbonates, which are valuable intermediates and functional solvents. Bis(2-methoxyethyl) carbonate (BMEC), synthesized from 2-methoxyethanol (MEG), has recently gained attention as a flame-retardant electrolyte solvent for lithium-ion batteries. However, the oxidative carbonylation of MEG is inherently limited by thermodynamic equilibrium due to the formation of water as a by-product. In addition, selenium-based catalysts, while highly active, suffer from gradual deactivation caused by the formation and leaching of soluble Se–carbonyl intermediates under continuous-flow conditions, posing a significant challenge for long-term operation and scale-up.

In this study, a recirculation packed-bed membrane reactor (PBMR) was developed to simultaneously address equilibrium limitation and catalyst instability. A water-selective LTA zeolite membrane prepared on the surface of tubular α-Al_2O_3 support was integrated with a Se/Al_2O_3 catalytic bed, enabling selective in-situ removal of water during the reaction. Owing to its strong hydrophilicity, well-defined pore size (~4 Å), and high mechanical stability, the LTA membrane exhibited excellent water selectivity while effectively retaining MEG and BMEC under high-pressure reaction conditions.

In contrast to conventional once-through membrane reactor configurations, the recirculating reactor design continuously recycles both reactants and dissolved selenium species, thereby suppressing Se loss and maintaining catalytic activity. A systematic evaluation of key operating parameters, including reaction temperature, pressure difference, reactant dilution, and flow rate, demonstrated that efficient in-situ water removal is the primary factor governing equilibrium shift and overall reactor performance. At optimized reaction conditions (MEG 2600 mmol, n(MEG/Se/DMAP) = 50:1:5, P = 3 MPa, CO/O_2 = 4:1, T = 70 °C, ΔP = 5 bar, flow rate = 500 mL min^{-1}), MEG conversion increased by approximately 30%p and BMEC selectivity was improved by about 15%p compared to a conventional packed-bed reactor.

The results demonstrate that a recirculating reactor equipped with membrane separation system enhances catalytic efficiency and stability in the oxidative carbonylation. This reactor design is scalable and can be applied to water-producing catalytic systems.

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DMB0142

Application of Tandem Catalysis in Membrane Contactor Reactors: An Efficient Pathway for CO2 to Fuels Processes

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Abstract Category: Reactor Modeling and Design - Reactor Design - Membrane reactor

Keywords: Membrane Reactor, Tandem Catalysis, Process Intensification

Abstract Body.
The efficient conversion of carbon dioxide (CO2) into high-value hydrocarbons is a key enabling pathway toward a sustainable and circular carbon economy, yet remains limited by thermodynamic constraints, product selectivity, and heat- and mass-transfer challenges in conventional reactor configurations. In this study, we propose and demonstrate an intensified process that integrates tandem catalysis with membrane contactor reactor (MCR) technology for the direct valorization of CO2 into aromatic hydrocarbons. A bifunctional Zn-ZrO2/ZSM-5 tandem catalyst was employed to enable sequential CO2 hydrogenation to oxygenated intermediates followed by methanol-to-aromatics (MTA) conversion within a single reactor system. To quantitatively assess the benefits of process integration, a macrokinetic modeling framework was developed that captures the coupled kinetics of CO2 hydrogenation, hydrocarbon chain growth, aromatization pathways, and competitive side reactions, while explicitly accounting for in situ water removal through the membrane interface. Modeling analysis reveals that selective extraction of water effectively shifts reaction equilibria, enhances forward reaction rates, and suppresses undesired reverse water-gas shift behavior, leading to an improvement in CO2 conversion of at least 50% relative to conventional packed-bed operation.

Experimental validation was performed under integral reactor conditions using approximately 20 g of catalyst. The MCR consistently outperformed a packed-bed reactor (PBR) baseline, achieving up to 53% higher CO2 conversion while maintaining favorable aromatic selectivity. In addition to reaction intensification, the MCR configuration enabled effective thermal regulation through the circulating sweep liquid, mitigating hot-spot formation associated with exothermic reaction steps. This dual functionality, simultaneous product separation and heat management, highlights a key advantage of membrane-assisted reactor design for tandem catalytic systems. Overall, the results demonstrate the strong synergy between tandem catalysis and membrane contactor reactor technology, offering a scalable and modular platform for intensified CO2 conversion. The proposed approach provides a promising pathway for the development of next-generation reactor systems aimed at sustainable production of hydrocarbon fuels and chemicals from CO2.

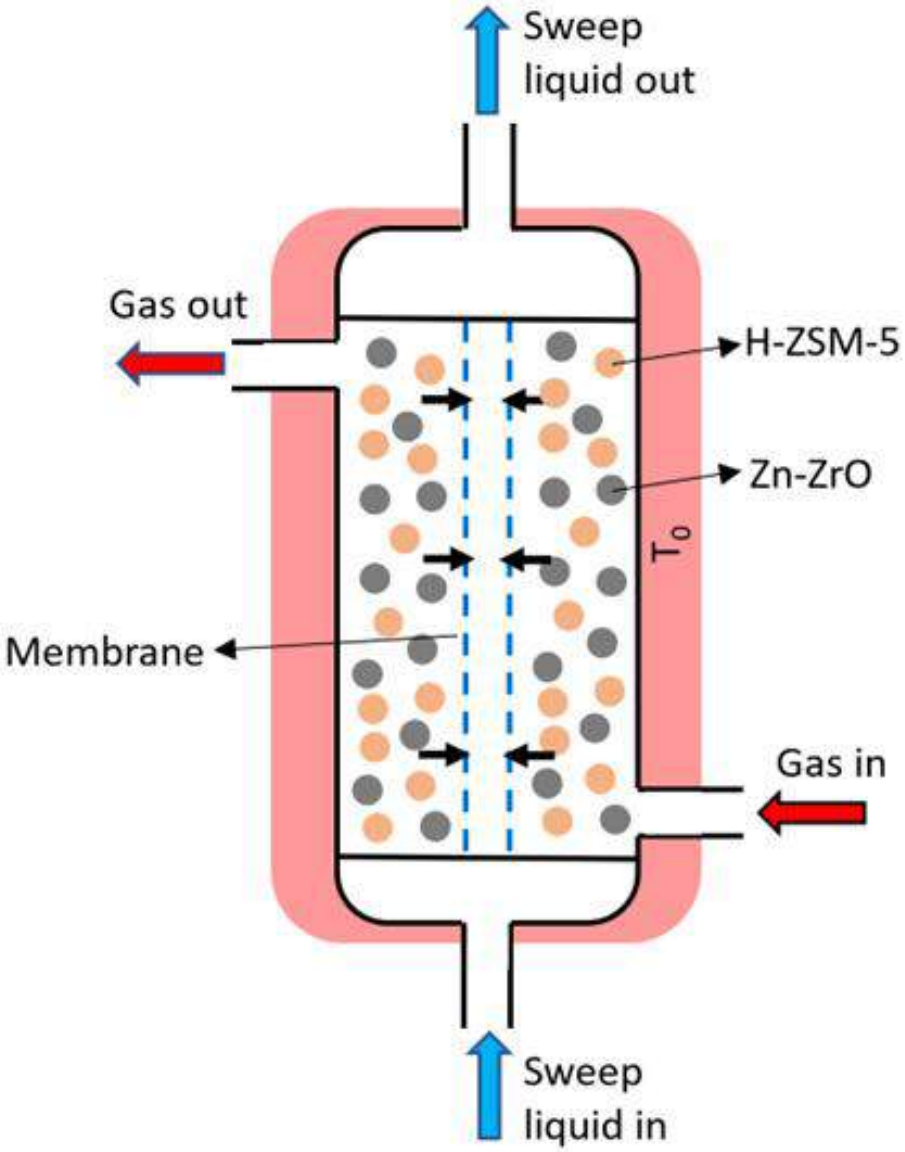

Figure 1. Schematic of the integrated tandem catalysis/MCR technical concept

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DMB0345

Overcoming an Equilibrium-Limited Dehydrogenation of a Liquid Organic Hydrogen Carrier by a Zeolite Membrane Reactor

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Abstract Category: Reactor Modeling and Design - Reactor Design - Membrane reactor

Keywords: zeolite membrane; membrane reactor; methylcyclohexane (MCH) dehydrogenation; H2 separation; liquid organic hydrogen carrier (LOHC)

Abstract Body.

Introduction. Efficient and economical hydrogen storage and transportation methods are essential for the practical use of hydrogen energy systems. Liquid organic hydrogen carriers (LOHCs) have attracted significant attention as they enable safe hydrogen storage under ambient conditions and controlled release through dehydrogenation.[1] Among various candidates, methylcyclohexane (MCH) and toluene (TOL) are promising due to their low toxicity, appropriate boiling points, and high hydrogen storage capacity.[2] However, MCH dehydrogenation is a highly endothermic reaction that typically requires high temperatures to achieve sufficient conversion, leading to catalyst deactivation and undesired side reaction.[3] Therefore, developing low-temperature and energy-efficient dehydrogenation processes is crucial for improving process efficiency and economic competitiveness.

Methods. A hydrogen-selective zeolite membrane was employed to enable low-temperature MCH dehydrogenation. By continuously removing hydrogen, the membrane reactor shifts the reaction equilibrium toward the product side, overcoming thermodynamic limitations and achieving higher conversion at reduced temperatures.[4] A DDR-type zeolite membrane with a pore size of 0.36 × 0.44 nm2[5] was used. Owing to the significant difference in kinetic diameters between hydrogen (0.29 nm[6]) and larger molecules such as MCH (0.60 nm[7]) and toluene (0.59 nm[7]), the membrane enables highly selective hydrogen separation.

Results and discussion. The hybrid zeolite membrane (Z) exhibited outstanding hydrogen permselectivity in the presence of both MCH and toluene, achieving separation factors exceeding 350. The use of Z into a membrane reactor (MR) significantly enhanced MCH dehydrogenation performance at low temperatures. At 220 °C, the Z-based MR achieved an MCH conversion of 75.3% ± 0.8%, which was substantially higher than that obtained in a conventional packed-bed reactor (56.4% ± 0.3%) and thermodynamic equilibrium conversion (53.2%). This improvement was attributed to the continuous and selective removal of hydrogen through the zeolite membrane, which effectively shifted the reaction equilibrium toward the product side. Furthermore, operation below 300 °C suppressed side reactions, particularly the demethylation of toluene, resulting in increased hydrogen purity and selective production of toluene as the hydrogen-lean LOHC. The membrane reactor also demonstrated stable and robust performance, highlighting its reliability.

These results demonstrate that hydrogen-selective zeolite membranes effectively overcome thermodynamic limitations in MCH dehydrogenation, enabling efficient low-temperature operation with improved conversion, selectivity, and energy efficiency while mitigating catalyst deactivation. Comparable performance to silica-based membrane reactors confirms their competitiveness. Overall, zeolite membrane-assisted reactors offer a promising and scalable pathway for energy-efficient hydrogen production from liquid organic hydrogen carriers.

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DMB0413

Modeling and Experimental Optimization of Membranes and Membrane Reactors for Methanol Synthesis from Biomass-Derived Syngas

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Abstract Category: Reactor Modeling and Design - Reactor Design - Membrane reactor

Keywords: Biofuels, membrane reactor, carbon membranes

Abstract Body.
Biofuels play a crucial role in decarbonizing the transport sector by offering low-carbon solutions compatible with existing technologies[1]. In 2022, global biofuel demand reached a record 170 billion liters and is expected to grow rapidly, driven by the need to reduce emissions in hard-to-abate sectors where alternatives are limited[2]. These include shipping, aviation, heavy industry, and heavy-duty transport. Methanol is a promising option due to its versatility as an energy carrier and chemical feedstock, although current production depends largely on fossil resources. The BioMeGaFuel project addresses this challenge by proposing an intensified, sustainable route for bio-methanol synthesis. It combines chemical looping gasification of low-value biomass with membrane-assisted methanol reactors, enabling near-zero CO2 emissions, improved equilibrium conversion, and high carbon utilization.

A phenomenological membrane reactor model for methanol synthesis was developed in MATLAB, implementing a kinetic law for the CO2 hydrogenation reaction network over a $Cu/ZnO/Al_2O_3$(CZA) catalyst[3] and carbon membrane permeation data from literature[4][5]. The reactor consists of an inner tubular membrane and an outer shell, with the catalyst packed in the annular space and the membrane interior as the permeation zone. As methanol synthesis system is overall exothermic, with most heat released near the inlet, a co-current configuration of feed and sweep gas was adopted. After validation, the model was used to optimize conversion and methanol yield at different gas hourly space velocities (GHSVs) by varying operating conditions, including pressure, pressure drop across the membrane, inlet temperature, number of membranes, and reactor geometry. Parallelly, carbon membranes were developed and tested to improve the state-of-art permeation results used as benchmark [5]. Membrane performance was evaluated using separation factors for H2O/CO, H2O/CO2, and H2O/H2 gas pairs.

The results on CO2 hydrogenation in membrane reactor achieved up to 15% higher CO2 conversion and 20% higher methanol yield compared to a conventional packed-bed reactor, reaching a final methanol yield of 92% at GHSV of 500 h^{-1}. Even at industrial-scale GHSV (10000 h^{-1}), improvements of 14% in conversion and 10% in yield were observed. To account for the presence of CO in the feed, a kinetic model for the CO–CO2–H2 reaction network over a commercial catalyst[6] has already been implemented and validated. In this case as well,

conversion and methanol yield are improved when using a membrane reactor. The final outcome of this research will be employed to design the reactor for implementation in a TRL5 demonstrator.

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MemCat, project number 101130047. Funded by the European Union. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the EU or EIC and SMEs Executive Agency (EISMEA). Neither the European Union nor the granting authority can be held responsible for them.

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KN0776

Sustainable Catalysis with Membrane or Plasma for Greenhouse Gas Valorization

Sibudjing Kawi

National University of Singapore,Singapore

Methane and carbon dioxide are major greenhouse gases whose emissions have contributed significantly to global warming over the past several decades. In this presentation, I will provide an overview of my group's research on developing advanced catalyst technologies for the efficient and emission-free utilization of these gases through their conversion into value-added products. I will then present our work on integrating our developed catalysts with membrane systems to enhance reaction conversion and product selectivity in greenhouse gas valorization reactions. One of these catalyst–membrane platforms offers a carbon-free pathway for hydrogen generation and is being further developed toward industrial-scale deployment in support of Singapore's low-carbon energy initiatives. Finally, I will highlight our collaborative research with Shell on electrified catalysis for methane coupling to produce light olefins under ambient conditions, enabled by low-temperature dielectric barrier discharge (DBD) plasma.

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DMB0482

Scale-up of the ceramic membrane reactor for continuous biomass gasification to produce clean hydrogen-rich syngas

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Abstract Category: Reactor Modeling and Design - Reactor Design - Membrane reactor

Keywords: Continuous biomass gasification, ceramic membrane reactor, SiC membrane, Ni reforming catalyst, H2-rich syngas

Abstract Body.
Purpose:
Biomass gasification offers a renewable route to hydrogen-rich syngas, but contamination by tars and particulate matter (PMs) limits its practical application. While integrated ceramic membrane reactors have shown promise for in situ purification, previous designs operated in batch mode with low throughput. This study aims to scale up a packed-bed ceramic membrane reactor for continuous biomass gasification to enable stable, high-throughput production of clean syngas.

Methods:
A continuous packed-bed ceramic membrane reactor was designed, integrating a porous SiC membrane tube (2 μm pore size) for PMs removal and monolithic Ni/Al2O3 catalysts for tar reforming. Corncob biomass (20–40 mesh) was continuously fed at 3–12 g min−1, with steam as the gasification agent. The reactor was operated at 800 °C under slight negative pressure. Performance was evaluated in terms of PMs/tar removal, syngas composition, flow rate, and H2/CO ratio over a 330-h long-term test.

Results:
The scaled reactor achieved PMs and tar removal efficiencies of ~99.9% and ~95.4%, respectively. Under optimized conditions (pre-pyrolysis at 200 °C, biomass feed 6 g min−1, steam 1.5 mL min−1), it produced syngas at ~10.2 L min−1 (N_2-free) with a stable H_2/CO ratio of ~1.4. Long-term operation over three 100-h cycles demonstrated consistent syngas composition (H2 ~51.1 vol%, CO ~25.8 vol%) and a H2/CO ratio of 2.0±0.1. Control experiments confirmed the complementary roles of the membrane (PMs retention) and catalyst (deep tar reforming).

Conclusions:
This work successfully demonstrates a scalable ceramic membrane reactor for continuous, stable production of clean H2-rich syngas from biomass. The integration of membrane filtration and catalytic reforming within a single unit effectively addresses contamination challenges while enabling high throughput and long-term operability. The study provides an engineering

framework for industrial-scale membrane reactors in sustainable biomass conversion.

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KN0717

Plasma Electrification for Power-to-X: Enabling Sustainable Fuel and Chemical Production

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Abstract Category: Invited Lecture - Keynote Lecture

Keywords: Plasma electrification; Plasma catalysis; Plasma chemical engineering; Power-to-X

Abstract Body.
The conversion of inert molecules (e.g., CO2, CH4, and N2) with strong chemical bonds into value-added fuels and chemicals has attracted significant interest. However, activating these molecules remains challenging due to their thermodynamic stability, which requires substantial energy input. Non-thermal plasma (NTP) has emerged as a promising electrification technology, enabling challenging chemical processes under mild conditions. Combining NTP with heterogeneous catalysis offers great potential for synergistic effects through plasma-catalyst interactions, enhancing the conversion, selectivity, and yield of end-products, as well as overall energy efficiency. Moreover, plasma processes can be switched on and off instantly, providing exceptional flexibility for decentralized fuel and chemical production using intermittent renewable energy sources. This presentation will highlight recent advances and challenges in plasma electrification for the production of e-fuels and e-chemicals, covering various chemical processes, including CH4 activation, CO2 conversion, and ammonia synthesis.

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DNR0081

Design and Analysis of a Novel Reactor for Homogeneous Oxidative Dehydrogenation of Ethane to Ethylene

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Abstract Category: Reactor Modeling and Design - Reactor Design - Novel Reactors

Keywords: Reactor Modelling, Homogeneous Kinetic Model, Ignition and Extinction, Monolith Reactor, Autothermal Operation

Abstract Body.

Introduction:

Ethylene is currently produced through ethane steam cracking, which is an energy intensive endothermic process that requires elevated temperatures, typically 1023-1173 K. Oxidative Dehydrogenation of Ethane (ODHE) has surfaced as a potential alternative that requires lower reaction temperatures and provides high conversions. Attempts to advance application of this chemistry have for the most part focused on catalytic approaches, with several catalysts that exhibit high ethane conversion and ethylene selectivity having been reported [1]. Little work has been presented though that incorporates (non-catalytic) homogenous chemistry. A potential means for overcoming the limitations of catalytic ODHE is to use gas phase rather than catalytic chemistry for ethylene production.

Methods:

We use a recently developed and experimentally validated 7-step 8-species based global kinetic model [2] for the gas phase ODHE to design a novel reactor configuration for autothermal operation [Fig 1 (a)] using a two-mode 1-D finite dispersion model. The reactor [Fig 1 (b)] consists of a disc (Length/Diameter <<1) with high thermal conductivity inert material such as SiC or SiSiC with properly sized perforations having effective heat and mass Peclet numbers Peh,eff<<1 and Pem,eff>>1 and transverse Peclet number (P)<1 with small temperature difference between fluid and solid wall, approaching the lumped thermal limit. These design conditions lead to largest region of autothermal operation and small temperature gradient in the solid along the flow direction by further ensuring the criterion where Da (Damköhler number) times Peh,eff<1.

Results/Discussion:

The model shows two operating conditions along the dimensionless reactor length for ethylene formation where in presence of strong heat back mixing and optimal geometrical configuration, the fluid temperature quickly approaches that of solid: (1) At extinction point [Fig 1 (c, e, g)], the oxidative chemistry dominates <70-75% of the reactor length. (2) Higher on ignited branch [Fig 1 (d, f, h)], the oxidative chemistry dominates <20% of the reactor length rendering rest available for the cracking chemistry which is reflected from gradual increase in ethylene concentration. Altogether, it is found that for feed temperatures in the range of 300-500K, practical range of space times (0.05 to 0.1s) and ethane to oxygen ratios in the range 2.5 to

4, it is possible to obtain high ethylene selectivity (>80%) and per-pass ethylene yields (>50%) by combining oxidative and non-oxidative chemistry.

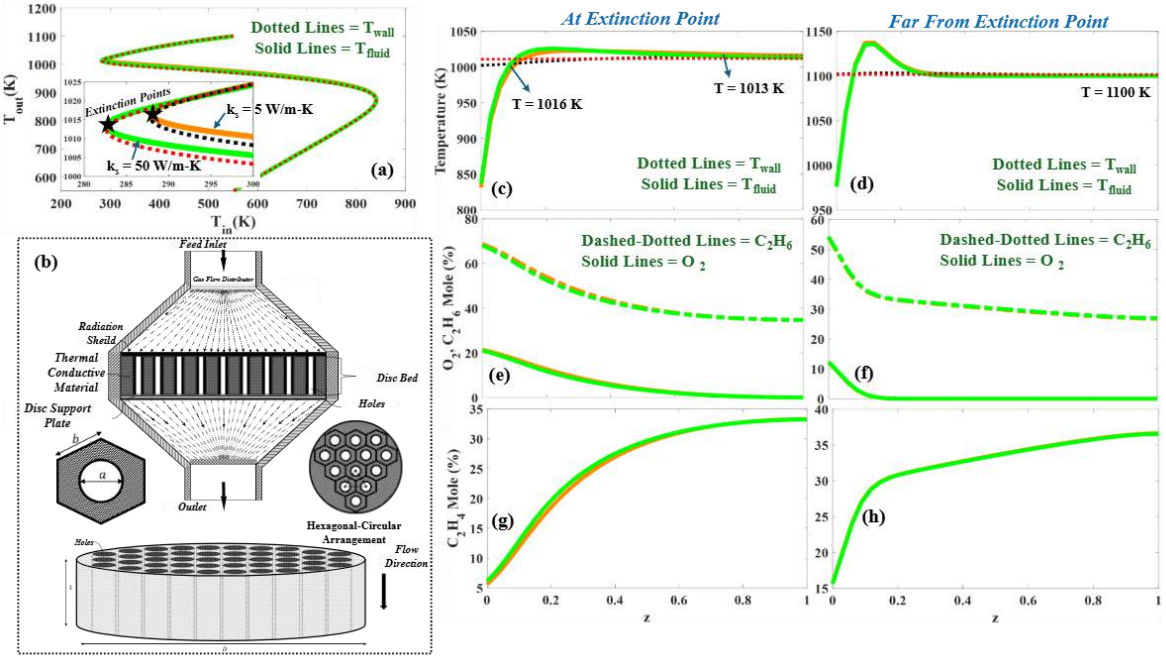

Fig. 1 Finite dispersion two-mode model simulations results at C_2H_6/O_2 feed ratio = 3:1, τ = 0.1 sec, L = 10 mm, a (Flow Diameter) = 0.5 mm, b (Outside Perimeter) = 0.6 mm; **(a)** Fluid and solid temperatures with inlet temperature T_{in} as a bifurcation variable plotted for two different material thermal conductivities (k_s = 5 W/m-K and 50 W/m-K) with extinction points marked as stars; **(b)** Reactor design schematic representing disc-type reactor with multiple perforations with L/D<<1 depicting hexagonal-circular arrangement; Solid and fluid temperature profile at: **(c)** extinction points; **(d)** far from extinction points (ignited branch); Ethane and oxygen composition profile at: **(e)** extinction points; **(f)** far from extinction points (ignited branch); Ethylene composition profile: at **(g)** extinction points; **(h)** far from extinction points (ignited branch).

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DNR0094

Process intensification in an Elastic Foam-bed Reactor: hydrodynamics, mass transfer and modeling

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Abstract Category: Reactor Modeling and Design - Reactor Design - Novel Reactors

Keywords: Process intensification, multiphase reactor, elastic bed, modeling

Abstract Body.
Elastic Foam-bed Reactor (EFR) was developed by combining polyurethane foam's elastic properties with crankshaft technology. The reactor consists of a column packed with two polyurethane foam blocks, forming a structured bed whose properties are modulated through piston-driven compression and decompression cycles. This motion promotes efficient gas-liquid mixing even at low velocities and allows continuous operation with complex systems like slurries or solid residues.

To evaluate the reactor in gas–liquid countercurrent and cocurrent downflow configurations, hydrodynamic and mass transfer studies were conducted. An experimental methodology was implemented to determine three key parameters over a range of fluid velocities from 0.5 to 11.5 mm/s:
(i) the liquid holdup (εl), determined using a KCl tracer method where a Dirac pulse of solution was injected and monitored by conductimetry;
(ii) the pressure drop monitored with a differential pressure gauge positioned upstream and downstream of the reactor;
(iii) the overall gas–liquid mass transfer coefficient (kla), estimated via oxygen stripping in deionized water using nitrogen and recorded with an oxygen probe.
These experiments were conducted under two operating modes: (I) Fixed Foam-bed Reactor (FFR), where the foam remains static, and (II) dynamic EFR mode, operated at 1 Hz and 80% compression, to benchmark the innovative EFR against the conventional FFR (Fig 1, a).

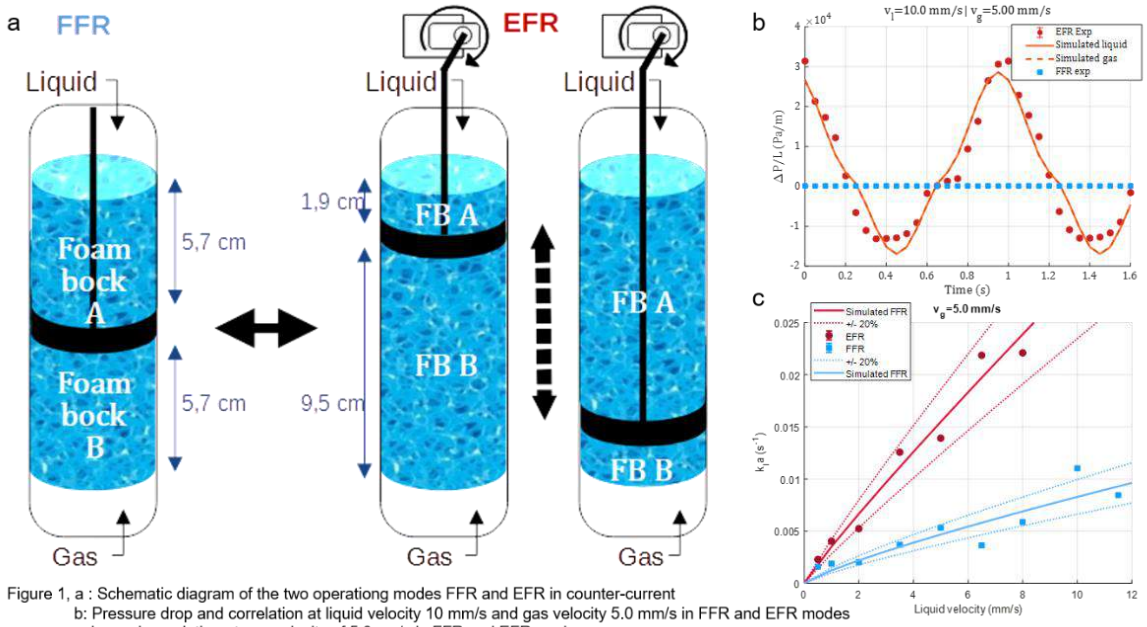

Figure 1, a : Schematic diagram of the two operationg modes FFR and EFR in counter-current
b: Pressure drop and correlation at liquid velocity 10 mm/s and gas velocity 5.0 mm/s in FFR and EFR modes
c: $k_l a$ and correlation at gas velocity of 5.0mm/s in FFR and EFR modes

The experimental campaign produced highly encouraging results. The Dispersed Plug-Flow (DPF) reactor model was used to determine liquid holdup and axial dispersion from the residence time distribution, which were then integrated into the calculations and correlations for kla and pressure drop. In co-current and FFR counter-current, liquid holdup exhibited typical TBR values around 20%, but increased significantly in counter-current EFR, reaching nearly 70%. In EFR mode, pressure drop exhibited sinusoidal oscillations synchronized with the crankshaft motion (Fig 1, b). This characteristic behavior was modeled using momentum balance and the Darcy–Forchheimer equation, incorporating the instantaneous piston velocity to capture the transient flow regime induced by the periodic compression. The controlled cycles significantly enhanced mixing and interfacial renewal, leading to a 1.5-fold increase in kla under identical operating conditions and demonstrating reduced diffusive limitations (Fig 1, c).
Correlations established predictive tools that support the optimization and scale-up of the EFR. A three-bed reactor arranged in series, with a total bed height ranging from 12 to 60 cm, is currently being studied for pilot-scale implementation.

A full comparison between static and dynamic modes for counter-current and co-current configurations for various flow rates will be presented during the conference.

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DNR0109

Catalytic CO2 Hydrogenation Reactions to Methanol: Catalysis, Intensification and Modelling

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Abstract Category: Reactor Modeling and Design - Reactor Design - Novel Reactors

Keywords: Ionic liquid sorbents, microkinetic modelling, CO2 conversion, reaction intensification

Abstract Body.

Keywords Ionic liquid sorbents; microkinetic modelling; CO2 conversion; reaction intensification

Purpose Efficient CO_2 utilization demands smarter routes to methanol, and conventional hydrogenation is held back by equilibrium limits. In situ removal of methanol and water with ionic liquids (ILs) presents an opportunity to break through these constraints and unlock higher conversions for more robust operation. This work explores the potential of IL-assisted synthesis through targeted IL screening and microkinetic modeling.

Methods Candidate ILs were examined through thermal exposure and sorption tests to evaluate stability, decomposition tendencies, and liquid-phase behavior at elevated temperatures. This was complemented by COSMO-RS predictions of methanol and water solvation to identify ILs with favorable affinity for selective product removal. A multisite microkinetic model [1,2] for CO_2 hydrogenation over Cu-based catalysts was applied to simulate intrinsic reaction rates and assess how IL-driven product extraction influences overall conversion and reactor performance.

Results The combined screening approach identified ILs with relevant thermal stability and sufficient methanol and water sorption capacity, though long-term stability under reaction conditions is still under investigation. These observations have direct implications for reactor design, emphasizing the need to optimally separate IL and catalyst to avoid deactivation while enabling vapor-phase product withdrawal. Microkinetic simulations show that effective in situ removal can substantially improve conversion, but performance depends on IL stability, regeneration capability, and thermal management.

Conclusion Overall, the results support the potential of IL-assisted methanol synthesis while highlighting key constraints that must be addressed in further process development.

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DNR0112

Pilot Testing and Reactor Modelling of Chemical Looping rWGS: Advantages of Countercurrent over Cocurrent Operation

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Abstract Category: Reactor Modeling and Design - Reactor Design - Novel Reactors

Keywords: CO2 capture and utilization, Iron oxide oxygen carrier, Reactor simulations.

Abstract Body.
This study investigates the chemical looping reverse water–gas shift (CL-rWGS) process in a pilot-scale packed-bed reactor, focusing on how cocurrent and countercurrent operation influence CO2 conversion, reactor productivity, and reaction behavior. Although CL-rWGS has shown promise at lab scale, its behavior and performance across different flow configurations remain insufficiently understood at larger scales. A key objective of this study is to quantify how reduction duration and gas-solid interaction patterns affect performance through thermodynamic and kinetic limitations, and to refine thermodynamic parameters for iron oxide-based oxygen carriers.

Experiments were conducted in a pilot-scale fixed-bed reactor (25.3 mol h-1 total flow, 84 vol% active gas, 973 K, 2.0 bara) using Fe2O3-MgAl2O4 oxygen carriers over multiple redox cycles. Cocurrent and countercurrent modes were tested at reduction durations of 5, 10, and 20 min. A one-dimensional pseudo-homogeneous reactor model incorporating equilibrium constraints was used to interpret gas-phase and solid-phase profiles. Bayesian optimization was applied to refine Gibbs free energy parameters, addressing discrepancies between NIST thermodynamic data and experimental behavior.

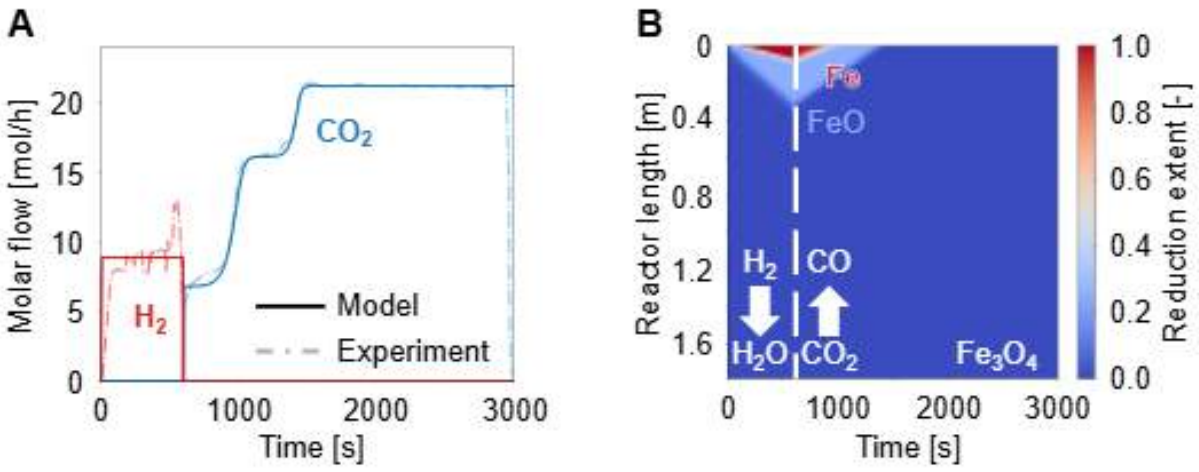

Figure 1. (A) Experimental and model molar outlet flow rates [mol/h] as a function of time [s] and (B) simulated reduction extent as a function of time [s] and reactor length [m] for CL-rWGS at pilot-scale.

Countercurrent operation achieved significantly higher average CO2 conversions of 46 % for 20 min reduction (compared to 36 % in cocurrent), exceeding gas-phase equilibrium. In countercurrent mode, CO2 first contacts FeO before reaching the Fe phase, improving oxygen carrier utilization. Cocurrent operation displayed stable but lower conversions, with overlapping oxidation fronts making Fe-FeO and FeO-Fe3O4 oxidation appear as a single step. Bayesian optimization showed that corrections of only a few kJ mol-1 in ΔG drastically improved model accuracy, highlighting nanoparticle-driven deviations from bulk thermodynamics. Model-experiment agreement was strong in countercurrent mode (see Figure 1) but less accurate in cocurrent, suggesting that unaccounted phenomena are at play.

This pilot-scale investigation demonstrates that countercurrent CL-rWGS provides superior CO2 conversion and more efficient oxygen-carrier utilization, driven by a favorable thermodynamic driving force along the reactor. The study reveals the high sensitivity of iron-oxide redox equilibria to small ΔG variations and provides corrected thermodynamic parameters that significantly improve predictive reactor modelling. These insights underline the importance of accurate oxygen-carrier thermodynamics and stable redox behavior for industrial CL-rWGS deployment. Future work should focus on refining kinetic models to enable optimized large-scale process operation, by improving heat-management strategies and identifying operating regimes that minimize carbon deposition.

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Rational Lab-Scale Reactor Design and Protocols for Tandem Alkane Cross-Metathesis in Polyolefin Recycling

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Olefin metathesis, Dehydrogenation, Alkane cross-metathesis, Plastic recycling, Polyethylene

Abstract Body.
Chemical recycling of polyolefin waste is attractive for carbon neutrality and plastic mitigation. Tandem alkane cross-metathesis (TACM, Fig. 1(a)) couples alkane dehydrogenation with olefin metathesis to convert polyethylene into saturated hydrocarbons under mild conditions (<300 °C). [1,2] However, the Mo-based metathesis-active catalytic species are extremely sensitive to trace H2O, O2, and oxygenates. We demonstrate that TACM performance is primarily governed by process-integrated reactor design. In the conventional ex-situ direct-charge batch (#1, Fig. 1(b)), brief exposure during catalyst transfer and feed charging limited C16-C6 TACM conversion to just 10-20%. The oven-housed in-situ fed-batch (#2, Fig. 1(c)) enables in-situ pretreatment and on-line delivery of dehydrated feed. Adding molecular sieve 5A to scavenge residual H2O further improves activity, yet reactor opening for polyolefin handling and coupled pretreatment remain constraints. The overhead-XCAD drop-in fed-batch (#3, Fig. 1(d)) preloads LDPE, applies vacuum, injects liquid feed, and introduces separately pretreated catalysts through independent ports without opening, preserving active sites and improving reproducibility with enhanced TACM conversion reaching 70-80% (Figs. 1(e-f)). With these process-integrated lab-scale reactor designs and handling protocols, TACM becomes a reproducible, accessible reaction that can be executed reproducibly in standard laboratory batch setups for many researchers.

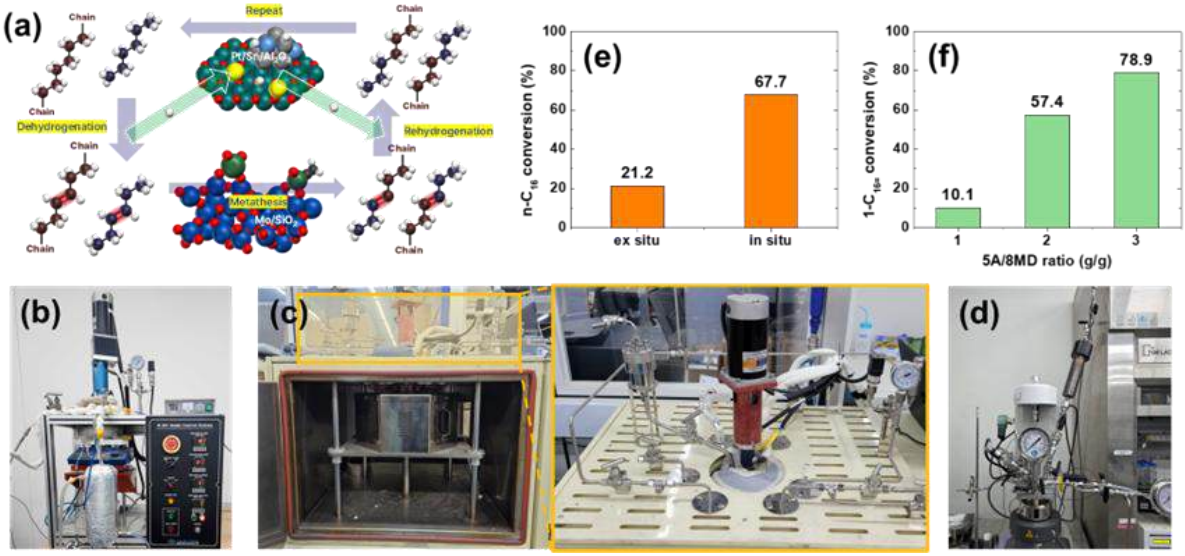

Figure 1. (a) schematic of heterogeneous TACM process, photographs of (b) the ex-situ direct-charge batch (Type #1), (c) the oven-housed in-situ fed-batch (Type #2), and (d) the overhead-XCAD drop-in fed-batch (Type #3), together with (e) the impact of in situ TACM addition on C16-C6 TACM performance and (f) the effect of 5A addition.

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DNR0125

Electrified dry reforming of methane via volumetric Joule heating of structured foam catalysts

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Abstract Category: Reactor Modeling and Design - Reactor Design - Novel Reactors

Keywords: Electrified dry reforming of methane; Joule heating; Structured catalysts; Decarbonization; Process intensification.

Abstract Body.

Introduction. The strong endothermic dry reforming of methane (DRM) is a reaction of interest to convert greenhouse gases into syngas. We have demonstrated a pilot-scale DRM process with a syngas productivity of 10k m3/h [1]. However, the conventional combustion heating generates unwanted CO2 emissions and suffers from heat transfer limitations. With the rising trend of renewable electricity, process electrification with Joule heating emerges as a promising alternative to combustion, facilitating decarbonization and process intensification [2-5]. In this regard, we have systematically studied the direct Joule heating of an internal SiSiC open-cell foam packed with Ni-based pellet catalysts for DRM reaction [6].

Methods. Commercial SiSiC open-cell foams (OD = 15 mm, L = 25 mm, 25 PPI) were adopted. 100 mg of Ni/Al2O3 catalyst (40-60 mesh), prepared by a wetness impregnation method, was mixed with 3 g of quartz sand (40-60 mesh, General-Reagent) and placed in the voids of SiSiC foam for Joule-heated DRM tests (CO2/CH4 = 2, 100 ml/min).

Results and discussion. The interconnected porous structure of SiSiC foam enables selective and volumetric heating of pellet catalysts in a packed bed configuration (Figure 1). The direct selective heating of internal structure requires extremely low input power, i.e., only 65 W to reach 800 °C compared to 143 W for external oven heating, and results in a reactor wall temperature approx. 300 °C lower than from the foam centerline, with the potential to significantly reduce reactor material requirements and cost. Additionally, volumetric Joule heating provides more uniform heating profiles and approx. 30 °C higher average temperatures over the catalytic bed with no cold spots observed, leading to enhanced CH4 and CO2 conversions reaching 94% and 64% at 800 °C, respectively, which are approx. 5-10% higher than external heating at the same outlet temperatures. The DRM ensures a significantly low specific energy demand of approx. 0.71 kWh/Nm³ for syngas production in an optimized process.

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DNR0238

STARBRIDGE™ Electrified Furnaces: Engineering-Scale 3D Modeling for Low-Carbon Steam Cracking, Reforming and Gas Heating

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Abstract Category: Clean Environmental Technologies - 선택 없음

Keywords: furnace, process heater, electrification, thermal radiation, decarbonization

Abstract Body.

The decarbonization of energy-intensive processes is a central challenge for the petrochemical industry. Fired heaters used in petrochemical applications such as steam crackers, reformers, and also process gas heaters for the steel industry are among the largest point sources of direct CO_2 emissions. Within Linde Engineering's STARBRIDGE™ platform, electrically heated furnaces are being developed and commercialized to replace conventional fired technologies and enable 90–95 % reductions in direct CO_2 emissions when powered by renewable electricity.

This contribution presents a comprehensive 3D furnace engineering model developed by Linde Engineering to support the design, scale-up, and project execution of STARBRIDGE™ electrified furnaces. The model is tailored for engineering applications, resolving all dominant physical effects while maintaining significantly lower computational effort than full CFD.

Thermal radiation is the dominant heat transfer mechanism and is treated in detail. Gas radiation is modeled using a Hottel-type zone approach combined with a weighted-sum-of-gray-gases model, enabling efficient yet realistic representation of participating media. Radiative exchange between heating elements, furnace walls, gas volumes and coils is solved using a ray-tracing method. Since radiation is non-local, the number of exchange coefficients increases rapidly with geometric complexity; this is addressed through a multi-grid strategy with efficient fine-grid reconstruction, allowing application to industrial-scale STARBRIDGE™ furnaces.

Furnace geometries are fully parametrized, enabling rapid setup of complex three-dimensional tube layouts, including multiple bends, coil tees, and electrically segmented tubes. Straight and bent coils are represented by cylindrical and toroidal elements, avoiding costly meshing while preserving geometric fidelity. Based on input parameters, the model automatically generates the complete 3D furnace geometry.

The furnace model is iteratively coupled with a tube-side process model by exchanging local tube wall temperatures and heat fluxes until convergence. This two-way coupling enables consistent prediction of tube metal temperatures, local heat fluxes, and process severity—key design criteria for STARBRIDGE™ applications. After convergence, the workflow automatically generates engineering reports in the form of tables and figures, directly supporting design reviews and project documentation.

The modeling approach has been validated against detailed CFD simulations and industrial plant data, including insights from the STARBRIDGE™ demonstration furnaces. Validation

confirms that the model reliably captures the radiative heat-transfer dominance and the characteristic differences between direct and indirect electrical heating concepts.

The presented work demonstrates how engineering-grade 3D modeling enables the industrialization of electrified high-temperature processes. It provides a digital foundation for the STARBRIDGE™ platform and supports the transition from demonstration to commercial deployment of low-carbon steam cracking and related furnace technologies.

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DNR0289

Rapid Pulsed Joule Heating for Energy-Efficient Nonoxidative Conversion of Methane to Ethylene

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Abstract Category: Reactor Modeling and Design - Reactor Design - Novel Reactors

Keywords: nonoxidative methane conversion; Joule heating; rapid pulsed heating; ethylene formation; energy efficiency

Abstract Body.
Introduction. Nonoxidative conversion of methane (NOCM) remains challenging due to methane's thermodynamic stability. Fe©SiO2 catalysts enable coking-free conversion to olefins, aromatics, and H2 above 950ºC, but conventional isothermal systems suffer from continuous coking and poor temporal control1,2. Joule heating (JH) provides superior temperature control, with programmable JH achieving over 75% C2 selectivity and 80% energy reduction3. This study employs rapid pulsed JH (RPJH) to enhance ethylene selectivity while minimizing energy consumption. We integrated NOCM in the RPJH reactor with acetylene hydrogenation to enhance ethylene production.
Methods. The JH reactor was assembled using Cu wire (0.04 mm o.d.), Cu sheets (0.02 mm), alumina tubes (0.6 mm i.d.), and carbon paper (CP) for resistive heating, connected to a DC power supply (EX80-30; ODA Technologies). CP was pretreated at 950°C in He flow (30 mL min-1, 2h). Temperature was monitored via infrared camera (PI 1M, Optris). For acetylene hydrogenation, a Pd/CeO2 catalyst was reduced at 250ºC in 5% H2/Ar (30 mL min-1, 1h), then passivated in 5% O2/Ar and packed downstream of the NOCM in RPJH.
Results and Discussion. The RPJH reactor achieved over 85% C2 selectivity at 10% methane conversion using millisecond heating-quenching cycles with 67% H2 and 30% CH4/Ar feed, effectively suppressing coke formation by minimizing secondary C-C coupling. The system demonstrated 47-fold higher energy efficiency than conventional continuous heating, consuming only 9.6 W. Integration of Pd/CeO2 catalyst (RPJH-HYD) enhanced ethylene yield 1.3-fold through selective acetylene hydrogenation, increasing ethylene selectivity from 56% to 70%. Temporally modulated temperature enabled precise reaction pathway control while minimizing energy consumption. H2 dilution improved CP stability by reducing coke accumulation, as evidenced by lower resistance changes and lower sp3/sp2 ratios compared with pure methane.

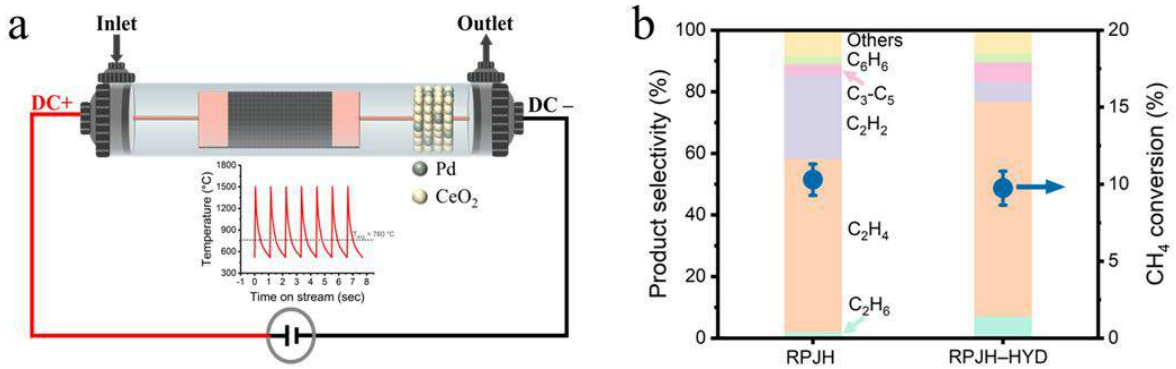

Figure 1. Schematic of RPJH reactor for NOCM integrated with acetylene hydrogenation (a). Comparison of CH4 conversion and selectivity between RPJH and RPJH–HYD (b).

Conclusion. NOCM to ethylene was achieved using an energy-efficient RPJH reactor with millisecond temperature switching that enhanced C2 selectivity by preventing coke formation. H2 dilution suppressed heavy hydrocarbons, achieving over 85% C2 selectivity with ethylene as the primary product. Acetylene was converted to ethylene via selective hydrogenation over a Pd/CeO2 catalyst. The system showed 47-fold higher energy efficiency than continuous heating, overcoming limitations of low productivity, poor selectivity, and high energy consumption.

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DNR0430

EMERALD: Experimental investigation of a novel eReactor concept based on radial electric current

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Abstract Category: Reactor Modeling and Design - Reactor Design - Novel Reactors

Keywords: Electrification, process intensification, innovative reactor design.

Abstract Body.

Introduction. The optimal design of eReactors must cope with a major topical challenge of endothermic catalytic processes (e.g., SMR): introduce strategies to match the varying heat demand of the reaction with the electrical power supply. To this scope, we propose a novel Joule heated eSMR reactor configuration based on radial electric current and on centrifugal gas flow (Figure 1A) [1].

Methods. Imposing the current, the variable cross-section (A_cross=2πr·H [m^2]) in the radial direction of the electric circuit leads to a non-uniform current density profile (J [A⁄m^2]). Hence, the local Joule's law exhibits a squared hyperbolic trend (q ̇_el=ρ_el·J^2 [W⁄m^3]∝1⁄r^2). Target reactive volume (100 ml) and GHSV (10 Nl⁄(h⁄g_cat)) were used to size the lab scale EMERALD reactor (Figure 1B). Temperature profiles were collected by seven thermocouples (Figure 1C) and the product gas compositions were analyzed by an online MicroGC. The temperature of the reactor casing (T_casing) was controlled by an external heating tape.

Results and discussion. Temperature profiles were strongly influenced by the relative heat flux (i.e., (Q_el) ̇-ΔH_reaction, Figure 1D); negative net heat fluxes (heating tape = power source) led to monotonically increasing temperature profiles from Profiles 1 to 6, nearly adiabatic conditions were observed from Profiles 7 to 10 and flat temperature profiles were collected, eventually positive net heat fluxes generated maxima in Profiles 11, 12, and 13. The product gas composition well aligned with the thermodynamic equilibrium line for each profile (i.e. from χ_(CH_4) (Profile1)=44.6% to χ_(CH_4) (Profile13)=70.8%). Both a simplified 1D pseudo-homogeneous model and detailed CFD simulations were used to rationalize the collected data enabling the validation of the EMERALD reactor prototype. Scaleup studies are ongoing.

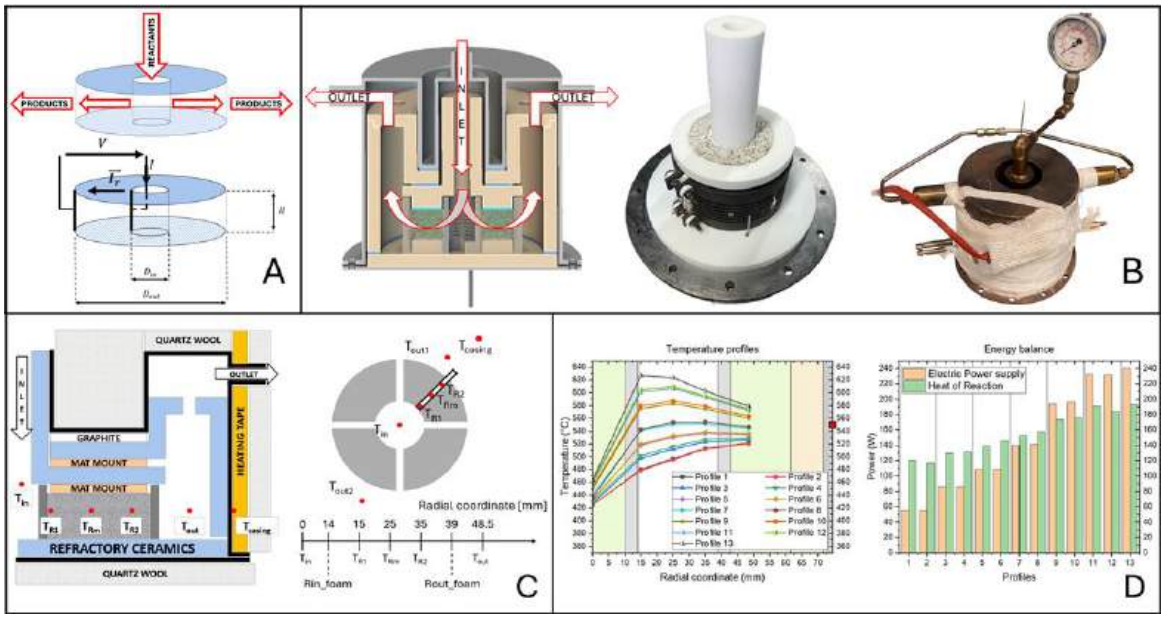

Figure 1. A) Design concept B) EMERALD lab scale reactor C) Reactor sketch D) Experimental results

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DNR0497

Electrification of ethylene production in a lab-scale electrothermal fluidized bed reactor through simulated steam cracking conditions.

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Abstract Category: Reactor Modeling and Design - Reactor Design - Novel Reactors

Keywords: Electrification, Joule Heating, Steam Cracking, CO2 mitigation, Ethylene

Abstract Body.
Ethylene serves as a fundamental precursor for chemical derivatives, including polyethylene and polyethylene terephthalate polymers. Conventional steam cracking processes emit approximately 1.6 tons of CO2 per ton of ethylene produced, with emissions dependent on feed composition. Electrification of chemical processes provides an alternative to traditional heating systems by enabling the use of renewable electricity and reducing CO2 emissions. Consequently, electrifying steam cracking represents a promising approach to mitigate the substantial CO2 emissions associated with ethylene production. This study examines ethylene production in a laboratory-scale electrothermal fluidized-bed reactor under simulated steam-cracking conditions. The experimental system utilizes graphite electrodes and a particle bed composed of graphite powder with an average particle size of 495 μm (0.12 m/s minimum fluidization velocity). The bed is contained within a 14/16 mmID/OD graphite hollowed cylinder deposited on stainless steel perforated plate located inside a 16.1/20 mmID/OD quartz tube. A feed mixture containing 45.3 vol% N2 and 54.6 vol% C2H6 simulates industrial steam cracking conditions. Experiments were conducted at electrothermal bed temperatures changing from 800 to 950 ºC to assess ethylene production under fluidization indexes ranging from 1.10 to 2.76, with residence times of 1.7 s and 0.49 s. Gas chromatography indicated conversion values between 28% and 62% and C2H4 selectivity values from 47% to 65%. C6+ compounds appeared under the tested conditions. Under electrothermal operation, specific energy consumption ranged from 0.197 to 0.213 kWh per mole of C2H4 for a residence time of 0.49 s (vs 0.132-0.164 kWh/mol C2H4 and 0.156-0.234 kWh/mol C2H4 in conventional ethane and naphtha steam cracking [1],[2], respectively, and 0.0467 kWh/mol C2H4 produced electrochemically [3]). Operational challenges persist at the required short residence times due to the insufficient contact between the gas and the hot bed for the intense heat transfer to reach steam cracking conditions without gas preheating. The results demonstrate that the electrothermal fluidized bed configuration enables sustainable and consistent ethylene production, despite design challenges for steam cracking conditions and the antagonistic requirements for low fluidization index for optimal power consumption. The results have been

modeled with the detailed kinetic model CRACKSIM [4], and good agreement between simulated and modeled data has been obtained. Simulations show the key role of residence time, with high ethylene selectivity achieved at short residence times. The particularities of the electrothermal fluidized bed design for optimal energy efficiency will also be discussed.

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DNR0565

A reduced order model for electrically heated catalytic reactors

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Abstract Category: Reactor Modeling and Design - Reactor Design - Novel Reactors

Keywords: Joule heating; Electrified steam methane reforming; Reduced-order model

Abstract Body.
Introduction: Decarbonizing energy-intensive chemical processes by using electricity from renewable sources offers a significant opportunity. Among electricity-driven technologies, Joule heating—where direct electric current is converted to heat—stands out due to its rapid thermal response and high thermal efficiency. Numerous experimental studies have reported promising results, particularly for energy-intensive endothermic catalytic reactions. However, scalability for industrial applications and systematic investigations of parameters, particularly for multiple catalytic reactions occurring simultaneously, remains largely unexplored.

Methods: A steady-state, 1-D electro-thermal-heterogeneous Reduced Order Model (ROM) is developed to represent an electrified tubular reactor with a catalyst washcoated on the reactor wall. The flow is assumed to be fully developed. Temperature-dependent thermophysical properties and heat losses to the surroundings through convection and radiation are included. The reaction kinetics of steam methane reforming (SMR) proposed by Xu and Froment [1] is used. The model is non-dimensionalized to gain insights into the reactor performance and enable systematic scale-up. Five dimensionless groups are obtained: thermal transport parameter (β), thermal Damköhler number (DaT), reaction Damköhler number (DaR), Nusselt (Nu), and Sherwood (Sh) numbers. Variation of these parameters enables accurate predictions across a vast design space for electrified tubular reactors.

Results and discussion: The ROM predictions for axial temperature profiles and methane conversion are in good agreement with experimental data reported by Wismann et al.[2]. Minor deviations arise as reactions are assumed to occur at the solid–fluid interface rather than within a porous wash-coated region. The dimensionless ROM reveals that higher β enforces solid–fluid thermal uniformity, whereas lower DaT enhances the non-uniformity, as shown in Figure 1. The developed ROM provides a computationally efficient yet accurate representation of an electrified SMR tubular reactor. Overall, the framework serves as a practical tool for analyzing and optimizing electrified catalytic reactors for low-carbon hydrogen production.

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DNR0621

Experimental testing and CFD modelling of an electrified ammonia cracking reactor

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Keywords: Ammonia decomposition; Process Intensification; Process Electrification.

Introduction

Ammonia is considered a promising hydrogen carrier due to its high hydrogen content and well-established storage and distribution infrastructure. Ammonia decomposition step is expected to be the bottleneck for industrial scale development. Since the reaction is significantly endothermic ($\Delta H°r$ =45.9 kJ/mol_{NH3}), efficient design and heat management in the catalytic reactor are of key importance for catalyst usage optimization and overall system performance. The proposed solution packs Ru catalyst pellets in thermally conductive periodic open-cell Al-alloy structures (POCS) in thermal contact with electrically heated wires[1].

Methods

The thermally insulated tubular reactor consisted of a stack of four aluminum POCS with diamond unit cells (dcell = 4 mm, porosity = 0.9) packed with a commercial catalyst (Heraeus, 2 wt% Ru/Al_2O_3, 1 mm spheres). A 400 W, ¼″ heating cartridge was placed at the reactor centerline, while two sliding thermocouples monitored half-radius and wall temperatures. Pure anhydrous ammonia was fed at gas hourly space velocities (GHSV) ranging from 2.5 to 10 Nl/h/g_{cat}. Power input, conversion and temperature profiles were collected over a temperature range of 400–525 °C and from 1 to 3 bar. A CFD reactor model was developed considering the heat transport properties of the POCS and the reaction kinetics derived by Franchi et al[2].

Results and discussion

As shown in Fig.1A, the system reaches NH_3 conversion approaching 100% at 2.5 Nl/h/g_{cat} with a thermal efficiency of 69% (defined as the ratio between the enthalpy change of the gases and the electric power supplied), while at 7.5 Nl/h/g_{cat} thermal efficiency approaches 88% with an NH_3 conversion >95%. The developed model predicts conversion, temperature profiles and thermal efficiencies for the whole span of experimental conditions considered – see some cases in Fig.1B. Finally, the validated model was used to design an industrial-scale ammonia cracking reactor operating at 7 bar, achieving almost complete conversion via constrained optimization of wire pitch, structured catalyst properties, and reactor geometry, while complying with thermodynamic, kinetic, and heat-transfer limitations.

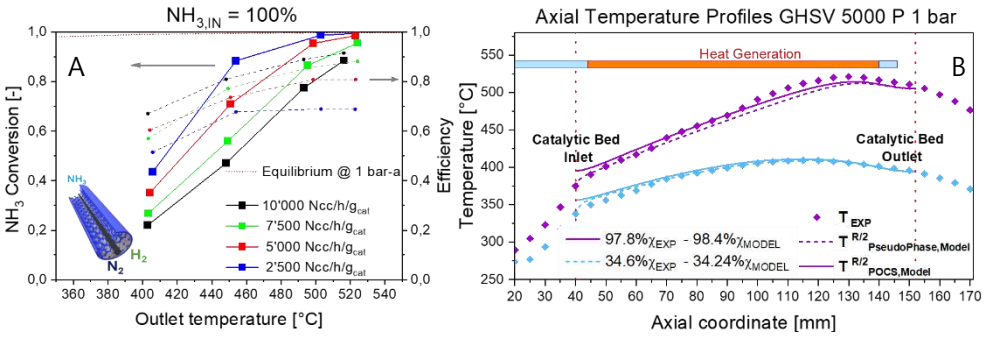

Figure 1 A) NH_3 conversion and thermal efficiency as a function of the outlet temperature and GHSV
B) Experimental data and model simulation comparison at GHSV 5000 Ncc/h/g_{cat} and 1 bar

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ISCRE29 & APCRE11
2026 / SEOUL, KOREA

DNR0366

Model-Driven AI Analysis and Optimization of a Novel Heat-Integrated Reactor for CO2 Methanation and NH3 Cracking

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Keywords: CO_2 utilization; H_2 generation; Machine learning

Introduction.

CO_2 methanation (Eq. 1-2) offers a viable pathway for carbon conversion into CH_4 [1]. Supplying carbon-neutral H_2 for this process still remains a challenge. NH_3 cracking (Eq. 3) can supply carbon-neutral H_2 [2]. These two reactions exhibit contrasting thermal behaviors, which demand different thermal management. Methanation is an exothermic reaction. High temperature (heat release) shifts it toward undesired CO formation (Eq. 2) [1,3]. Although it is an equilibrium endothermic reaction, NH_3 cracking is controlled by the kinetics. Low temperatures (heat consumption) limit NH_3 cracking kinetics and equilibrium [2,4]. A thermal control through an optimized design is essential to balance reaction rates in both processes. A heat-exchanging thermally-coupled reactor (Fig.1a) offers an effective strategy by integrating the exothermic-endothermic reactions in a single system.

$$CO_2 + 4H_2 \rightleftarrows CH_4 + 2H_2O\,, \Delta H^\circ = -165\frac{kJ}{mol} \quad (1)$$

$$CO_2 + H_2 \rightleftarrows CO + H_2O\,, \Delta H^\circ = +41\frac{kJ}{mol} \quad (2)$$

$$NH_3 \rightleftarrows 1.5H_2 + 0.5N_2\,, \Delta H^\circ = +46\frac{kJ}{mol} \quad (3)$$

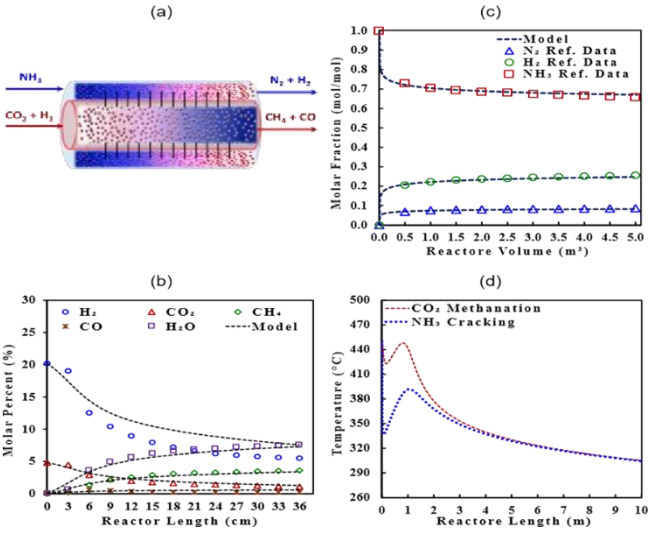

Figure 1: (a) thermally coupled reactor, (b) CO_2 methanation, (c) NH_3 cracking, and (d): temperature distributions

Novel computation tools, such as AI modeling, can enable optimization of CO_2/NH_3 utilization in this reactor, leading to maximized H_2 delivery, CO_2 reduction, and CH_4 yield. This study develops an AI tool to optimize a thermally-coupled reactor integrating CO_2 methanation with NH_3 cracking.

Methods.

A database, which is generated by a mathematical model, is utilized to train AI tools (MLP, CFF, and RBF). The best AI design is combined with an optimization procedure to explore the best operation with the highest CO_2 conversion and H_2 and CH_4 yields.

Results and discussion.

The validated mathematical model against CO_2 methanation and NH_3 cracking (Fig.1b-c) is used to design the reactor. The temperature profiles (Fig.1d) show that the cracking reaction can capture the released heat in the methanation side and benefit from it to convert more NH_3.

Acknowledgments.

This work was supported by the National Research Foundation of Korea(NRF) grant funded by the Korea government(MSIT) (RS-2020-NR049541). This work was supported by the National Research Foundation of Korea(NRF) grant funded by the Korea government(MSIT)(RS-2025-02306122).

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ISCRE29 & APCRE11
2026 / SEOUL, KOREA

DNR0458

Novel Autothermal Cracker concept for Ethylene production

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Abstract Category: Reactor Modeling and Design - Reactor Design - Novel Reactors

Keywords: Autothermal Cracking, Novel reactor design, Kinetics, Ethylene, Decarbonization

Abstract Body.
Introduction. Conventional steam cracking furnaces remain heavily reliant on fossil fuels and are energy intensive and globally account for 0.75% of total CO2 emissions. Here we propose a novel autothermal cracker (ATC) with a radically different reactor design [1] in which steam cracking reactions occur at much shorter residence times (<10 ms) and higher temperatures (>1200 °C) than in conventional furnaces.

Methods. The ATC concept hinges on very fast mixing of the in-situ produced very hot steam (>1600°C) and the “cold” hydrocarbon feed. Preliminary commercial scale design options were evaluated using computational fluid dynamics (CFD). Proof of concept experimental studies, using pre-mixed feeds, were conducted with ethane, naphtha, and pyrolysis oil. The experimental data were used to adapt and improve existing kinetic models, as conventional steam cracking kinetics are not directly applicable to the ATC concept. These kinetic models were subsequently integrated into the CFD model to optimize the commercial scale reactor design in conjunction with an integrated cracker plant design.

Results and Discussion. The experimental work with pre-mixed feed (hydrocarbon and steam) at temperatures and residence times prevailing in the envisioned auto-thermal reactor, showed significant improvements in both selectivity towards desired products and yields. However, the commercial scale reactor should be capable of very fast mixing of steam, very short times in the mixing/reaction zone with limited recirculation. The CFD results showed that for most of the selected configurations, including side and inline feed injections as well as co-current and counter-current flow arrangements, it was not possible to simultaneously meet the stringent residence time, fast mixing and temperature requirements. A major improvement was achieved with a counter-current lance-feeding concept, see Figure 1.

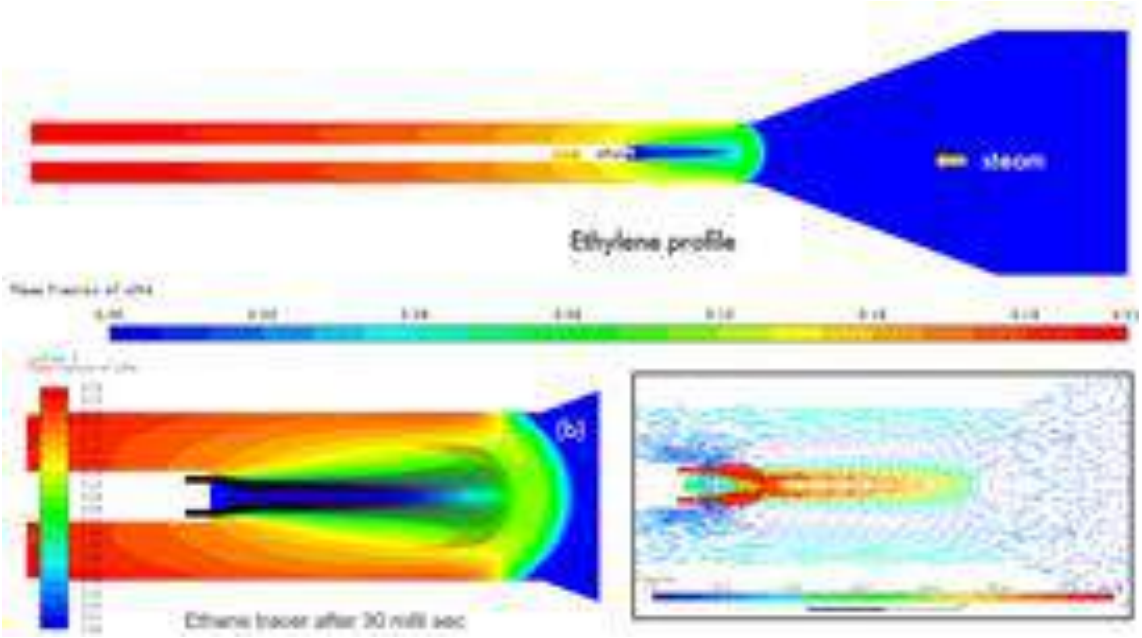

Figure 1 (a) ATC reactor concept (b) Flow & mixing profile

Here ethane is injected via a lance at very high velocities, forming a jet within the steam flow. This configuration demonstrated in the CFD simulations a significantly improved mixing and residence time distribution compared to the more straightforward initial reactor concepts. The reactive CFD simulations predicted significant yield improvement compared to conventional ethane cracking, typically 10-15%.

Acknowledgments
The authors thank the experts of Linde for the very constructive collaboration.

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ISCRE29 & APCRE11
2026 / SEOUL, KOREA

DNR0529

CFD modelling of reactive CO2 absorption in structured packings

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Abstract Category: Reactor Modeling and Design - Reactor Design - Novel Reactors

Keywords: CFD modelling, absorption, structured packing, CO2 capture

Abstract Body.

Introduction:

CO_2 absorption using amines is a mature and widely applied technology. Its efficiency depends on operating conditions, solvent type, and the effectiveness of gas-liquid contact. In recent years, structured packings have emerged as a well-established device for gas-liquid contact, due to their higher mass transfer efficiency, higher capacity, and lower pressure drop compared to random packings. The present work focuses on developing a multiphase Eulerian CFD model to predict hydrodynamics, mass transfer, and CO_2 absorption in monoethanolamine (MEA) for an in-house structured packed column.

Methodology and Results:

The computational domain consists of a packed column of 28 cm height and 5 cm diameter (Figure 1), containing structured packing of 4.979 cm diameter. The column is filled with MEA solution up to 28 cm, while a gas mixture of 28.2 wt% CO_2 and 71.8 wt% N_2 is introduced from the bottom at a velocity of 0.021 m/s. Flow abatement zones of about 5% of the column height are included at the inlet and outlet to minimize boundary effects.

The governing momentum, energy, and species transport equations are solved using OpenFOAM v8.0. Hydrodynamics are first investigated, followed by modeling CO_2 absorption in MEA with chemical reaction forming carbamate. Mass transfer between phases is taken into account using a Sherwood number-based mass transfer model, i.e, Sh = f(Re, Sc). The predicted outlet CO_2 concentration and capture efficiency at different gas velocities has to be validated against in-house experimental data. The effective interfacial area across the column is estimated from the gradient of the liquid volume fraction, i.e., [1].

$$CO_2 + H_2O + 2MEA \overset{K_1}{\leftrightarrow} MEACOO^- + MEAH^+$$

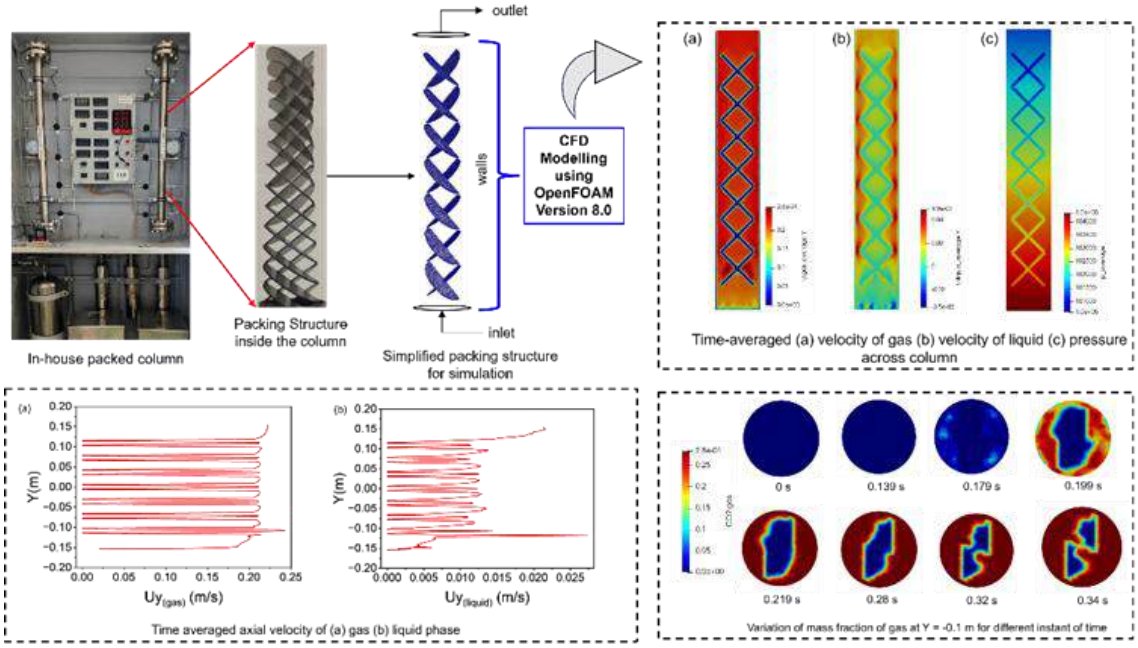

Figure 1: Schematic overview of the experimental packed column, structured packing geometry, and corresponding CFD model, along with simulated hydrodynamics.

Figure 1 shows the time averaged axial velocity profiles of both gas and liquid phases across the column, at Ug = 0.021 m/s. Within the packed region, both phases exhibit the strong variations in velocity, which indicates the complex nature of multiphase flow caused by the packing structures. The time-averaged velocity across a cross-sectional slice and the CO2 mass fraction contours at y = -0.1 m also presented.

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ISCRE29 & APCRE11
2026 / SEOUL, KOREA

DNR0687

MODELING OF A CATALYTIC CANDLE FILTER FOR DUST AND TAR REMOVAL FROM SYNGAS

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Abstract Category: Reactor Modeling and Design - Reactor Design - Novel Reactors

Keywords: Syngas cleanup, catalytic tar removal, filtration, multifunctional reactor

Abstract Body.

Introduction. Particulate matter (PM) and tars in biomass-derived syngas pose significant operational challenges in its further processing and conversion. Catalytic candle filters (CCFs) have been experimentally researched as multifunctional devices for simultaneous tar and PM removal from syngas. However, mathematical models for design and performance analysis of CCFs have been seldom reported. A transient model inspired from the classical unit collector approach is proposed in the present study to obtain insights into the coupled particle filtration and catalytic tar conversion in a CCF.

Methodology. The porous region of a cylindrical CCF is discretized into an array of concentric annular slabs, with each slab comprising an array of spherical unit collectors with a catalyst washcoat (catalytic collectors) separated by void space. The catalytic collectors provide surface for particle deposition while acting as a washcoated substrate for tar conversion. Transient mass balances are used to model deep-bed filtration of particles with a multivariate size distribution across the porous region, assuming Brownian motion and interception as the primary filtration mechanisms. Voidage-dependent partition coefficients are used to model the onset of cake filtration. Further, conservation-based transport equations with literature kinetics are used to model tar conversion, with careful consideration of the mass-transfer resistances incurred on account of boundary layer formation and particle deposition. The set of equations are solved using Python-3 to predict time-resolved evolution of species concentrations, filtration efficiency, and pressure drop.

Results and discussion. Fig. 1 (a) shows the temporal variation of concentrations of differently-sized particles with time at the CCF outlet, for total particulate concentration of 1.54×10-3 kg/m3 in the raw syngas. While the filter has overall removal efficiency > 90% at all times, larger particles are associated with lower exit concentrations, and dominance of the interception mechanism is observed. Fig. 1 (b) represents the variation of model tar species' concentrations along the radial position in the porous domain at t=1.75 h. C6H6 exhibits a higher conversion (85%), as compared to C7H8 (41%) and C10H8 (57%). Owing to low tar concentrations in the feed syngas, the conversion of tars does not have a significant effect on the concentrations of major syngas components (CO, H2, CO2, etc.). Further insights were obtained into the role of different filtration mechanisms, mass-transfer resistances in CCF performance, and will be presented in the full manuscript.

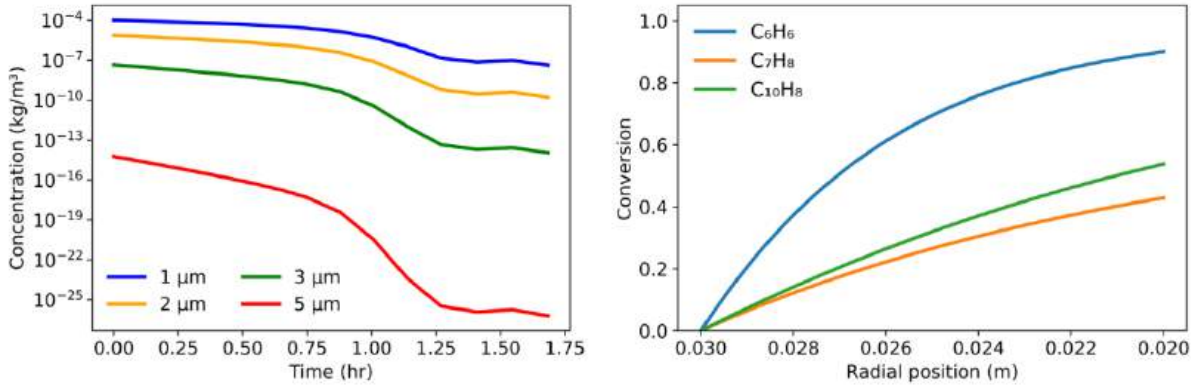

Fig. 1. (a) Temporal variation of particle concentrations at CCF outlet, (b) Variation of tar concentrations along the radial position of CCF

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2026 / SEOUL, KOREA

DPR0099

Detailed Modeling of Autoclave Reactors

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Abstract Category: Reactor Modeling and Design - Reactor Design - Polymerization Reactors

Keywords: Autoclave reactors, Low-density polyethylene and copolymers, Molecular weight distribution, Fixed pivot technique, Free-radical polymerization, gPROMS

Abstract Body.
Purpose:

Developing new polymer grades often involves significant challenges, particularly in identifying operating conditions that achieve the desired molecular weight distribution (MWD) in reactors with imperfect mixing and complex kinetics. This presentation describes how an integral modeling approach helps in accelerating polymer grade development, in evaluation of new reactor designs, and in optimization of operating conditions that preserves polymer properties when changing throughput.

Methods:

Comprehensive models of industrial autoclave reactors were developed by integrating advanced modeling concepts:
(a) The advanced SAFT-γ Mie Equation of State, which represents molecules as chains of functional groups [1], ideally suitable for the modeling of polymers.
(b) Kinetic model that considers elementary reaction steps in free radical co-polymerization and solves for the evolution of MWD using the fixed pivot technique (FPT) [2].
(c) A multi-zonal approach that models the reactor as a network of perfectly mixed reactors to handle complex flow patterns. The inter-zonal flows are derived from “cold-flow” Computational Fluid Dynamics (CFD) simulations.

The integrated reactor model is built on Siemens’ gPROMS® advanced process modeling platform using Siemens’ gPROMS properties thermodynamic engine and Siemens’ Hybrid Multizonal gPROMS-CFD tool for automatic processing of results of CFD simulations performed with Siemens’ Star-CCM® or ANSYS Fluent®.

Results:

- The use of rigorous thermodynamics allows incorporation of temperature and pressure effects on the heat of reaction and improving temperature predictions. This also allows accurate prediction of the on-set of two-phase behavior of reacting mixtures, accounting for polydispersity and branching (Figure 1A).
- Detailed kinetic modeling allows prediction of MWD including the high molecular weight shoulder seen in many LDPE and copolymer grades (Figure 1B).
- Multizonal modeling with a sufficiently large number of zones (200-300) allows the model to respond to changes in design details, such as impeller geometry, and positioning of injection ports

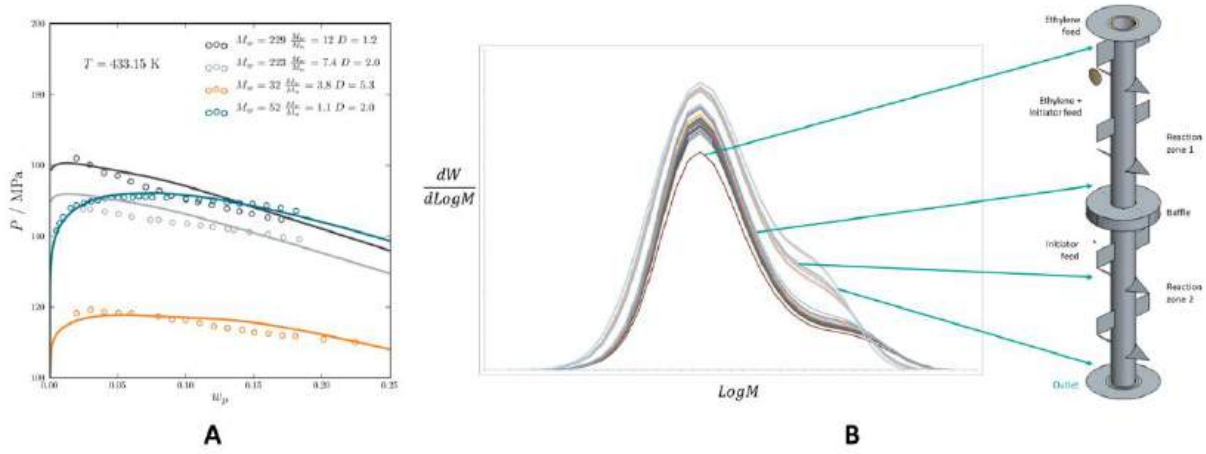

Figure 1: A. Cloud curves of ethylene + polyethylene of different weights and degree of branching (D) comparing SAFT-γ Mie predictions and experimental data [3], B: evolution of MWD across reactor

Conclusions:

The integrated modeling approach offers several benefits that enhance the accuracy of autoclave reactor models. Implementation on the gPROMS platform allows (i) adjusting kinetic parameters to match plant data, and (ii) optimizing operating conditions that achieve desired product properties, such as melt index and resin density.

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ISCRE29 & APCRE11
2026 / SEOUL, KOREA

DPR0626

Size control of polystyrene particles in suspension polymerization with a stirred tank

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Keywords: suspension polymerization; polystyrene; particle size distribution

Introduction. Polystyrene (PS) is a versatile thermoplastic widely applied in packaging, electronics, and construction due to its high transparency, electrical insulation, mechanical strength, low density, and cost–effectiveness. It can be produced through bulk or suspension polymerization, with suspension polymerization serving as the predominant industrial method for manufacturing expandable polystyrene (EPS). Suspension polymerization is a heterogeneous free radical process in which monomer droplets are dispersed in an aqueous continuous phase, offering efficient heat transfer, precise temperature control, low impurity content, and easy post–treatment. In this process, styrene monomers are first dispersed into fine droplets within an aqueous medium containing dispersants. Subsequently, at elevated temperatures (80–120 °C), the initiator, such as benzoyl peroxide (BPO), decomposes to initiate the polymerization reaction within the droplets. The particle size distribution (PSD) of the resulting polymer critically governs its properties, especially for EPS, influencing insulation, storage stability, processability, mechanical strength, and foaming behavior. It is understandable that the control of droplet size and stability is the key point for optimizing the reaction process and product quality. In this study, the effect of rotation speed, suspension agent tricalcium phosphate (TCP) concentration, co–dispersant sodium dodecyl benzenesulfonate (SDBS) concentration on the final PSD were studied, and the underlying mechanism was discussed. The findings in this study provide effective guidance for the formulation design of industrial PS production.

Methods. The recipe contains distilled water, TCP, SDBS and sodium sulfate in the continuous phase, and styrene, BPO, polyethylene wax in the disperse phase. The oil fraction is 50%. suspension polymerization was operated at 90°C in a stirred tank with tilted six-blade agitator. PSD of the final PS particles was characterized by laser diffraction particle sizer.

Results and discussion. The measured results suggest that increasing the rotation speed decrease the particle size, and the distribution becomes narrower, as shown in Figure 1. This can be attributed to the rapid rise in turbulent energy dissipation within the reactor, which is cubic power function of agitation speed. According to Kolmogorov's local isotropy theory, higher turbulence intensifies shear forces, thereby enhancing droplet breakage. Consequently, the dynamic balance between droplet breakage and coalescence shifts toward breakage, leading to a reduction in the droplet and particle size, narrowing the distribution. We also studied other factors, such as concentration of TCP and SDBS, tubular baffles and PH, on the PSD.

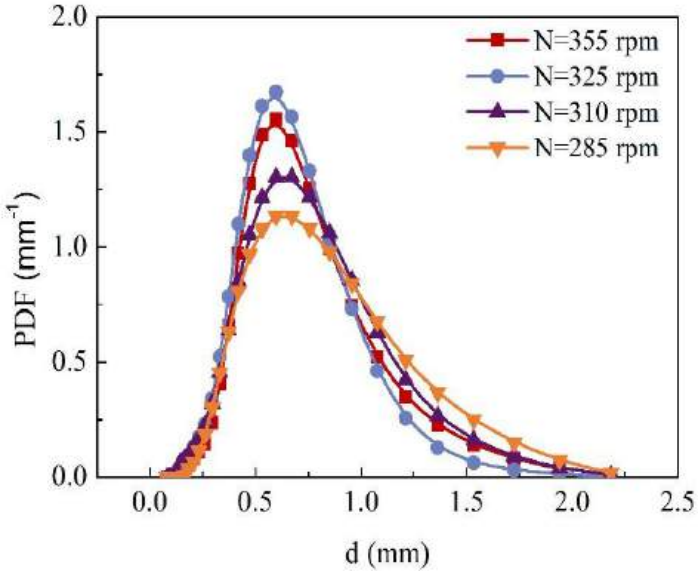

Figure 1 The effect of operating rotation speed on PSD

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

DPR0633

Optimization of Slurry Loop Reactors by Understanding the Complex Mesoscale Behaviors of swelling particles

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Abstract Category: Reactor Modeling and Design - Reactor Design - Polymerization Reactors

Keywords: Swelling particle, Fluidization, Loop reactors

Abstract Body.

Introduction.

Slurry loop reactors have been extensively used in chemical industry, for example, ethylene copolymerization. A classical engineering problem is the timely removal of reaction heat which would otherwise cause particle swelling and aggregation, and thus reactor fouling, operation instability, or even blockage, imposing a high safety risk in production [1]. Lack of knowledge on the mesoscale information of particle swelling and aggregation poses great challenge on the prediction of the macroscale behavior [2].

Methods.

This work conducts an experimental study on the fluidization of polyethylene particles in an elevated-temperature liquid-solid fluidized bed. The measurement of pressure drop under different temperatures is used to study the effect of temperature on fluidization regimes. And then we develop a swelling-dependent two-fluid model, the CFD with Eulerian-Eulerian method was used to simulate the swelling particle behaviors in loop reactors.

Results and discussion.

Based on the experiment of swelling particle fluidization, four regimes can be identified through static bed height and pressure drop measurements, i.e., stable fluidization, noncohesive-swelling fluidization, cohesive-swelling fluidization, and full defluidization. Simulation resluts resolves the particle aggregation and plug accumulation in the upstream of the pump and the upper horizontal pipe, revealing the fundamental of reactor blockage. The mesoscale structure, when developing to a certain extent, can cause a sharp increase of pump power consumption. Based on the simulation, a reactor optimization scheme was heuristically proposed to minimize or eliminate the plug regions by employing two pumps and two cycles.

Acknowledgement

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Oral Presentation

Process Intensification

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

PTL9699

Scale-up of a compact Fischer-Tropsch structured reactor

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Abstract Category: Process Intensification - Process Intensification / TEA / LCA

Keywords: Fischer-Tropsch synthesis; Periodic Open cellular structures; Structured reactor.

Abstract Body.

Introduction. Industrial-scale Fischer–Tropsch (FT) plants typically employ multi-tubular fixed-bed or slurry bubble column reactors designed to process large gas throughputs. The increasing interest in decentralized syngas sources motivates the development of compact FT reactors, whose scale-up requires robust reactor models and effective heat-management strategies due to the critically exothermic nature of the reaction [1].

Methods. Several highly conductive AlSi10Mg Periodic Open Cellular Structures (POCS) [2] were tested to boost heat transfer in a pilot FT reactor at Politecnico di Milano [3-4]. The lattice elements were packed with 20 wt.% Co/Al_2O_3 catalyst particles (300 μm), occupying the central 20 cm of a jacketed tubular reactor 1 m long with ~1-inch I.D.. Experiments were run at 25 barg, H_2/CO = 2.1 and GHSV ≈ 4 Nl/h/gcat. Axial catalyst T-profiles together with outlet gas composition were used to estimate an overall heat-transfer coefficient representative of each POCS tested. The resulting data from the experimental campaign were used to develop a 2D pseudo-homogeneous reactor model implemented in gPROMS®.

Results and discussion. The validated 2D model was applied to the preliminary design of a scaled-up FT reactor, consisting of a single ~1 inch tubular reactor with a 1 m long structured catalytic bed. The catalytic bed is modeled as a homogeneous POCS packed with catalyst, while in practice it is obtained by stacking five 20 cm-long packed POCS elements, Figure 1. The feasibility was assessed in experimental campaigns, where POCS elements with different axial lengths (10 and 20 cm) were operated under comparable conditions [4]. This modeling framework provides a reliable basis for the rational scale-up of structured FT reactors. The conduction-driven heat-transfer mechanism promoted by the Al POCS is beneficial for both highly exothermic reactions, as FT synthesis, and endothermic processes.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

PTL0155

Thermochemical conversion, and process integration solutions for biomass-derived feedstocks and their upgrading into usable fuel blends

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Abstract Category: Process Intensification - Process Intensification / TEA / LCA

Keywords: Fuel blends, pyrolysis, process integration

Abstract Body.

The transition toward sustainable energy systems is especially important for the Nordic region, where ambitious climate targets coexist with the availability of large amounts of biomass and industrial residues. The EU-Interreg Aurora project FORBLEND addresses this challenge by exploring sustainable fuel blending concepts based on locally available renewable resources. This study presents an overview of ongoing work within the project, combining laboratory results and preliminary process simulations to evaluate low-carbon fuel pathways suitable for Nordic conditions.

The work focuses on the thermochemical conversion of biomass-derived feedstocks and their upgrading into usable fuel blends. Experimental observations are supported by steady-state process modelling using Aspen Plus, which is applied to represent key unit operations such as conversion reactors, gas cleaning, and separation units. Attention is given to the selection of thermodynamic property models, as accurate description of phase behaviour and reaction equilibria is essential for biomass-based systems. The Redlich–Kwong equation of state is selected due to its reliable performance at elevated temperatures and moderate pressures, especially for gas mixtures containing hydrogen, carbon monoxide, carbon dioxide, and light hydrocarbons. Reaction behaviour is evaluated using equilibrium-based approaches, allowing comparison with experimental trends while keeping the model computationally efficient.

Initial simulation results suggest that process integration and appropriate fuel blending strategies can improve energy efficiency and carbon utilization compared to conventional fossil-based fuels. Sensitivity analyses indicate that operating conditions and feedstock composition strongly influence system performance, highlighting the importance of region-specific design for Nordic applications. Future work within FORBLEND will extend this modelling framework by incorporating techno-economic assessment and life-cycle considerations, as well as closer integration with experimental data. Overall, this study contributes to the early-stage evaluation of sustainable fuel blends and supports the development of low-carbon energy solutions for the Nordic region.

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KN0629

AI Assisted CO2 Conversion Process for Value Added Chemical Production

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Abstract Category: Invited Lecture - Keynote Lecture

Keywords: CO2 Utilization, Reactive Capture and Conversion, Process Systems Engineering, Explainable AI, Bayesian Optimization

Abstract Body.
The successful implementation of Carbon Capture and Utilization (CCU) requires a seamless transition from molecular-level innovation to system-level integration. Reactive Capture and Conversion (RCC) has emerged as a promising strategy to streamline this transition by merging capture and conversion into a single, energy-efficient workflow. However, the development of these systems is often hindered by the vast search space of potential materials and the intricate complexity of process configurations.
Our framework addresses these challenges by integrating advanced Machine Learning with rigorous Process Systems Engineering . At the initial stage, we employ Graph Neural Networks and Bayesian Optimization to perform high-throughput screening of amine-based absorbents and catalysts. This molecular-level strategy allows us to identify optimal candidates with high CO2 loading capacity and catalytic activity while minimizing computational costs. To bridge the gap between material discovery and industrial application, we have developed an automated process synthesis platform centered on Superstructure Optimization. This approach is particularly effective for the electrochemical CO2 reduction reaction, where numerous process alternatives exist. By linking our optimization model with automated design software, we can explore an extensive process design space that was previously inaccessible through manual methods. The system automatically evaluates thousands of configurations, including various separation sequences and heat integration schemes, to identify the most techno-economically viable pathways. Finally, we address the critical issue of catalyst durability. By implementing Explainable AI on cyclic voltammetry data, we have established a methodology to decode complex degradation patterns. This allows for a clear distinction between extrinsic factors, such as poisoning, and intrinsic factors, like active site dissolution. These insights provide a definitive roadmap for designing resilient electrochemical systems. This integrated AI-assisted approach demonstrates a systematic pathway toward the rapid commercialization of sustainable carbon resource technologies.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

PTL0232

Environmental and Economical Assessment of Membrane-based Blue Hydrogen Process: Integrating Carbon Capture and Oxygen-enriched combustion

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Abstract Category: Process Intensification - Process Intensification / TEA / LCA

Keywords: Blue hydrogen, Gas separation membrane, Process siulation

Abstract Body.

Purpose

Blue hydrogen production via steam methane reforming (SMR) integrated with carbon capture is widely recognized as a practical bridge technology toward clean energy. However, conventional amine-based capture systems suffer from significant energy demands for solvent regeneration. This study proposes and evaluates a novel hybrid process that integrates SMR with membrane-based carbon capture (CCM) and oxygen-enriched combustion (OEC) using gas separation membranes to enhance energy efficiency and economic feasibility.

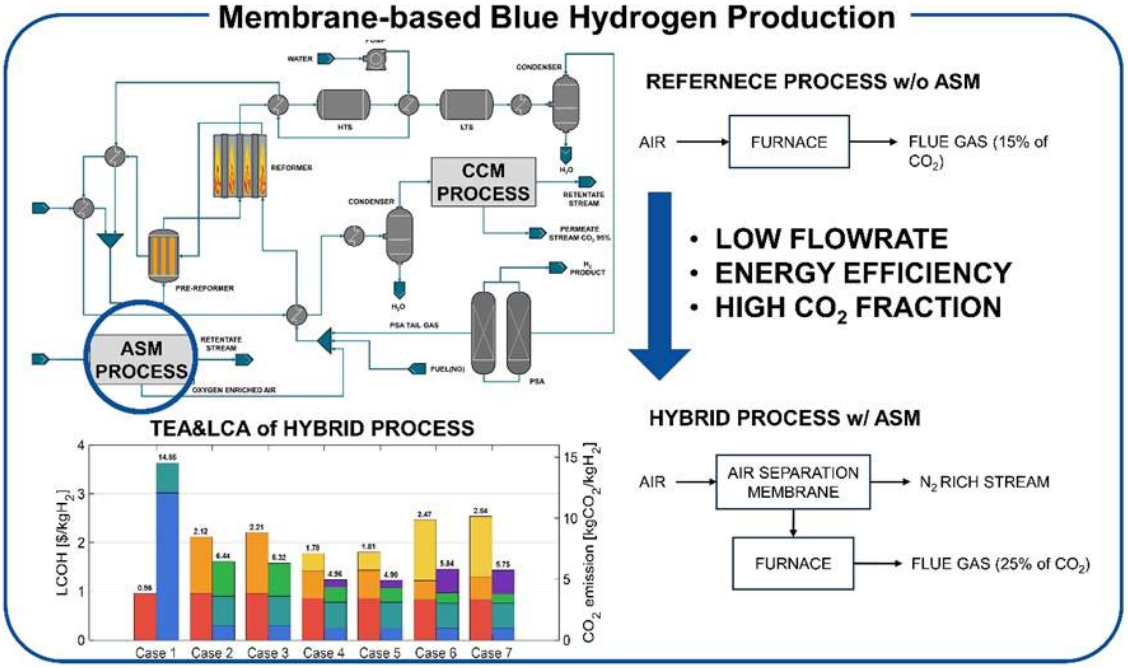

Figure 1. Overview of the proposed process

Methods

A comprehensive process simulation was developed using gPROMS to model the integrated process. As illustrated in Fig. 1, the study framework encompasses the hybrid process schematic, rigorous unit-operation models (reformer, WGS reactors, furnace, membrane modules), and a summary of key performance indicators. The study evaluated various operational configurations, including feed compression versus permeate vacuum modes and single- versus two-stage membrane arrangements. Detailed Techno-Economic Analysis (TEA) and Life Cycle Assessment (LCA) were conducted to calculate the Levelised Cost of Hydrogen (LCOH) and total specific CO2 emissions. Sensitivity analyses on membrane properties and energy prices were performed to benchmark the hybrid process against conventional hydrogen production technologies.

Results

Simulation results identified the optimal configuration as using 30% oxygen-enriched air produced via vacuum pumping, combined with post-combustion CO_2 capture via feed compression at 11 bar. This scenario achieved an LCOH of $1.78/kg H2, representing a 16% cost reduction compared to the membrane-based capture scenario without OEC ($2.14/kg H2). Total specific CO2 emissions were reduced to 4.9 kg CO2/kg H_2, with direct emissions limited to approximately 1 kg CO2/kg H2. While 40% oxygen enrichment minimized the individual capture cost, it resulted in a higher overall LCOH due to the significant increase in capital expenditures of air separation membranes. Additionally, sensitivity analysis indicated that improving air separation membrane selectivity could further lower the LCOH to approximately $1.51/kg H2.

Conclusions

The proposed hybrid membrane-based process presents a competitive and sustainable strategy for blue hydrogen production. The integration of moderate OEC (30%) significantly reduces furnace fuel consumption and flue gas volume, thereby optimizing downstream capture costs. These findings demonstrate that membrane-integrated systems offer a robust pathway for achieving the 2050 net-zero emission goals, particularly if future improvements in membrane selectivity are realized.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

PTL0381

High-Pressure Sorption-Enhanced Reverse Water Gas Shift Process: a Comparative Study of LTA and FAU Zeolites

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Abstract Category: Process Intensification - Process Intensification / TEA / LCA

Keywords: non-conventional reactor engineering, sorption enhanced reverse water gas shift, carbon monoxide

Abstract Body.

Introduction

Carbon monoxide (CO) is a key intermediate for the production of synthetic fuels (e-fuels), enabling more favorable downstream synthesis routes such as methanol and Fischer–Tropsch processes compared to direct CO_2 conversion. The reverse Water Gas Shift (rWGS) reaction is a promising upstream step for CO production, although it is thermodynamically limited, especially at low temperatures. Sorption Enhanced Reaction (SER) strategies, based on the in situ removal of water, offer an effective route to shift the reaction equilibrium toward CO formation and intensify the process. This work investigates the application of SER to the rWGS reaction under high-pressure conditions, focusing on the role of water-selective zeolite adsorbents and potassium-modified catalysts.

Materials and Methods

Experiments were carried out in a fixed-bed reactor operating at 20 atm, using a mechanical mixture of catalyst and water adsorbent. A commercial catalyst (MET-951, Meryt) was modified with potassium to inhibit methanol formation during CO2 hydrogenation. LTA-type zeolites were employed as water adsorbents due to their high adsorption capacity and strong affinity for H_2O. The experimental setup represents a laboratory-scale simulation of a CO2 hydrogenation process, allowing direct comparison between conventional rWGS operation and sorption-enhanced conditions.

Results

The application of the SER strategy led to a marked intensification of CO production compared to conventional rWGS experiments. The CO molar flow increased significantly when water was selectively removed from the reaction environment by the zeolite adsorbent. Integration of the CO production profiles showed that sorption-enhanced operation achieved up to a twofold increase in total CO production relative to the baseline conventional reaction. These results confirm the effectiveness of potassium promotion in suppressing methanol formation and highlight the strong impact of water adsorption on shifting the rWGS equilibrium.

Conclusions

High-pressure sorption-enhanced rWGS is an effective strategy for intensifying CO production from CO2 hydrogenation. The combination of potassium-modified catalysts and LTA-type zeolites enables substantial improvements in CO yield by overcoming thermodynamic

limitations through in situ water removal. This approach represents a promising route for improving the efficiency of upstream CO generation in e-fuel production chains.

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PTL0601

Techno-Economic Assessment of Hydrogen Production from Agricultural Residue-Derived Bio-Oil via Steam Reforming

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Abstract Category: Process Intensification - Process Intensification / TEA / LCA

Keywords: Agricultural residue, Pyrolysis, Steam reforming, Hydrogen, Aspen Plus®, Techno-economic assessment

Abstract Body.
Hydrogen production from renewable biomass presents a promising pathway toward sustainable energy systems; however, achieving large-scale technical and economic viability requires a systematic evaluation. This study assesses an integrated biomass-to-hydrogen process that combines the pyrolysis of agricultural residues with steam reforming of the resulting bio-oil, using an equilibrium-based Aspen Plus simulation. The novel process model incorporates pre-processing, pyrolysis, steam reforming, water-gas shift (WGS) reaction, and a hydrogen purification unit. Sensitivity analysis reveals that reformer temperature, steam-to-carbon (S/C) molar ratio, and WGS temperature are key parameters influencing hydrogen yield and syngas composition. Optimal operating conditions-steam reforming at 700 °C with an S/C ratio of 2-3, followed by WGS at 250 °C-maximize hydrogen production while minimizing residual hydrocarbons and carbon monoxide. A Techno-economic assessment across plant capacities of 100-100000 kg/h indicates that small-scale operations are economically unviable due to limited revenue. Economic performance improves significantly at larger capacities through economies of scale, reduced unit capital costs, and enhanced energy efficiency. At capacities ≥10000 kg/h, the process shows favorable economic indicators, including high internal rates of return, profitability indices above unity, and payback periods as low as 3 years under favorable market conditions. Economic uncertainty analysis reveals that commercial viability is strongly influenced by hydrogen and by-product prices, as well as the costs of agricultural residues. Heat-duty analysis highlights the potential for internal heat integration, further improving process efficiency. Overall, the study demonstrates that integrated pyrolysis of agricultural residues and steam reforming of residue-derived bio-oil is a technically feasible and economically viable pathway for large-scale renewable hydrogen production.

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DNR0398

Digital Twin Guided Reinforcement Learning for Stable and Energy-Efficient Operation of Complex Reactive Systems

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Abstract Category: Reactor Modeling and Design - Reactor Design - Novel Reactors

Keywords: Digitally augmented reactors; Gas-solid reactive systems; Digital twin modeling; Energy-efficient reactor operation

Abstract Body.
Complex industrial reactive systems are frequently characterized by strong nonlinear reaction-transport coupling, long residence times, partial observability, and delayed responses between operational actions and reaction outcomes. These features challenge conventional reactor operation and design methodologies, particularly when long-term stability and energy efficiency must be achieved simultaneously. This study aims to introduce a novel reactor operation paradigm in which operational intelligence is explicitly incorporated as part of reactor design, rather than treated solely as a downstream control problem.
A hybrid digital twin–guided reinforcement learning framework is proposed for the operation of complex reactive systems. The digital twin integrates a first-principles mechanistic reaction model with a data-driven residual correction module, preserving thermodynamic and mass–energy balance consistency while capturing unmodeled dynamics arising from multiphase interactions and operational disturbances. Using this digital twin as a surrogate environment, an offline reinforcement learning strategy is developed to learn long-horizon operational policies without unsafe online exploration. The methodology is demonstrated on an industrial-scale gas–solid reactive system characterized by multi-hour residence times and strong energy–reaction coupling.
Compared with conventional operation strategies, the learned operational policy reduces variability in key reaction performance indicators, suppresses large corrective operational actions, and achieves a sustained reduction in cumulative energy-intensive inputs over extended operating horizons. Rather than focusing on short-term setpoint tracking, the framework improves long-term operational consistency by accounting for delayed system responses and cumulative energy effects. These improvements are obtained without modifying the physical reactor configuration, highlighting the effectiveness of digitally enabled operation.
The proposed framework introduces the concept of digitally augmented reactors, where the effective behavior of a reactor is jointly determined by physical structure, reaction kinetics, and learned operational intelligence. In this sense, reactor operation becomes an additional degree of freedom in reactor design. Although demonstrated on a gas–solid reactive system, the methodology is broadly applicable to other complex reaction systems with long time constants and strong energy coupling, such as fixed-bed and moving-bed reactors. This work provides a new pathway for advancing reactor design and operation in energy-intensive chemical and process industries.

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PTL0048

Ultrasound enhanced continuous crystallization

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Abstract Category: Process Intensification - Process Intensification / TEA / LCA

Keywords: crystallization, ultrasound, microreactors

Abstract Body.
Continuous crystallization has the potential to replace traditional batch crystallization as one of the most important separation and purification processes especially in the pharmaceutical industry. The development and application of microfluidic technology has enabled on-demand synthesis of pharmaceutical products using miniaturized continuous platforms. To achieve end-to-end local drug production, the integration of continuous crystallization in small scale reactors is desirable. However, major drawbacks which need to be overcome are i) the susceptibility of these small devices to clog in the presence of solid particles, and ii) to achieve control over the different crystallization phenomena. Ultrasound has emerged as a promising intensification technique, offering enhanced nucleation and improved crystal properties. This presentation will highlight the role of ultrasound in continuous crystallization processes and assess its potential for process intensification.
We investigated ultrasound-assisted crystallization in continuous tubular crystallizer setups. Experiments were conducted using model systems under varying ultrasonic frequencies, power densities, and reactor geometries. Furthermore, we studied both cooling and anti-solvent crystallization. To accompany the experiments, a population balance-based model was developed that captures ultrasound enhanced mixing and the increased nucleation rates. This modeling framework was then extended with CFD and acoustic modeling to predict scale-up performance.
Ultrasound application significantly accelerated nucleation and reduced induction times compared to silent conditions. Furthermore, sonication in continuous cooling crystallization improved particle size control and reduced agglomeration, enabling narrower size distributions. The ultrasound assisted anti-solvent crystallization of o-aminobenzoic acid resulted in enhanced polymorphic control and increased yield. The population balance and CFD modeling of this system revealed the importance of turbulent micromixing induced by cavitation for maintaining small crystal sizes and high productivity. Advancing to hydrothermal interzeolite conversion reveals that ultrasound promotes rapid phase transformation and uniform crystal morphology by intensifying local mass transfer. Across all studied systems, ultrasound integration resulted in higher productivity and improved reproducibility without compromising crystal quality.
Ultrasound integration in continuous crystallization offers significant benefits across diverse crystallization processes and material classes, including organic compounds (e.g., APIs) and inorganic frameworks (e.g., zeolites). It enables faster nucleation, improved polymorph control, and mitigation of clogging. Mechanistic evidence suggests that cavitation-driven micro-mixing and localized supersaturation are key contributors to these benefits. These findings confirm ultrasound as a broadly applicable intensification strategy for continuous crystallization.

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PTL0086

Early Detection of Thermal Runaway in Chemical Reactors via Electrical Conductivity Monitoring

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Abstract Category: Process Intensification - Process Intensification / TEA / LCA

Keywords: Early Warning Detection System (EWDS), Thermal runaway, Exothermic reactions, Reactor safety and control.

Abstract Body.
Purpose:
In the context of energy transition and industrial decarbonization, the chemical industry is adopting innovative reaction systems and intensified processes. While these technologies improve efficiency and sustainability, their limited operational maturity can introduce hazards, particularly in highly exothermic reactions prone to thermal runaway. Early Warning Detection Systems (EWDS) provide a critical layer of protection when reliable reactor models are unavailable, or system predictability is compromised. Conventional EWDS, based on temperature monitoring, are limited by sensor delays and spatial dependence, reducing their effectiveness in detecting rapid or localized thermal excursions. This work aims to propose and experimentally validate an alternative EWDS approach based on electrical conductivity monitoring, offering faster and more sensitive detection of runaway onset, using a refined version of the Strozzi and Zaldivar criterion.
Methods:
The study uses the acid-catalyzed esterification of acetic anhydride with methanol as a representative highly exothermic reaction. Experiments were conducted in bench-scale stirred reactors equipped with temperature, optical, and conductivity sensors. Comparative analyses included kinetic evaluation and model-based stability assessments to benchmark the performance of the conductivity-based EWDS against conventional temperature-based detection.
Results:
Experimental results show that conductivity variations consistently precede temperature signals, enabling earlier identification of runaway onset. The conductivity-based EWDS detected instabilities with an error of approximately 1 °C relative to analytical benchmarks, compared to about 3 °C for conventional temperature-based detection. Additionally, conductivity signals anticipated the temperature maximum by over 250 s, providing a substantially extended warning window for corrective action. Figure 1 compares the divergence trends determined analytically and using temperature- and electrical conductivity-based data.
Conclusions:

The proposed conductivity-based EWDS significantly improves reactor monitoring by enhancing sensitivity and response time. This approach offers a robust tool for the safe operation and scale-up of innovative reaction systems, supporting the reliable deployment of advanced and sustainable chemical processes.

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PTL0258

High-Gravity Vortex Drying for Intensified Secondary Drying of Pharmaceutical Powders

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Abstract Category: Process Intensification - Process Intensification / TEA / LCA

Keywords: process intensification, rotating vortex dryer, high-gravity fluidization, secondary pharmaceutical drying

Abstract Body.
Purpose. Secondary drying is a critical step in the pharmaceutical manufacturing of amorphous solid dispersions (ASDs). Residual solvents remaining after spray drying (typically 1-10 wt%) must be further reduced to meet product specifications. Conventional secondary drying technologies, such as tray or vacuum ovens, often require long residence times, exhibit non-uniform temperature profiles, and consume significant energy. Such limitations are particularly problematic for thermally and mechanically sensitive ASDs [1]. To address this, we investigate the use of an intensified rotating vortex dryer, enabling gentle yet rapid drying of pharmaceutical powders. The rotating vortex dryer is a high-gravity (HiGee) unit where the centrifugal force field exceeds gravitational acceleration, designed to enhance gas–solid interactions and achieve process intensification [2], herein applied to drying for the first time.

Methods. The drying performance of the vortex dryer is evaluated using a celecoxib:PVP K30 (1:2 w/w) ASD as a representative case. The drying unit consists of a mechanically rotating cylindrical chamber equipped with a tangential gas distributor, generating a strong vortex flow and a HiGee centrifugal field. In the HiGee field, gas drag balances centrifugal forces rather than the drag-gravity balance in conventional fluidized beds. Momentum transfer from gas to powder results in stable fluidization under HiGee conditions, thus intensifying gas–solid mass and heat transfer while achieving high throughput in a compact unit. Powder fluidization behavior is visualized using high-speed imaging, while drying kinetics are monitored via online gas-phase humidity measurements. Residual moisture content is determined offline and compared with a conventional vacuum tray dryer operated as a benchmark.

Results. Preliminary experiments demonstrate stable fluidization of the pharmaceutical powder with no observable particle attrition, as confirmed by SEM analysis. Online humidity measurements indicate rapid water removal, and offline analysis shows that the vortex dryer achieves drying rates up to 1-2 orders of magnitude higher than those of the vacuum tray dryer for similar overall drying extent.

Conclusions. The rotating vortex dryer enables substantial process intensification at near-ambient temperatures and with low blower energy per unit of water removed. These findings highlight the potential of vortex technology as a compact, energy-efficient secondary drying

solution for sensitive pharmaceutical solids. Ongoing studies focus on organic solvent removal (methanol and dichloromethane), physical stability of the ASD, and systematic evaluation of operating parameters.

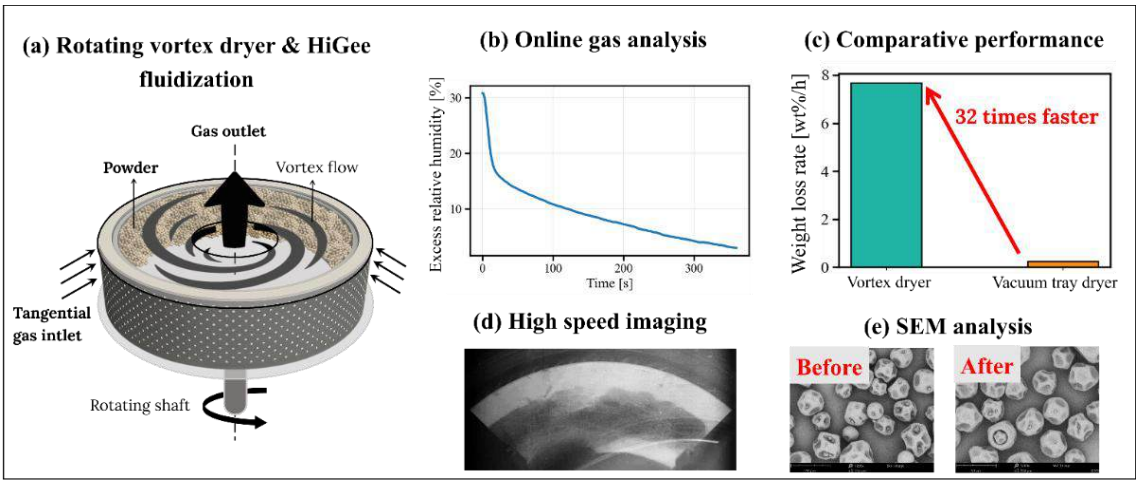

Fig. 1. (a) Schematic representation of the vortex dryer, (b) online relative humidity profile during drying, (c) comparative drying performance, (d) HiGee fluidization image, (e) SEM analysis before and after vortex drying.

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2026 / SEOUL, KOREA

PTL0486

Solid-liquid mass transfer characteristics of porous corn straw particles in the stirred tank

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Abstract Category: Process Intensification - Process Intensification / TEA / LCA

Keywords: Mass transfer coefficient, Porous particle, Dissolution method, Solid-liquid mixing

Abstract Body.

Purpose:

Corn straw (CS) is a major anaerobic digestion feedstock in China, yet its low density and hydrophobicity cause floating and scum formation, reducing efficiency and stability[1]. Additionally, CS has a porous structure formed by the cross-linking of cellulose, hemicellulose, and lignin, which has the capacity for liquid penetration[2]. During the mixing, the liquid penetrates the particle, which can be regarded as a liquid-solid mass transfer process. As a result, the density of CS particles will increase, thereby influencing the drawdown and suspension behavior in the stirred tank. Yet current research lacks effective methods for evaluating solid-liquid mass transfer rates of floating CS particles, especially in non-Newtonian systems. Accurate mass transfer modeling is essential for optimizing reactor design and operation, but traditional models are often limited to specific experimental conditions, reducing their robustness in complex scenarios. Machine learning offers a promising alternative with greater robustness, accuracy, and versatility than conventional models, yet its black-box nature makes balancing performance and interpretability challenging.

Methods:

This study developed a measurement technique for determining the solid-liquid mass transfer coefficient of porous CS particles in the stirred tank by utilizing the dynamic changes in electrical conductivity during salt particle dissolution, based on the dissolution method. Simultaneously, the effects of particle size, solid loading, liquid viscosity, impeller type, off-bottom distance, and rotational speed on the solid-liquid mass transfer coefficient are investigated. At last, the mass transfer of CS particles in the stirred tank was modelled by a hybrid model using symbolic regression (SR) and machine learning.

Results:

The results showed that the natural sedimentation behavior of straw particles was closely related to the liquid viscosity, particle size, and solid loading. Besides, small particles had a higher mass transfer rate due to their larger specific surface area. Increasing the rotational speed and off-bottom distance could improve the wetting rate and mass transfer rate of the particles, but higher solid loading would prolong the wetting time. Orthogonal experiment results indicated liquid viscosity was the most significant factor affecting mass transfer rate, followed by solid loading and rotational speed. The hybrid model was better than the SR model, achieving an R2 of 0.734, and overall exhibited superior predictive capability.

Conclusions:

These findings provide practical strategies for optimizing agitation systems not only to improve

solid-liquid mixing but to enhance mass transfer in anaerobic digesters treating lignocellulosic biomass.

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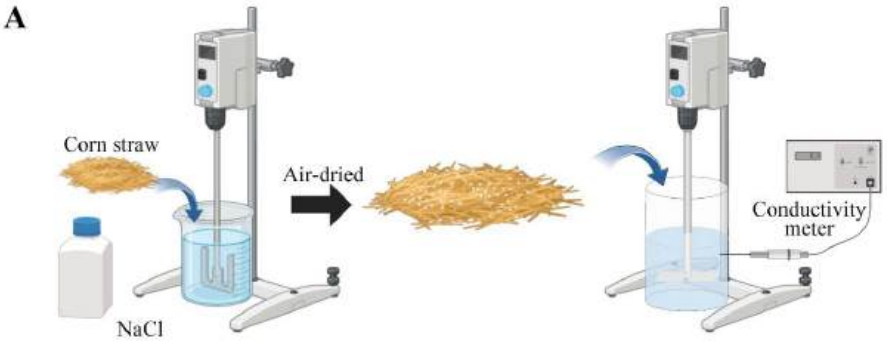
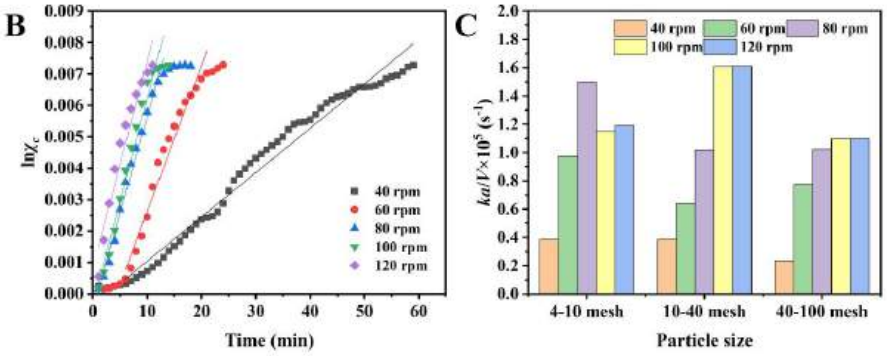
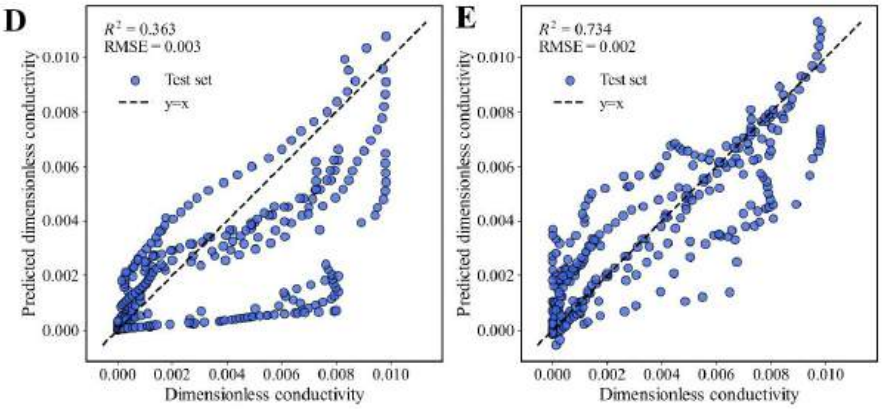
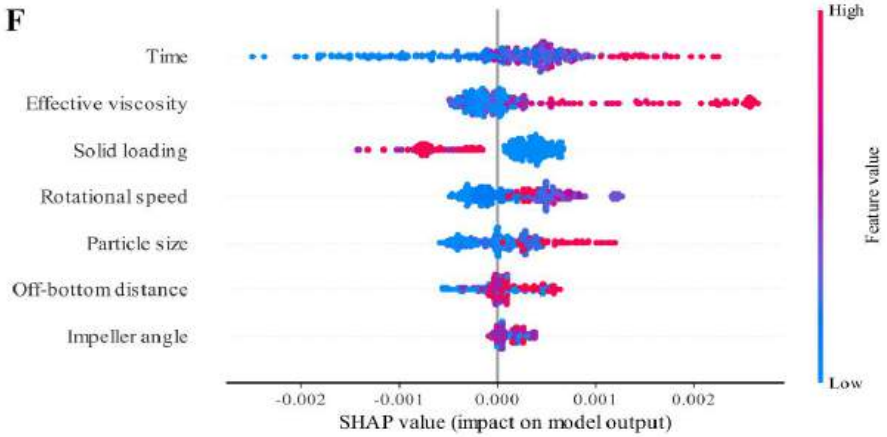






Prediction performance on test set of (A) symbolic model and (B) hybrid model



ISCRE29 & APCRE11
2026 / SEOUL, KOREA

PTL0519

Autonomous Chemical Process Design and Simulation Using LLM Agents: An Integrated Design-to-Simulation Framework

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Abstract Category: Process Intensification - Process Intensification / TEA / LCA

Keywords: LLM, Process Design, Process Simulation, Chemical Flowsheet Design, Aspen Plus

Abstract Body.
With recent advances in large language models (LLMs), the way research is conducted is being revolutionized. From generating code to designing experiments, LLMs have shown strong capabilities not only in human-like conversation but also in supporting research and development tasks. These developments naturally raise questions about the limits of LLM utilization in different areas of scientific research. In this study, we aim to explore the potential for automating chemical process design using LLM-based agents, with the long-term goal of enabling rapid generation and evaluation of multiple process configurations for process intensification and design exploration.

By leveraging LLMs' ability to follow natural language instructions and their inherent domain knowledge, we develop a multi-agent architecture for autonomous process design and simulation setup. The proposed system decomposes the overall workflow into clear and structured steps that can be addressed sequentially by specialized agents, each responsible for a specific stage of the design-to-simulation process. A commercial process simulator is employed to generate and evaluate simulation models.

The proposed framework is evaluated through case studies in which LLM-based agents generate process designs and corresponding simulation models. The results show that, with carefully curated workflows and well-defined agent assignments, the system is able to produce simulation-ready process flowsheets and reduce the level of manual intervention required in model development.

These findings demonstrate that LLM-based multi-agent systems can serve as practical tools for bridging conceptual process design and process simulation. By enabling autonomous generation of multiple simulation models, the proposed framework provides a foundation for future studies on automated process optimization and intensification. While the performance remains dependent on problem characteristics, the results highlight the potential of LLM-driven automation for accelerating process design workflows.

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PTL0644

Breaking the ASF Constraint: Catalytic Surface Resonance as a Route to Controlled1 Chain-length Selectivity

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Abstract Category: Process Intensification - Process Intensification / TEA / LCA

Keywords: Catalytic resonance, ASF distribution, Fischer Tropsch, nonlinear frequency response

Abstract Body.
The Anderson–Schulz–Flory (ASF) distribution provides a statistical description of Fischer–Tropsch (FT) product selectivity under steady-state conditions. While optimization of FT product selectivity through control of the ASF chain-growth parameter (α) has been widely studied, this approach inherently relies on steady-state assumptions. In this work, we introduce the first application of the nonlinear frequency response (NFR) framework to catalytic surface resonance, to analyze and predict how periodic modulation of surface kinetic parameters reshapes FT product chain-length selectivity beyond steady-state ASF descriptions. A mechanistic chain-growth kinetic model, formulated in a continuous stirred-tank reactor (CSTR), is employed, in which a periodic modulation of the propagation rate parameter kp is imposed to represent nominal catalytic surface resonance operation. The resulting nonlinear periodic reactor response is analyzed using the nonlinear frequency response method, which yields an explicit expression for the time-averaged shift in the FT product distribution as a function of forcing amplitude and modulation frequency. Steady-state analysis confirms an optimum jet-fuel-range selectivity (C9−16) at α = 0.85. Under dynamic operation, the FT product distribution departs systematically from steady-state ASF predictions and exhibits a pronounced resonance band between 4 and 15 Hz, within which the C9−16 carbon selectivity increases sharply and reaches a maximum near 14 Hz. Parametric analysis further reveals that the optimal forcing frequency depends on intrinsic kinetic timescales, with higher propagation rates shifting the resonance to higher frequencies while reducing the attainable enhancement. Compared with steady-state operation at the optimal static α, catalytic resonance enables time-averaged FT product distributions that not only achieve higher selectivity toward the desired jet-fuel fraction, but also avoid undesirable increases in light hydrocarbons, demonstrating the potential of dynamic catalysis to extend selectivity control beyond the limits implied by steady-state ASF descriptions.

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2026 / SEOUL, KOREA

PTL0250

Geometry-Driven Process Intensification of Continuous Biodiesel Synthesis in 3D-Printed Meandering Milli-Reactors

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Abstract Category: Process Intensification - Process Intensification / TEA / LCA

Keywords: Biodiesel; Continuous processing; Milli-reactor; Meandering channel; 3D printing; DoE; GLM

Abstract Body.

Introduction. Continuous biodiesel synthesis in micro/milli-reactors offers intensified heat/mass transfer, safer operation, and compact footprint compared with batch systems [1–2]. Meandering milli-channels can further enhance mixing via curvature-induced secondary flows, yet combined optimization of junction geometry and operating variables for continuous biodiesel production remains limited. This work uses geometry screening + DoE-GLM optimization to maximize biodiesel yield and triglyceride (TG) conversion.

Methods. Alkali-catalyzed transesterification of palm oil with methanol was performed in 3D-printed meandering milli-reactors (2 mm ID, 1 m length) under steady continuous flow. T- and Y-inlet configurations with 30°, 45°, and 60° inlet angles and different meandering layouts were tested. Biodiesel yield was quantified by HPLC (FAME content after purification). A multi-factor DoE-GLM model evaluated main/interaction effects of temperature, KOH concentration, MTO ratio, total flow rate, and channel design, and identified optimal conditions.

Results and discussion. The GLM model revealed that KOH concentration was the most influential factor governing biodiesel yield (LogWorth = 25.446), with yield increasing strongly as catalyst concentration increased (Fig. 1a). Among the reactor configurations, channel design emerged as the next dominant contributor to performance, confirming that geometry-driven mixing significantly impacts continuous transesterification outcomes (Fig. 1b). Several statistically significant interaction terms such as MTO×Total Flow Rate, Temperature×Flow Rate, Channel Type×Flow Rate, and Channel Type×KOH concentration further indicate that the intensification benefits are jointly controlled by hydrodynamics and inlet/channel architecture. Based on the GLM predictions, the optimum operating point was identified as 51 °C, 6 wt% KOH, MTO = 6:1, and total flow rate = 1 mL min^{-1}, using the SSY60 meandering reactor (Fig. 1c). Experimental validation under these conditions confirmed high biodiesel yield and improved triglyceride (TG) conversion trends, while detailed effect magnitudes and geometry-specific performance comparisons will be presented in the full manuscript.

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PTL0311

Scale-Up Performance of Electrified Steam and Plasma Cracking of Naphtha for Ethylene Production

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Abstract Category: Process Intensification - Process Intensification / TEA / LCA
Keywords: Electrification, Naphtha Cracking, Decarbonization, Techno-Economic Analysis, Life Cycle Assessment

Abstract Body.
Electrification of endothermic cracking reactors offers a promising route to decouple ethylene production from fossil fuel combustion. This study compares electrified steam cracking and plasma arc cracking of naphtha from an industrial scale-up perspective, focusing on process design, production cost, and greenhouse gas emissions. Industrial-scale reactor and process models were developed for both pathways, with the plasma arc cracking configuration informed by pilot-scale experimental data. Industrial-scale reactor models were developed for both pathways, with the plasma cracking configuration informed by pilot-scale experimental data. At the reactor level, plasma arc cracking enhances C2 hydrocarbon selectivity to 26.09%, compared with 23.50% for electrified steam cracking. At the overall plant level, this translates into a higher ethylene yield of 0.42 tonne ethylene per tonne naphtha for plasma cracking, relative to 0.28 tonne ethylene per tonne naphtha for electrified steam cracking. However, this intensified reaction environment is accompanied by a substantially higher specific electricity consumption, reaching 43.47 MW per tonne ethylene for the plasma cracking plant compared with 10.35 MW per tonne ethylene for the electrified steam cracking plant. To assess implications beyond the reactor scale, an integrated techno-economic and life cycle assessment framework was applied, linking cracking energy demand to production cost and greenhouse gas emissions under multiple electricity supply scenarios and methane by-product utilization routes. System-level analysis shows that plasma cracking combined with methane utilization, carbon capture, and renewable electricity can achieve low greenhouse gas emissions, but its high electricity intensity leads to elevated production costs that limit near-term economic feasibility. In contrast, electrified steam cracking coupled with methane utilization and renewable electricity provides a more balanced pathway, maintaining favorable reaction performance while improving system efficiency and reducing emissions. These results highlight a fundamental trade-off in electrified naphtha cracking: enhanced reaction selectivity achieved through process intensification imposes significant energy penalties at industrial scale. The study highlights the importance of reactor-to-system integration when evaluating electrification strategies for large-scale ethylene production.

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PTL0356

Process Intensification using Anisotropic POCS – experimental and numerical assessment

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Abstract Category: Process Intensification - Process Intensification / TEA / LCA

Keywords: Process intensification, Structured catalyst supports, POCS, Lattice materials, Catalytic reactors

Abstract Body.

Introduction. Periodic Open Cellular Structures (POCS) have been proposed as advanced catalyst carriers for process intensification of catalytic reactors. POCS offer an improved trade-off between mass transfer and pressure drop, a key aspect in e.g. aftertreatment devices and other applications of environmental catalysis. Using reactive CFD simulations, we demonstrate that by modifying the diamond cell topology, specifically by tuning the strut–flow angle α, it is possible to enhance the support performances even outperforming the state-of-the-art honeycomb monoliths1.

Methods.

An experimental study was here conducted on 4 POCS (diamond cell) with identical porosity and strut diameter but different strut–flow angles α, produced by SLA 3D printing and washcoated with 3%Pd/CeO_2. External mass transfer coefficients were measured using rich-H2 oxidation as probe reaction2 since it is active enough to be operated under mass transfer-controlled conditions at temperatures below the resin HDT. Pressure drops were measured feeding air in a separate setup at ambient temperature. One-to-one CFD simulations of the printed samples were also performed using the catalyticFoam framework3 to include the system non-idealities. To interpret the results, the Merit Index4 (MI) is used.

$$MI = \frac{-\ln(1 - X_{O_2})}{\frac{\Delta p}{\rho u^2}}$$

Results and discussion. Fig. 1(a) shows the modified POCS geometry along with the 3D printed washcoated structure. Fig. 1(b) shows the measured merit indexes (circles) and the corresponding CFD simulations of structures with different α, being α = 54.7° the standard diamond geometry. An excellent agreement is reached between experimental and simulated data. Moreover, the modified diamond lattice with small α offers up to 1.5× the mass transfer coefficients of advanced honeycomb structures (HC OFA=0.85) at the same pressure drop, demonstrating its strong potential as an enhanced structured substrate for process intensification.

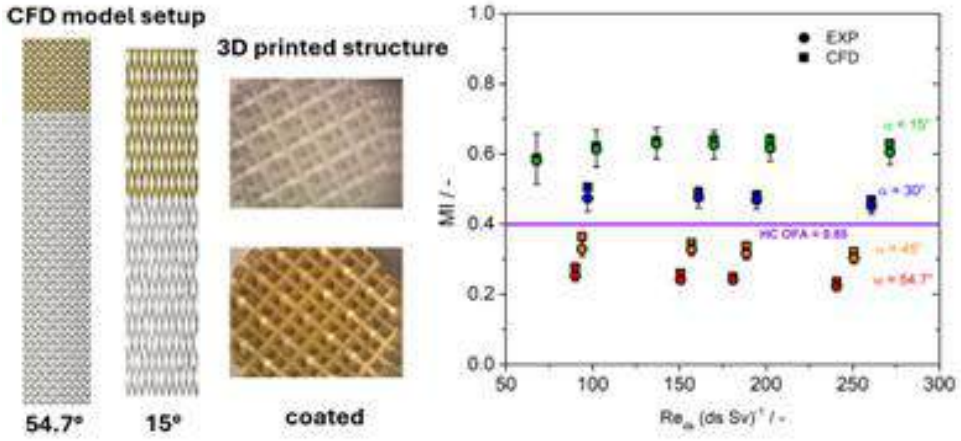

Figure 1 – Measured and simulated Merit Indexes for different POCS geometries

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PTL0401

Thermally stable TR-PBO hollow fiber membrane reactor for process intensification of catalytic reactions

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: Membrane reactor, process intensification, in-situ water removal, equilibrium shift

Abstract Body.

Water generated in situ during catalytic reactions often undermines conversion, selectivity, and catalyst stability. Thermodynamically, water accumulation constrains equilibrium, reducing attainable conversion. Water competes with reactants for active sites, causing deactivation via site blocking and catalyst restructuring. Moreover, water promotes undesired side reactions; for example, it facilitates the Water–Gas Shift (WGS) reaction during Fischer–Tropsch synthesis, increasing CO2 formation, and it accelerates reduction of PdO to Pd during methane combustion, leading to activity loss. Conventional mitigation strategies, including adsorbents and inorganic membranes, can remove water but require regeneration, and their selectivity can deteriorate at elevated temperatures. To address these limitations, we develop robust polymeric membranes for selective water removal and evaluate them in membrane-reactor configurations under reactive gas mixtures. We investigate thermally rearranged polybenzoxazole (TR-PBO) hollow-fiber membranes that maintain stability up to 440 ℃ while exhibiting high water perm-selectivity. Integrating the membrane enables reaction and separation in a single unit, avoids cyclic regeneration steps, and simplifies downstream purification. Incorporating TR-PBO membranes into catalytic reactors provides three advantages: (i) continuous water extraction shifts the equilibrium of the reverse WGS reaction toward CO, increasing CO2 conversion; (ii) reduced water activity mitigates water-related deactivation of Pd catalysts; and (iii) suppression of water-mediated pathways improves olefin selectivity. Overall, polymeric membrane reactors provide a strategy to relieve equilibrium constraints, protect catalysts from water-driven deactivation, and suppress water-mediated side reactions. By combining high-temperature stability with durable perm-selectivity and pressure tolerance, robust polymeric membranes enable process intensification, higher conversion, and improved selectivity, supporting more sustainable catalytic chemistry and more carbon-efficient CO2 utilization.

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PTL0706

Radio-Frequency–Driven Propane Dehydrogenation over Pt-based Catalysts

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Abstract Category: Process Intensification - Process Intensification / TEA / LCA

Keywords: Propane dehydrogenation, PtSn catalysts, Electrified catalysis, Radio-frequency

Abstract Body.
This work highlights the radio frequency heating for catalytic propane dehydrogenation using Pt-based catalyst in a parallel plate applicator. Propane dehydrogenation (PDH) is a key industrial reaction for propylene production but is highly energy-intensive due to its endothermic nature and reliance on conventional furnace heating. Electrified heating strategies offer a potential pathway to improve energy efficiency and enable reduction of reactor volume. We use radio-frequency (RF) heating as an alternative energy input for PDH reaction using Sn-promoted Pt/Al2O3 catalysts supported on structured monolith reactors. Reaction performance under RF heating was compared directly to conventional furnace heating at identical operating conditions (500 °C, C3H8/H2/Ar feed). RF heating successfully achieved and sustained PDH-relevant temperatures and enabled stable reactor operation using PtSn catalysts. Relative to unpromoted Pt, Sn addition significantly increased propylene selectivity (>90%) and suppressed methane formation by more than a factor of five. RF-heated experiments exhibited propane conversions and propylene yields comparable to conventional heating, with higher initial activity observed under RF conditions. A strong correlation was identified between catalyst electrical conductance and RF heating efficiency, with more conductive formulations requiring higher RF power to reach the same operating temperature. Finite element method (FEM) simulations were conducted to demonstrate RF heating of catalyst-coated monoliths in a parallel plate applicator, which showed good qualitative agreement with experimental observations. A scale-up analysis was also performed by increasing the monolith diameter, revealing an optimal size that maximizes heating efficiency. These results demonstrate that RF heating can effectively drive PDH using industrially relevant catalysts in structured reactors while revealing a critical coupling between catalyst material properties and reactor heating behavior. The findings provide new reaction-engineering insight into RF-driven catalytic systems and highlight the importance of material property optimization for electrically heated heterogeneous reactors.

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PTL0707

Methanol Synthesis in a Sorption Enhanced Fluidized Bed Reactor with Continuous Sorbent Feeding (SEFBR+CSF)

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Abstract Category: Process Intensification - Process Intensification / TEA / LCA

Keywords: non-conventional reactor engineering, sorption enhanced methanol synthesis, selective segregation

Abstract Body.
Sorption Enhanced Methanol Synthesis (SEMS) is a process-intensification strategy that presents a major drawback as it typically operates under discontinuous conditions. This limitation arises because the process relies on the selective adsorption of a reaction co-product by a solid sorbent to shift the kinetics and thermodynamic equilibrium, thereby increasing the single-pass conversion. However, once the sorbent becomes saturated, the intensification effect ceases. The process configuration recently patented by our group proposes a fluidized-bed reactor with continuous solid inlet and outlet streams, which are used for the continuous flow of the sorbent particles. By exploiting density and size differences between sorbent and catalyst, a segregated fluidized bed can be achieved in which the catalyst remains in the jetsam phase, while the sorbent behaves as flotsam and is continuously removed from the reactor. In this way, regenerated sorbent is continuously supplied and saturated sorbent is withdrawn, enabling truly continuous operation of the intensification strategy. An additional advantage of this approach is the reduction of thermal stress on the catalyst associated with in situ regeneration, which is usually a major cause of accelerated catalyst deactivation.

The reactor proposed for this process uses a commercial copper–zinc–alumina (CZA) catalyst (BASF K3-110) and a sorbent, in this case a 3A zeolite.The zeolite is introduced through the lower lateral inlet and withdrawn from the reactor through the upper lateral outlet. Achieving this configuration requires proper solid segregation, ensuring that the catalyst remains in the lower section of the reactor to maintain a constant catalyst inventory. To this end, particle sizes and gas velocities (ug) were carefully adjusted. The operating pressure was 20 atm and temperature was varied between 220-280 ºC.

The solids segregation was characterized verifying that low gas velocities (i.e., low ug/umf ratios) favor effective segregation and minimize catalyst loss from the process. Under these conditions, the system achieved effective process intensification under continuous operating regime.

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PTL5686

Electrified Sorption-intensified Ammonia Production Process over Serial Ruthenium Catalysis / Zeolite-supported Halide Capture

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Abstract Category: Process Intensification - Process Intensification / TEA / LCA

Keywords: electrified catalysis, ammonia synthesis, magnetic heating, sorption intensification, ruthenium catalysts, halide-modified zeolites

Abstract Body.

Purpose: The transition to renewable energy systems requires flexible, carbon-neutral pathways for chemical fuel synthesis. Hydrogen is increasingly regarded as a key energy vector, yet its storage and transport remain technological challenges. Ammonia, with its high hydrogen density and established global logistics, is a compelling hydrogen carrier – provided its synthesis can be decarbonised and decentralised. This work aims to develop an electrified, sorption-intensified ammonia production route capable of operating beyond centralised Haber–Bosch facilities. Specifically, we investigate the in
tegration of magnetically heated ruthenium catalysis with halide-assisted sorption using tailored zeolite materials, enabling efficient single-pass ammonia yields under renewable-compatible, intermittently powered conditions.

Methods: The process couples inductively driven magnetic heating of Ru-based catalysts with sequential halide-promoted sorption stages designed to selectively capture and release ammonia. Magnetic nanoparticles serve as both heat mediators and structural supports, allowing rapid, localised thermal control without external furnaces. Zeolite frameworks modified with halide species provide enhanced ammonia affinity, intensifying conversion through continuous product removal. The catalyst–sorbent materials were comprehensively characterised using NH_3-TPD to quantify acidity and sorption performance, STEM-EDX for nanoscale elemental mapping, VSM for magnetic responsiveness, and complementary methods assessing morphology, stability, and thermal behaviour. Process metrics were evaluated under varied magnetic field intensities and dynamic operating regimes and sorbent configurations to quantify ammonia production rates and system stability.

Results: The electrified catalytic system achieved over 1% ammonia yield in a single pass even without the sorption step, confirming the high intrinsic activity of the magnetically heated Ru catalyst. Incorporation of the halide-modified sorbent enabled semi-stable operation under repeated sorption–desorption cycles, while maintaining effective magnetic heating behaviour. The combined catalytic–sorptive configuration exhibited sustained performance without observable degradation in heating efficiency and some loss of sorbent capacity. These findings validate the compatibility of magnetic induction heating with integrated solid sorption, and highlight the role of halide species in promoting ammonia uptake under reaction conditions.

Conclusions: This study demonstrates a viable pathway for decentralised, electrified ammonia production, leveraging renewable electricity for direct catalytic heating and product intensification via sorption. The integration of magnetically heated Ru catalysis with halide-enhanced zeolite sorbents enables significant single-pass ammonia conversions and stable process operation. The concept provides a promising foundation for modular, flexible ammonia synthesis units aligned with distributed renewable energy generation.

Oral Presentation

Heterogeneous/Homogeneous Catalysis

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HTT0173

Thermocatalytic CO2 conversion into oxygenates on Febased catalyst under high pressure conditions

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: CO2 hydrogenation, High-pressure catalysis, Iron catalysts

Abstract Body.

Reaction pressure is a powerful but underutilized engineering parameter for tuning both catalyst structure and product selectivity in CO2 hydrogenation. Dense-phase CO2 at elevated pressure can strongly modify gas-phase nonideality (fugacity), transport properties, and interfacial solvation, thereby reshaping catalytic reaction networks. Here we show that reaction pressure acts as a decisive “engineering handle” to switch both the working phase and product selectivity of a potassium-promoted iron catalyst (K–Fe2O3) during CO2 hydrogenation. Catalytic tests were performed at 330 °C over 3.5–10.0 MPa under identical feed composition and space velocity (H2/CO2 = 3; GHSV = 6000 mL gcat-1 h-1; 100 h). At moderate pressure (3.5 MPa), the catalyst exhibited classical CO2–FTS behavior with high CO2 conversion and extensive hydrocarbon chain growth. In contrast, increasing pressure to ≥ 7.0 MPa suppressed C5+ hydrocarbons and substantially enriched oxygenates, reaching ~23% oxygenate selectivity at 10.0 MPa.

To link dense-phase operation to catalyst restructuring, spent catalysts were analyzed by XRD and 57Fe Mössbauer spectroscopy. Low-to-moderate pressures yield the canonical Fe3O4/Fe5C2 assemblage associated with RWGS and chain growth, whereas high pressure induces the emergence and eventual dominance of FeCO3. The progressive enrichment of FeCO3 from 7.0 to 10.0 MPa correlates directly with the observed shift from hydrocarbon-rich to oxygenate-rich products. Operando DRIFTS reveals systematic differences in carbonate-/hydroxyl-related surface features between mild- and highpressure– derived catalysts, supporting a mechanistic picture in which dense-phase CO2 (high CO2 fugacity, together with in situ water) promotes surface carbonation and stabilizes COOcontaining intermediates, thereby redirecting the catalytic cycle toward oxygenateterminated pathways.

Overall, this work provides a proof-of-concept that dense phase CO2 operation can drive a pressure-induced phase/selectivity switch in iron catalysts without changing formulation, offering a mechanistic basis for designing supercritical CO2 enabled CO2 hydrogenation routes to oxygenate.

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CO2 hydrogenation to methanol on ZrO2-supported Cu and Cu-In2O3: comparative catalysis and in-situ IR

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: CO2 hydrogenation, Methanol synthesis, In-Cu catalysis, ZrO2, DRIFTS, FTIR

Abstract Body.

Introduction. CO2 emissions are a major driver of global warming, making CO2 capture and valorization increasingly relevant. Among the available routes, CO2 hydrogenation to methanol is attractive, although the reaction network also forms by-products such as CO, methane, and DME. The industrial Cu/ZnO/Al2O3 catalyst used for syngas-to-methanol (CO2:CO:H2) provides good conversion but also promotes RWGS, thus limiting selectivity [1]. Therefore, alternative catalytic systems are being pursued. Here, In2O3-based catalysts and Cu supported on ZrO2 are investigated, since In2O3 can achieve higher methanol selectivities [2].

Methods. Cu and/or In2O3 were deposited on ZrO2 by deposition–precipitation via an oxalate gel route starting from the corresponding metal nitrates [3,4]. The catalysts (Cu/ZrO2, In2O3/ZrO2, and Cu-In2O3/ZrO2) were characterized by N2 physisorption (77 K), H2-TPR, CO2-TPD, XRD, XPS, and STEM-EDX. Catalytic tests were performed in a fixedbed reactor at 23 bar and 200–300 °C using H2:CO2:N2 = 15:5:3, followed by postreaction characterization. Transmission FTIR and DRIFTS (static and flowing) were additionally carried out on the best-performing sample to investigate surface chemistry, active sites, and reaction pathways.

Results and discussion. Catalytic tests confirmed that Cu enhances In2O3 activity, increasing methanol yield [3], likely aided by InCu alloy formation that promotes H2 spillover. However, Cu-In2O3/ZrO2 was not competitive with Cu/ZrO2, which showed higher TOF, consistent with stronger Cu–ZrO2 synergy and higher Cu dispersion. In Cu-In2O3/ZrO2, Cu is dispersed between In2O3 and ZrO2; only a smaller fraction resides on ZrO2, while a substantial portion is also present on/with In2O3. Consequently, Cu primarily plays a promotional role, and the catalytic behavior resembles that of an In2O3/ZrO2 system rather than a Cu/ZrO2 catalyst. Cu/ZrO2 also produced DME (the methanol dehydration product), which can increase CO2 conversion. The performances are shown in Figure 1. Static and flow spectroscopy indicated a formate-to-methoxy-to-methanol pathway; formates may originate from direct CO2 hydrogenation or from carbonate hydrogenation. Finally, a dynamic formate-methoxy interconversion was observed, and methanol feeding led to formaldehyde and DME production.

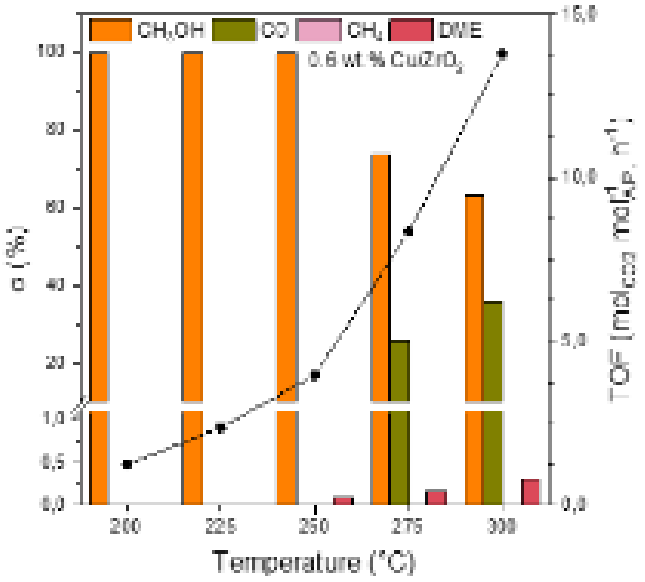

Figure 1 – Product distribution and turnover frequencies (TOF) for 0.6 wt.% Cu/ZrO2.

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HTT0293

Effects of Zn and Mn promoter over mesoporous cobalt-based catalyst for CO2 hydrogenation to hydrocarbons

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: CO2 hydrogenation, mesoporous structures, Fischer -Tropsch synthesis (FTS)

Abstract Body.

Introduction: CO2 hydrogenation reaction via a reverse water-gas shift (RWGS) reaction mainly produces CO and HØ O, and various hydrocarbons can be formed by Fischer– Tropsch synthesis (FTS) reaction including wide-range hydrocarbons. Co-based catalysts exhibit higher hydrocarbon selectivity with smaller CO byproduct at low temperatures. Therefore, ordered mesopore-structures can provide high surface area and low catalyst deactivation. Since the Co-based catalysts enhance methanation activity at high temperatures, Mn metal oxide promoter having abundant oxygen vacant sites are applied to enhance hydrocarbon productivity. Since the roles of Zn promoter over the Co-based FTS catalyst have not been well investigated, the ordered mesoporous Co3O4–MnO2–ZnO metal oxides were investigated to verify the roles of Mn and Zn metal oxide promoters with their different reduction behaviors, metal dispersion and oxygen vacant sites to catalytic activity and product distribution.

Methods: Highly ordered mesoporous mixed metal oxides catalysts were prepared by using the well-known nanocasting method with a KIT-6 hard template. Co, Mn, and Zn metal precursor were impregnated through an incipient wet impregnation (IWI) method. Then, the KIT-6 hard template was removed by using NaOH solution. Catalytic performance of the mCoMnZn metal oxides catalysts were evaluated by using a fixed bed tubular reactor. Results and discussion: All the synthesized catalysts showed a highly ordered mesoporous structures as shown in Figure 1. The ZnO-promoted catalysts at an optimal Zn/Co ratio of 0.7 showed a higher CO2 conversion with highest C2+ hydrocarbons selectivity. CO2 hydrogenation activity with small amount of CO byproduct was related with the presence of abundant oxygen vacant sites due to the presence of Mn promoter and high metallic cobalt with Zn promoter. Zn promoter increased the dispersion by forming larger active sites and by changing crystallite size. Furthermore, the Co3O4-MnO-ZnO ternary metal oxide system enhanced the catalytic stability by preserving ordered mesoporous structure under the reaction condition. The stable preservation of proper oxidation states of Co nanoparticles and strong interactions with highly dispersed metals were crucial to get high catalytic activity and stability as shown Figure 1.

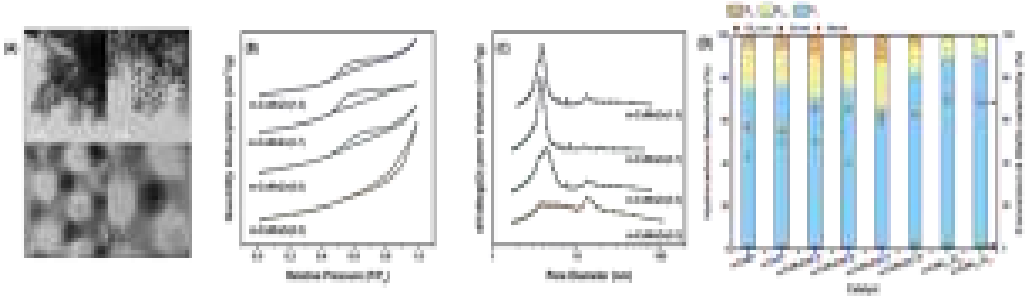

Figure 1. (A) TEM images of the m-CoMnZn(0.7), (B) N2 adsorption-desorption isotherms, (C) Pore size distribution on the fresh catalysts and (D) Catalytic performance on the mCoMnZn catalysts

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MKF9704

Hybrid heterogeneous transfer learning for kinetics models

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Keywords: Hybrid ODE; Heterogeneous Transfer Learning; Kinetics Models; Hydrotreatment

Introduction. Hydrocracking units [1] use hydrotreatment reactors to remove nitrogen impurities from heavy feedstocks. The energy transition is driving the evolution of refining processes toward renewable feedstocks, creating a need for predictive models based on limited experimental data. Although kinetic models (ordinary differential equations, or ODEs) [2, 3, 4] offer interpretability and respect physical trends, they are difficult to recalibrate for these new chemistries such as tire feedstocks due to limited experimental data and incomplete chemical knowledge. Heterogeneous transfer learning (HTL) neural networks have emerged to address data scarcity [2], but these data-driven models often fail to extrapolate beyond the regions for which they were trained. This work overcomes this limitation by integrating HTL within the ODE itself.

Methods. Following the source and target ODEs defined in our previous work [2], the target ODE contains feature/s which are not present in the source ODE. Part of each ODE is replaced with a neural network (NN_S for the source and NN_T for the target), which has the same architecture in both domains. The NN's inputs are heterogeneous yet share overlapping features, enabling HTL within the ODEs:

$$Source: \frac{dy}{dt} = f\left(y(t), \overline{\boldsymbol{x}}_S, \overline{\boldsymbol{\theta}}_S, NN_S(\hat{\boldsymbol{x}}_S, W_S)\right)$$
$$Target: \frac{dy}{dt} = f\left(y(t), \overline{\boldsymbol{x}}_T, \overline{\boldsymbol{\theta}}_T, NN_T(\hat{\boldsymbol{x}}_T, W_T)\right)$$

where $\boldsymbol{x_S} = (\overline{\boldsymbol{x}}_S, \hat{\boldsymbol{x}}_S)$ and $\boldsymbol{x_T} = (\overline{\boldsymbol{x}}_T, \hat{\boldsymbol{x}}_T)$ are feature vectors divided into two parts across domains: a kinetic part $(\overline{\cdot})$ associated with some of the kinetics parameters whose structure and boundaries are known, and a black-box part $(\hat{\cdot})$ encoded using a NN (NN_S; NN_T) parametrized with W (W_S; W_T). y is the variable of interest to predict using minimal data. An efficient HTL framework is proposed and compared to DHTLM [2] and the reference kinetic model [2] (fitted on target data using Metropolis-Hastings within Gibbs [2]). For simulated data, the reference kinetic model was used to generate the data (the perfect model); for real data, it serves as the best available approximation. Evaluation uses mean absolute error (MAE) on test sets with varying training sizes. Only the feedstock properties across domains were encoded with NN. Further experimentation will involve replacing additional ODE components.

Results and discussion. Figure 1 shows mean prediction error on test sets for simulated (left) and real (right) data versus training size. The bands show min-max error intervals. For simulated data, the hybrid ODE HTL framework achieves lower errors and tighter intervals than DHTLM (except for n_t=20). For real data, DHTLM shows slightly lower errors; however,

DHTLM cannot extrapolate beyond training regions as it lacks physical knowledge. Compared to the kinetic model reference, the hybrid ODE framework demonstrates superior stability and tighter intervals on simulated data and better prediction error for real data, for almost all training sizes. This work enables the data-efficient modelling of renewable feedstock processes while preserving physical interpretability and extrapolation capabilities.

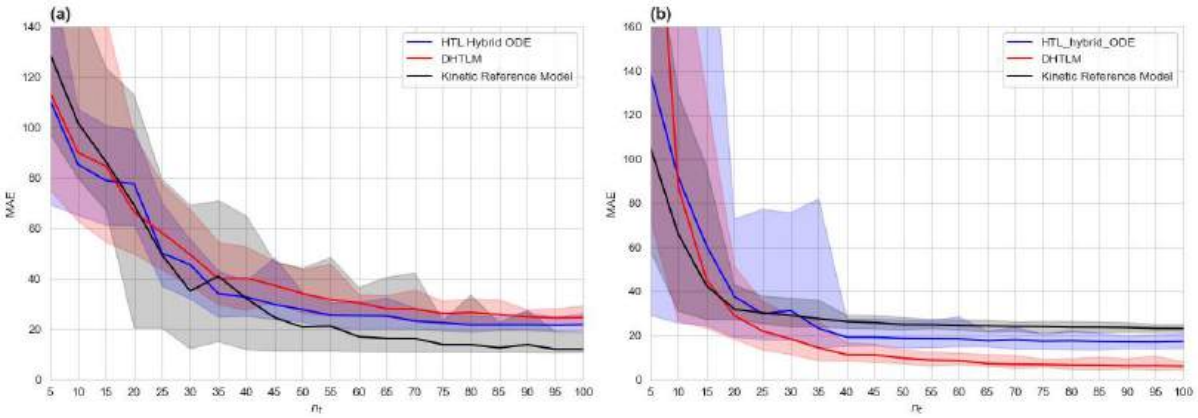

Figure 1: Comparison of the Hybrid ODE (blue), DHTLM (red), and the kinetic reference model (black) on simulated (left) and real (right) data sets. The plot shows mean prediction error (solid line) on test sets versus training size of the target domain. Bands represent min-max error intervals across test sets.

Acknowledgments

We would like to thank Ben Gao for his advice and exchange of ideas.

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ISCRE29 & APCRE11
2026 / SEOUL, KOREA

HTT0541

Investigation the Interface between Cu and Boron oxide as an active site for CO2 to Methanol

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Abstract Category: Hydrogen - Hydrogen Storage (LOHC, NH3, MeOH etc)

Keywords: Carbon dioxide;, Methanol, Heterogeneous catalyst, Hydrogen

Abstract Body.

Introduction.

Copper is the most widely studied non-noble metal for CO2-to-methanol, yet the identity of its true active site remains debated. Here we hypothesize that an interfacial Cu–O–B ensemble formed on defect-engineered boron nitride (d-BN) stabilizes Cu^+ and provides strong Lewis-acidic B sites. This study investigates the Cu–O–B interface and demonstrates that it can serve as an active site.

Methods. Defect BN was obtained by ball-milling h-BN; hot-water washing yielded d-BN-W. Colloidal Cu nanoparticles (≈7.7 nm) were deposited identically on each support and activated in H2. Structure and dispersion were probed by TEM/HAADF-STEM and H2-TPR. Interfacial chemistry and oxidation state were quantified by XPS/Auger (modified Auger parameter, Cu^+ fraction). Mechanistic fingerprints were obtained by operando DRIFTS (formate/methoxy). Catalytic tests used CO2/H2 = 1:3 at 200–240 °C.

Results and discussion. On h-BN, Cu particles sintered to ~7.95 nm and reduced in a single low-temperature TPR peak (255 °C). On d-BN, particles redistributed to 4.19 nm, and TPR displayed an additional, higher-temperature component, consistent with stronger Cu–O–B interaction. After washing (d-BN-W), overlayer removal increased surface Cu–O–B interfacial component. XPS/Auger revealed a parallel increase in Cu^+ fraction.

Consequently, the site-normalized methanol rate followed d-BN-W > d-BN □ h-BN, while CO (RWGS) and CH4 were suppressed as the interface was exposed.

Figure 1. Schematic illustration of Cu/BN series catalyst for CO2 to methanol.

Exposing interfacial ensembles with higher Cu^{+} and Lewis acidic site has a synergy that lowers barriers for the formate/methoxy sequence. These results provide a mechanistic insight for designing Cu catalysts via interface engineering rather than bulk composition in CO2 to methanol.

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HTT0570

Copper Oxide-Zeolite Tandem catalysis for direct multicarbon oxygenates synthesis from CO2 hydrogenation

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal
Keywords: Tandem Catalysis, Zeolite, Oxygenates, CO2 hydrogenation

Abstract Body.

Introduction.

Direct and selective higher oxygenates synthesis from CO2 has been tremendously attractive but challenging [1-3]. Herein, tandem hydrogenation and carbonylation reactions were coupled to achieve one-step methyl acetate (MA) and ethanol (EA) synthesis from CO2. The thermally stable Cu-ZnO@SiO2 and 8-membered rings (8-MRs) in FER were applied to produce an optimal CO/DME ratio by CO2 hydrogenation and realize efficient carbonylation to MA for its further hydrogenation to EA.

Methods.

SiO2 encapsulated Cu-ZnO nanoparticle catalysts were prepared though a reverse micelle approach. The Cu/Zn mole ratio was varied by modified precursor mole ratios by copper and Zn nitrate trihydrate and Brij C10 was employed as a non-ionic surfactant. The CuZnO@SiO2 catalysts were collected dried and calcined from the micelle-formed precursors. FER was synthesized via hydrothermal synthesis method, After obtained Naform NFER zeolite, it was transformed to H-form by ion-exchange.

Results and discussion.

For the selective ethanol formation from CO2 hydrogenation, we integrated tandem hydrogenation-carbonylation strategy to achieve one-step MA and EA synthesis. Specifically, CO2-to-methanol and CO2-to-CO over Cu-ZnO@SiO2 (Fig. 1A) generated appropriate ratios of methanol/CO intermediates. Subsequent the carbonylation of CO and dimethyl ether (from methanol dehydration) occurred on nano-ferrierite (NFER, Fig. 1B), enabling MA production from direct CO2 hydrogenation. Thermally stable Cu-ZnO sites in CZ@Si and the 8-membered ring (8-MR) channels in NFER crucially optimized the CO/DME ratio, which significantly facilitates the efficient MA intermediate for further ethanol production via triple tandem catalysis. Moreover, the Figure 1C demonstrates more than 50% of MA selectivity at ~20% CO2 conversion over CZ@Si/NFER system.

In conclusion, we bridged the dimethyl ether (DME) carbonylation over zeolite as the intermediate step to form the selective methyl acetate intermediate, which was facile to be hydrogenated to ethanol. Higher hydrocarbon formations were largely prohibited with the minimized propagation and hydrogenation of CHx* monomers, enabling selectively converted CO2 toward ethanol synthesis achieving CO2 conversion around ~30% and ~50% ethanol selectivity.

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HTT0625

Experimental and Theoretical Evidence for the Rearrangement of Ru Catalyst for CO2 Hydrogenation: An In situ TEM and DFT Study

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: CO2 Hydrogenation, Ru catalysts, Formic acid, In situ TEM, Density Functional Theory (DFT)

Abstract Body.
Ruthenium (Ru) catalysts supported on nitrogen-doped carbon (NDC) exhibit remarkable activity for the hydrogenation of CO2 to formic acid. However, the heterogeneity of binding sites in the support often leads to catalyst deactivation, as Ru species on weaker binding sites (e.g., bare carbon or graphitic-N) are prone to detachment or agglomeration during the reaction. This study provides experimental and theoretical evidence for a strategy to enhance catalytic stability by promoting the homogenization of active structures via thermal treatment. To investigate this, a model catalytic system utilizing Ru supported on sheet-like NDC with abundant strong binding sites was synthesized and subjected to thermal treatment up to 400 °C in an inert N2 atmosphere. The morphological dynamics of Ru species were monitored in real-time using in situ heating transmission electron microscopy (TEM). In situ TEM analysis revealed a progressive rearrangement where Ru aggregates on weak binding sites decomposed and redispersed into isolated single atoms as the temperature increased. Complementary density functional theory (DFT) calculations were performed to elucidate the thermodynamic driving forces behind this structural evolution. The calculations suggested that the migration of Ru atoms to thermodynamically stronger binding sites, such as pyridinic-N or pyrrolic-N, is energetically more favorable than re-aggregation or remaining on weaker graphitic-N sites. Consequently, the catalyst treated at 400 °C demonstrated superior stability, retaining 95% of its initial activity after five consecutive recycling runs for CO2 hydrogenation. This work offers fundamental insights into the rearrangement mechanism of Ru species, supported by both direct observation and theoretical verification.

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KN0719

Catalysis-Driven Practical Solutions for Carbon Neutrality

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Abstract Category: Invited Lecture - Keynote Lecture

Keywords: Catalyst, Greenhouse Gas Mitigation, Industrial Decarbonization, Carbon Neutrality

Abstract Body.

The development of human civilization has been accompanied by a steady increase in energy consumption. Since the 18th century, fossil fuel–based energy systems have enabled significant improvements in industrial productivity and quality of life, while simultaneously giving rise to structural environmental challenges such as air pollution and greenhouse gas emissions. Catalysts has been utilized as a key technological solution capable of reconciling industrial growth with environmental protection.

Catalysts used for exhaust gas purification in automobiles, power generation facilities, and other stationary sources have contributed substantially to air quality improvement and energy efficiency. In parallel, process catalysts in the chemical industry have enabled the efficient production of high value-added materials. However, the large-scale emission of carbon dioxide from fossil fuel combustion has accelerated climate change, which is now an ongoing global crisis. Following the Paris Agreement in 2015, countries established national greenhouse gas reduction targets, and carbon neutrality by 2050 has become a shared global objective. Recent discussions at COP30 further emphasized that meaningful emission reductions before 2030 will be critical in shaping the future trajectory of climate change, leading major economies to pursue industry-wide decarbonization roadmaps toward 2035. Catalytic technologies are increasingly recognized as practical and immediately deployable solutions for greenhouse gas mitigation, as they can deliver substantial emission reductions while leveraging existing industrial infrastructure. By enabling reaction activation at lower temperatures, catalysts reduce direct process emissions (Scope 1) and simultaneously decrease energy consumption, thereby lowering indirect emissions associated with electricity use (Scope 2). Catalysts are also applied to mitigate unburned methane emissions from LNG-fueled marine engines and gas turbines, as well as exhaust gases generated during the use of low-carbon and carbon-free fuels such as ammonia, methanol, and hydrogen. In the semiconductor industry, catalysts play a critical role in abating greenhouse gases with extremely high global warming potential, including perfluorinated compounds (PFCs) and nitrous oxide (N2O).

Hydrogen is further gaining attention as a key energy carrier for achieving carbon neutrality by 2050, and catalysts are indispensable across hydrogen production and utilization pathways, including methane reforming, ammonia cracking, water electrolysis, and fuel cell applications. In addition, the recovery and recycling of precious and valuable metals from

spent catalysts enhance resource circularity and contribute indirectly to greenhouse gas reduction.

Overall, catalytic technologies are expanding their applications across diverse industrial sectors and are emerging as essential enablers of greenhouse gas mitigation and global decarbonization.

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2026 / SEOUL, KOREA

HTT0384

Inhibition of Excessive NiO-MgO Solid Solution Formation via BaO Addition for Dry Reforming of Methane

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Dry reforming of methane, Ni-based catalyst, crystallite size, solid solution

Abstract Body.

Inhibition of Excessive NiO-MgO Solid Solution Formation via BaO Addition for Dry Reforming of Methane

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Keywords: Dry reforming of methane; Ni-based catalyst; crystallite size; solid solution

Introduction.

Dry reforming of methane (DRM) is an attractive route for the simultaneous utilization of CH4 and CO2, a representative greenhouse gas. However, its industrial application is constrained by catalyst deactivation [1]. Ni-based catalysts are economically viable but suffer from sintering and carbon deposition. CeO2, a reducible support, can suppress carbon deposition by promoting the oxidative removal of deposited carbon via mobile oxygen. Ni0 sintering can be inhibited through NiO-MgO solid solution formation, but excessive solid solution lowers the formation of the active Ni0 phase due to the excessive interaction between NiO and MgO. In this study, we introduced BaO into the Ni-MgO-CeO2 (NMC) catalyst to prevent excessive NiO-MgO solid solution formation, thereby maximizing the formation of the Ni0 phase after the pre-reduction process, an active species for the DRM reaction.

Methods.

All catalysts were synthesized by the co-precipitation method with varying the MgO and BaO contents. The catalysts were pre-reduced at 750 oC in a 5% H2/N2 flow for 3 h and tested at 800 oC for 12 h. The catalytic properties were examined through comprehensive physicochemical analyses.

Results and discussion.

NMC catalyst forms a NiO-MgO solid solution, which enhances the interaction between NiO and MgO, thereby improving resistance to sintering. However, excessive formation of solid solution decreases the fraction of readily reducible Ni species, decreasing the formation of Ni0 active sites after the pre-reduction. Introducing BaO can limit overly extensive formation of NiO-MgO solid solution, resulting to the increase of the formation of active metallic Ni (Ni0) species, leading to improved catalytic performance. Excessive BaO loading can weaken NiO-support interaction and increase Ni0 mobility during the reduction, thereby accelerating Ni0 sintering.

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2026 / SEOUL, KOREA

HTT0507

Fe Modification Complementing Zeolite Encapsulation for Coke-Resistant Ni@S-1 in Dry Reforming of Methane

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Dry reforming of methane; Zeolite; Encapsulation; Coke suppression; Alloy

Abstract Body.

Introduction.

Dry reforming of methane (DRM) converts the greenhouse gases CO2 and CH4 into valuable syngas (H2 and CO), yet widely used Ni-based catalysts suffer from severe coke formation during DRM. Zeolite encapsulation could suppress coke formation by confining ultrafine Ni nanoparticles within the zeolite framework[1]. However, at higher Ni loadings, complete encapsulation becomes increasingly difficult, resulting in partially surface-exposed Ni that grow larger and readily promote coke formation. In this study, Ni@S-1 with different Ni loadings are benchmarked against surface-impregnated Ni/S-1 to elucidate the loading dependence of zeolite encapsulation, and Fe is introduced onto higher-loading Ni@S-1 to complement encapsulation by regulating surface Ni via Ni-Fe alloy formation and redox cycling, enabling effective coke suppression and identification of an optimal Fe/(Ni+Fe) ratio.

Methods.

Ni@S-1 catalysts with different Ni loadings (1-3 wt%) were synthesized via a hydrothermal encapsulation route using a Ni-phyllosilicate (Ni-PS) precursor prepared from Ni(NO3)2, NH3 aq., and TEOS, followed by hydrothermal crystallization with TPAOH and TEOS and calcination. For comparison, 1-3 wt% Ni/S-1 were prepared by conventional impregnation. Fe/Ni@S-1 catalysts with Fe/(Ni+Fe) molar ratios of 0.20-0.55 were obtained by impregnating Fe(NO3)3 aq. onto Ni@S-1. After H2 reduction, the DRM tests were conducted at 600 °C in a fixed bed reactor with CH4: CO2: Ar: He = 20: 20: 40: 10 mL/min (GHSV: 2,000 L/g-Ni/h).

Results and discussion.

TEM showed that 1-2wt% Ni@S-1 maintained ultrafine Ni NPs (3-4 nm), whereas 3 wt% Ni@S-1 exhibited partial surface exposure and particle growth; in contrast, Ni/S-1 displayed much larger and broadly distributed Ni particles. Under DRM at 600 °C, coke formation increased with Ni loading for all catalysts, but Ni@S-1 consistently outperformed Ni/S-1 at identical Ni contents. Nevertheless, 3 wt% Ni@S-1 still accumulated substantial coke (27 wt%), indicating an intrinsic limitation of encapsulation at high loading. To address this, Fe was introduced onto 3 wt% Ni@S-1, where moderate Fe levels improved metal dispersion via Ni-Fe alloy formation. Catalytically, 0.25Fe/Ni@S-1 preserved conversions comparable to Ni@S-1 (~45% CH4 and ~55% CO2) while reducing coke from 27 wt% to 5 wt%. In-situ CO2/CH4

pulse qualitatively indicated enhanced CO_2 activation and slightly weakened CH_4 decomposition on Fe/Ni@S-1, consistent with Fe redox cycling that facilitates coke removal. Overall, Fe modification complements zeolite encapsulation by regulating surface-exposed Ni at high loadings, offering a general strategy for coke-resistant catalyst design.

Acknowledgments
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2026 / SEOUL, KOREA

HTT0523

Sorption enhanced carbon dioxide methanation employing a bifunctional zeolite-based material with fine-tuned nickel clusters.

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: enhanced methanation, nickel cluster tuning, carbon dioxide valorisation

Abstract Body.
Introduction. The urgent need to mitigate climate change has highlighted the interest in carbon dioxide (CO2) utilization technologies, particularly in processes that yield valuable products while reducing atmospheric CO2 levels. One such promising approach is sorptionenhanced methanation (SEM) of CO2, aimed at producing high-purity methane (CH4) by overcoming the thermodynamic limitations of conventional methanation reactions. In this process, water is continuously removed via sorption on a zeolite based catalyst, thereby shifting the equilibrium towards methane formation. This technique offers significant potential for improving both conversion efficiency and product purity in applications such as synthetic natural gas (SNG) production. The bifunctional material is composed by zeolite 13X which act as adsorbent for water and support for the active metal; nickel provides the catalytic active sites, and cerium increases the CO2 adsorption capacity.
Methods. Different catalysts prepared with different nickel precursors and the same nominal content (5%Ni2.5%Ce13X) have been tested in sorption enhanced methanation. The experiments were conducted at 240 °C, 1 atm in a packed bed reactor, using 16 ml/min of H2, 4 ml/min of CO2 and 80 ml/min of He. Gas analysis was performed using an online microGC. Extensive catalyst characterization was performed using SEM, TEM, N2physisorption, pyridine-FTIR, CO2-TPD and H2-TPR.
Results and discussion. The experimental results highlighted the impact of the nickel precursor used in the catalyst synthesis. The steady state conversion employing the catalyst prepared with nickel nitrate was 11% while the one made with the best precursor achieved 48%. Among the different precursors used, different particle sizes and activity were observed. A linear correlation between the nickel cluster surface area and steady state conversion was obtained. The experiments also demonstrated the possibility to obtain a pure stream of methane from carbon dioxide and hydrogen during the sorption enhancement period. An increased activity provided by the best precursor implies a longer sorption enhancement operation, higher productivity and lowering energy duty costs. Other reactions which employ nickel as active metal could benefit by this preparation method.

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2026 / SEOUL, KOREA

HTT0554

Kinetic Roles of Surface Carbon in Methane Dry Reforming on Rh and Ni by Operando Raman Spectroscopy

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Methane Dry Reforming, Ni-based catalysts, Rh-based catalysts, Operando Raman spectroscopy, Carbon deposition, Deactivation

Abstract Body.

Please refer to the attached PDF file. I am also reporting the abstract text below, since the form forces me to fill this part.

Introduction.

Methane Dry Reforming (MDR) is a promising solution for biogas and CO2-rich natural gas valorization. However, its industrial scalability is hindered by catalyst deactivation due to carbon deposition [1]. In our investigation, we have combined kinetic tests in an annular reactor with spatio-temporal operando Raman spectroscopy to elucidate the carbon formation pathway and its kinetic implications on MDR in a comparative analysis between Rh and Ni.

Methods.

The catalysts (4 wt.% Rh/α-Al2O3 and Ni/α-Al2O3), coated as a thin layer (thickness 10-30 μm, length 20 mm) on the external surface of an alumina tube, were prepared via incipient wetness impregnation of an α-Al2O3 support with a solution of the active phase precursor (Rh(NO3)3 and Ni(NO3)2). A sapphire window aligns with the catalytic bed, enabling the acquisition of time-resolved and spatially-resolved operando Raman spectra through a laser probe (488 nm), and a JASCO ® NRS-4100 spectrometer.

Results and discussion.

Our MDR spectro-kinetic analysis conducted between 550 °C and 700 °C (representative operando spectra shown in Figure 1.a) demonstrates that on Rh carbon deposition follows a nucleation and filaments base-growth mechanism, mainly driven by multiple surface precursors (“Surface Route” in Figure 1.b) [2]. Instead, on Ni two distinct types of carbon are identified: (I) an early graphitic fraction derived from CHÀ decomposition, which is mainly responsible for a rapid early loss of catalytic activity, and (II) defective carbon, formed via Cdiffusion into Ni and subsequent filaments tip-growth or encapsulation (“Diffusion route” in Figure 1.b), which dictates the long-term deactivation dynamics. While on Rh deactivation can be avoided under oxidative feeds (high CO2/CH4 ratios or O2 co-feed) thanks to a strong interaction of the local chemical environment with the surface carbon (“Oxidative route” in Figure 1.b), on Ni the weaker Csolid–CO2 interconnection prevents complete removal of early deposited graphitic carbon, making the catalyst more prone to deactivation. These mechanistic insights provide a consistent picture of both the nature and impact of deposited carbon under varying COØ /CHÀ ratios, temperatures, and space velocities,

highlighting the role of the active metal in determining both the carbon morphology and its kinetic influence.

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2026 / SEOUL, KOREA

HTT5687

Redox-Basic Functional Balancing of Ni-Based Catalysts for Synergistic Coupling of Dry Reforming of Methane and the Reverse Water-Gas Shift Reaction

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Synergistic DRM–RWGS, Redox–basic balancing, Ni-based catalysts

Abstract Body.

Redox-Basic Functional Balancing of Ni–Based Catalysts for Synergistic Coupling of Dry Reforming of Methane and the Reverse Water–Gas Shift Reaction

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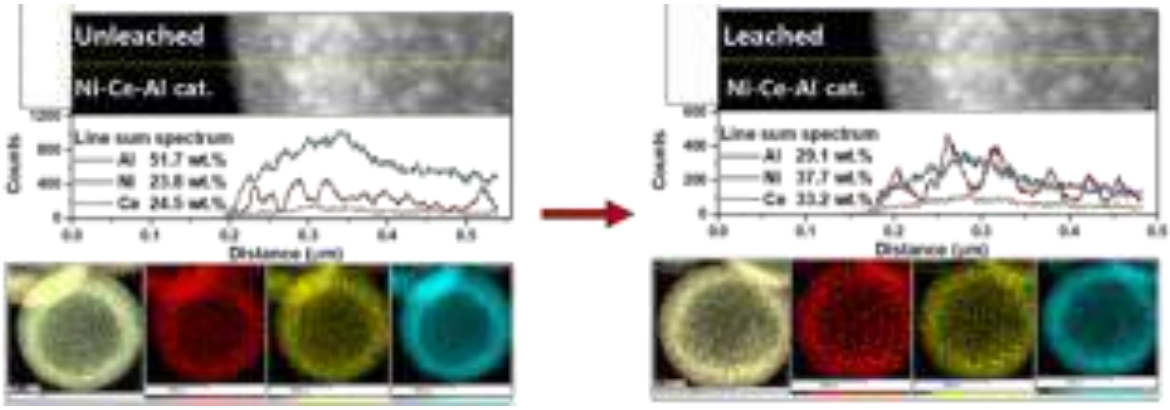
Keywords: Synergistic DRM–RWGS; Redox–basic balancing; Ni-based catalysts Introduction.

The Synergistic Coupling of Dry Reforming of Methane and the Reverse Water–Gas Shift Reaction (SCDR, $CH_4 + 3CO_2 \rightarrow 4CO + 2H_2O$) provides a CO_2-intensified route for generating CO-rich syngas without external hydrogen. Under $CH_4:CO_2 = 1:3$ conditions, H_2 produced via DRM ($CH_4 + CO_2 \rightarrow 2CO + 2H_2$) is immediately consumed by RWGS ($CO_2 + H_2 \rightarrow CO + H_2O$), suppressing carbon deposition and maintaining an oxidizing atmosphere. Efficient SCDR catalysis therefore requires materials capable of CH_4 activation, CO_2 dissociation through oxygen-vacancy pathways, and stabilization of oxy-carbon intermediates under redox-dynamic conditions [1, 2].

Methods.

Spray pyrolysis was employed to synthesize homogeneous Ni–Ce–Al microspheres.

Selective phase exposure (SPE) via controlled alkaline leaching removed γ-Al_2O_3 while exposing $NiAl_2O_4$–CeO_2 interfaces, increasing Ce^{3+}, enhancing lattice-oxygen mobility, and suppressing $CeAlO_3$ formation. Surface basicity was independently adjusted through post-synthetic MgO deposition by incipient wetness impregnation (1–5 wt%), which preserved the redox framework without promoting $MgAl_2O_4$.



Results and discussion.
SPE restructuring yields a porous $NiAl_2O_4$–CeO_2 network rich in oxygen vacancies and highly reducible Ni species, while MgO loading selectively enhances medium-strength basicity. Operando DRIFTS shows complementary roles: Ce-based redox sites promote HOCO* and HCOO* turnover, whereas MgO stabilizes bidentate carbonates, shifting the

DRM/RWGS interplay. Optimal MgO loading improves CO_2 activation and intermediate conversion, leading to higher CH_4 conversion, greater CO selectivity, and better carbon resistance. These results demonstrate that independent tuning of redox and basicity functions provides a rational strategy for optimizing of SCDR catalysis for CO_2-intensified syngas production.

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2026 / SEOUL, KOREA

KN0194

Active Site Structures on Transition Metals and Oxides and their Mechanistic Roles in Alcohol Conversion

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Abstract Category: Invited Lecture - Keynote Lecture

Keywords: Partial oxidation

Abstract Body.

Introduction. Catalytic partial and total oxidation of alkanes and alkanols is of significant practical relevance for exhaust emission control, the upcycling of small molecular building blocks, and the generation of heat and energy. These reactions share kinetically coupled catalytic oxidation–reduction cycles with common mechanistic requirements, most notably the involvement of reactive oxygen species in C–H bond activation. Reaction turnovers depend on the relative rates of these cycles and, consequently, on the structure of the active sites that bind reacting intermediates. Here, we describe the effects of oxygen content as well as the chemical and electronic states of oxygen adatoms on alkanol conversion, and we identify hierarchical oxygen-deficient layers on oxide shells as active structures responsible for C–H bond activation in alkanols.

Results and discussion. Using Cu as the reference catalysts, spectroscopic and microscopic characterizations confirm diverse Cu speciation of Cu+ single atoms embedded in TiO2 surfaces, Cun+-O2- on small CuOx clusters (~1 nm, on C and TiO2), and Cu0-Cu0 on reduced Cu nanoparticles. Rate assessments under differential conditions show distinct kinetic regimes, in terms of reaction orders with respect to O2 and alcohols, kinetic parameters in the activation of methanol and ethanol, because of the different coordination environment of the reactive oxygen adatom and Cun+ center. A thermochemical deconstruction of the activation barrier, within the context of transition state theory, shows the correlation of the activation barrier to the various kinetic descriptors for oxygen assisted C-H activation, i.e., hydrogen atom addition energy (HAE), oxygen vacancy formation energy, and hydroxyl desorption energy. These descriptors are related to each other, quantitatively described and confirmed here with density functional theory calculations. With integral time resolved X-rays absorption studies, we probe the gradual depletion of the reactive oxygen species from CuOx nanoparticle surfaces, leading to a commensurate reduction of the Cu2+. These reconstruction of the surface leads to the formation of strained outer layers on CuOx cores, and to an increase in the C-H bond activation rates of methanol, as also verified with the transient dynamic switching studies of CH3OH and CH3OH-O2 reaction, probing the time-dependent oxygen contents and C-H activation rates. Extending this knowledge, we investigate other metals and their speciation on rates and establish periodic reactivity trends for alcohol dehydrogenation vs. partial oxidation.

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2026 / SEOUL, KOREA

HTT0327

Regulating the Acidity of MCM-22 Zeolite Catalysts for Aromatization from Light Hydrocarbons

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Aromatization, MCM-22, Acidity control

Abstract Body.

Introduction

Zeolites are well-known for producing aromatic compounds due to the acid sites. Especially, Brønsted acid site (BAS) play an important role in acetylene aromatization [1]. In this study, MWW-type zeolite and MCM-22 catalysts with controlled acid sites were prepared. We propose a new bottom-up synthetic method to control the BAS.

Methods

The typical MCM-22 was synthesized by hydrothermal method [2]. The acidity of MCM-22 was controlled by adjusting the composition of mother solution and denoted as NS-MCM-22. The synthesized catalysts were characterized by XRD, NH3-TPD, SEM, and TEM. The activity tests were conducted at 700 oC [2]. To investigate the reaction pathway, the commercial ZSM-5 sample was pre-tested by in-situ FT-IR at 200 oC.

Results and discussion

As a result of XRD analysis, typical patterns of MWW-type zeolite were observed in all samples. It was confirmed that NS-MCM-22 exhibited left-shifted BAS peaks with similar amounts of BAS across all samples. Figure 1a-b shows the catalytic performance of MCM-22-type catalysts. NS-MCM-22 catalysts showed higher C2H2 conversion and BTX yield than MCM-22. Figure 1c shows the pre-tested in-situ FT-IR spectra of ZSM-5. The intermediates of aromatization reaction were detected [3]. After C2H2 desorption, the peaks of the intermediates were more clearly identified. Similarly, MCM-22 type catalysts will be investigated by in situ FT-IR analysis

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HTT0298

Pr-doped Pd/CeO2 catalysts for CH4 oxidation: unveiling the promoting role of Pr through in-operando techniques

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Methane oxidation, palladium, ceria, praseodymia, operando characterizations

Abstract Body.
Introduction. Pd-supported catalysts have been recognized as the most promising materials for CH4 oxidation to CO2, while ceria exhibited excellent properties as Pd support. More recently, Pr-doping of the ceria support proved to enhance metal-support interaction, stabilizing oxidized Pd species and counteracting water-induced deactivation phenomena.
Methods. Nanostructured Ce-Pr supports were prepared through hydrothermal synthesis and impregnated with 2 wt.% of Pd. The samples were named Pd/Ce(100-X)Pr(X), where X indicates the atomic percentage of Pr in the support (0, 10, 25, 50%). Pd-Ce-Pr systems with different compositions were tested and deeply investigated with some advanced techniques, such as Near-Ambient Pressure X-ray Photoelectron Spectroscopy (NAP-XPS), in-situ/operando FTIR spectroscopy, and in-operando Transmission Electron Microscopy (TEM) gaining new insights into the promoting role played by Pr during methane oxidation.
Results and discussion. A mild Pr-doping was associated with an enhancement of Pd/ceria catalytic activity towards methane oxidation: indeed, Pd/Ce90Pr10 resulted to be the most performing sample, both in dry and wet conditions. Further Pr addition was instead linked to lower activity. According to in situ FTIR, a higher Pr content was related to a strong affinity with carbonate species: indeed, Pr-rich materials were covered by stable bi- and poly-dentate carbonates, showing a limited CO2 desorption tendency (Fig. 1-a). NAP-XPS showed that the catalysts containing a low Pr percentage exhibited a variegated mix of reduced and oxidized Pd species throughout the course of the reaction up to 500 °C (Fig. 1-b); a higher Pr loading was instead associated with the presence of too stable oxidized palladium forms, with detrimental effects on catalytic activity. An intermediate Pr doping represents therefore the best compromise in terms of stability of both Pd active species and reaction intermediates. In-operando TEM confirmed the oxygen depletion of the Pd particle during heating, particularly around 600°C (Fig.1-c); this behavior was reversible after cooling, where PdO was reformed.

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HTT0524

C=C enantioselective hydrogenation over Pd/MOF

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Pd nanoparticle, enantioselective hydrogenation, MOF modification, electron density, ligand modification

Abstract Body.

Heterogeneous enantioselective hydrogenation of C=C bonds is a key transformation for the synthesis of fine chemicals and pharmaceutical intermediates, yet establishing clear design principles for such catalysts remains challenging[1]. A major difficulty arises from distinguishing the intrinsic electronic effect of the metal surface from structural factors such as particle size or pore geometry. This study aims to construct a well-defined standard platform based on functionalized MIL-53 Metal–Organic Frameworks (MOFs) that allows systematic control of the electronic state of Pd nanoparticles. Using this platform, we investigated the relationship between the Pd surface electronic properties, product desorption behavior, and the resulting chiral selectivity.

MIL-53-X supports (X = H, NH_2, OH, NO_2) were synthesized via a hydrothermal method, and Pd nanoparticles were deposited by a chemical reduction approach. The resulting Pd/MIL-53-X catalysts were characterized by XRD, TEM, N_2 physisorption, FT-IR, XPS, and CO-adsorption IR spectroscopy. Catalytic performance was evaluated through the enantioselective hydrogenation of α-phenylcinnamic acid (PCA) in the absence and presence of benzylamine (BA) as an additive. Time-resolved ATR-IR spectroscopy was also employed to qualitatively monitor adsorption and desorption behaviors of the product under reaction conditions.

All Pd/MIL-53-X catalysts exhibited comparable particle sizes (2.1–2.8 nm) and surface areas, confirming that the structural parameters remained constant. Variation of the organic linker effectively influenced the electronic nature of Pd, leading to distinct catalytic performances. Catalysts containing electron-donating groups (–NH_2, –OH) showed higher turnover frequencies and enantioselectivities than those bearing the electron-withdrawing –NO_2 linker. The presence of BA further enhanced the overall reaction rate and ee, particularly for the Pd/MIL-53-NH_2 catalyst. Characterization results supported that linker modification successfully tuned the electronic interaction between Pd and the MOF framework, which in turn affected the adsorption–desorption behavior of the product during the reaction.

A MOF-based model platform was successfully established to examine electronic effects in heterogeneous asymmetric catalysis while minimizing structural variation. The results demonstrate that controlling Pd electron density through linker functionalization enhances both activity and enantioselectivity by facilitating product desorption and maintaining active chiral surfaces. This work provides a rational framework for designing high-performance asymmetric hydrogenation catalysts via electronic modulation at the metal–support interface.

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HTT0618

Environmentally Benign Co/Sn Catalysts: The Role of Mesoporous Silica Supports in Propane Dehydrogenation

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Propane dehydrogenation, Co-based Catalyst, Mesoporous silica supports, Metal–support interaction

Abstract Body.

Introduction

Propane dehydrogenation (PDH) is an attractive route for on-purpose propylene production; however, industrial processes still rely largely on platinum-based or chromium oxide catalysts, raising concerns about cost and toxicity. Cobalt-based catalysts have therefore emerged as promising non-noble alternatives due to their ability to selectively activate C–H bonds. Nevertheless, the rational design of Co-based PDH catalysts remains challenging, as performance is highly sensitive to cobalt speciation, metal–support interactions, acidity, and coke-induced deactivation[1]. In particular, the influence of support topology on the stabilization of active cobalt sites and on balancing activity, selectivity, and stability remains insufficiently understood.

Methods

A series of Co/Sn catalysts supported on mesoporous silica materials was synthesized to investigate the effect of the support on performance. Mesoporous silica supports (TUD-1, UVM-7, MCM-41, HMS, DMSN, and FSM-16) with distinct pore architectures were prepared via support-specific synthesis routes[2], followed by in situ incorporation of tin (4 wt% SnO_2) and subsequent impregnation of cobalt (3 wt% Co). Catalytic performance was evaluated in a fixed-bed quartz reactor using propane diluted in nitrogen, with products analyzed online by gas chromatography. Catalyst performance was assessed by propane conversion, propylene selectivity, yield, and time-on-stream stability, and correlated with structural and surface properties.

Results and discussion

The catalytic performance of Co/Sn catalysts(Fig. 1a-c) was strongly governed by the mesoporous silica support, demonstrating that support topology controls activity, selectivity, stability, and deactivation behavior in propane dehydrogenation. Among the investigated materials, Co/Sn@MCM-41 exhibits the highest propylene yield (26%), combining elevated propane conversion (27.7%), high propylene selectivity (94.3%), and a propylene formation

rate of 7.57 mmol.gcat-1.h-1. XPS and H2-TPR analysis indicated that this superior performance correlates with a higher population of surface-accessible Co2+ species, moderated metal–support interactions, and a controlled acidity dominated by weak and medium-strength acid sites. Consistent with ongoing discussions on oxidic versus reduced cobalt species in PDH, H2-TPR showed that Co/Sn@MCM-41 exhibits the highest Co2+/Co0 ratio (0.66), highlighting the importance of Co2+ stabilization[3] by the MCM-41 support. Supports promoting stronger cobalt anchoring or excessively strong acidity, which favors less accessible cobalt species and enhanced side reactions, resulting in lower propylene yields. Deactivation was accompanied by coke deposition (kd = 0.025 h-1), as evidenced by TGA, while regeneration over four cycles confirmed efficient recovery of catalytic performance. Overall, these results establish a structure–surface–performance relationship and highlight support engineering as an effective route to stabilize active cobalt species in environmentally benign PDH.

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HTT0654

Carbonate-mediated CO2 and CH4 Conversion over Metal Oxide-based Catalysts for Value-added Product Production

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Methane, Carbon dioxide, CH3COOH, CH3OH

Abstract Body.
Introduction. The catalytic conversion of CO2 and CH4 into value-added chemicals offers a promising route toward sustainable chemical processes. However, the simultaneous transformation of these thermodynamically stable molecules remains challenging due to the lack of efficient activation pathways. Here, we present a CO2 and CH4 activation strategy inspired by the CO2 adsorbent shuttling behavior between metal oxide (MO) and metal carbonate (MCO3). In this approach, MCO3 supplies pre-activated CO2, enabling its sequential reaction with CH4 to produce CH3COOH [1]. Furthermore, reaction optimization and catalyst modification allow control over product selectivity and improved productivity [2].
Methods. Catalytic reactions of CO2 and CH4 were carried out in a fixed-bed continuous-flow reactor. Metal oxide-based catalysts exhibiting carbonate-forming characteristics were employed. The sequential activation of CO2 and CH4 over representative metal oxide catalysts was investigated to explore pathways toward selective oxygenate formation, including CH3COOH and CH3OH. Mechanistic investigations were performed using multiple characterization and analytical approaches to elucidate the role of carbonate-mediated activation pathways and their influence on product selectivity.
Results and discussion. The catalytic behavior of CO2 and CH4 conversion was strongly governed by carbonate-mediated activation pathways. When CO2 was pre-activated on MO-based catalysts, subsequent exposure to CH4 enabled efficient formation of oxygenated products, demonstrating the importance of sequential activation.
Systematic variation of reaction conditions revealed that surface carbonate species function as dynamic reservoirs of activated CO2, facilitating C−C bond formation through acetate-type intermediates. In particular, sustained CH3COOH synthesis was achieved when sequential CO2 & CH4 activation, and desorption of CH3COOH was recycled, highlighting the critical role of carbonate shuttling between oxide and carbonate phases. Furthermore, altering the activation sequence of CO2 and CH4 redirected product selectivity, with sequential CO2 activation favoring C2 oxygenates, while alternative protocols promoted C1 products such as CH3OH. These results highlight how carbonate-mediated pathways enable tunable and selective CO2 and CH4 conversion over metal oxide catalysts.

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CET0213

Continuous hydrodeoxygenation of bio-derived oils in a pilot-scale reactor toward marine fuel applications

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: Sustainable marine fuels, bio-oil upgrading, continuous hydrodeoxygenation

Abstract Body.

The marine shipping industry is a significant contributor to global emissions of sulfur and carbon. The recent regulations, including the sulfur cap by the International Maritime Organization, have led to the search for cleaner fuel alternatives in maritime transport. Bio-oil is a promising alternative for marine fuel-oriented applications. However, the direct utilization of bio-oils is limited due to their high oxygen and water content, and limited miscibility with conventional marine fuels. Hydrodeoxygenation (HDO) represents a promising upgrading strategy by selectively removing oxygenated functionalities and improving fuel-relevant properties. The aim of this study is to investigate the continuous HDO behavior and product quality in a pilot-scale reactor, with the goal of exploring the potential for marine fuel applications.

In this study, continuous flow HDO experiments were performed in a high-pressure fixed-bed reactor at 250 °C and 300 bar H2 using commercial hydrotreating catalysts. Three experimental cases were investigated under identical operating conditions: i) fast pyrolysis biooil (FPBO) over BASF SHF1; ii) FPBO over BASF HPJ3; and iii) gasification tar (GT) over BASF HPJ3. Liquid products were collected every 30 minutes to evaluate time-on-stream behavior and to define steady-state operation. Product characterization focuses on elemental composition, degree of deoxygenation, changes in key oxygenated species, such as acetic acid, and evolution of water content. Due to limitations in gas quantification, product distributions were evaluated on a liquid-phase basis.

Stable reactor operation was achieved for all investigated cases, as evidenced by the reproducible production of liquid over consecutive collection intervals. For FPBO, consistent phase separation into aqueous and organic phases was observed for both catalysts. FPBO upgraded over SHF1 yielded 56.4 ± 7.1 wt.% organic phase, while HPJ3 produced a comparable distribution of 57.9 ± 1.1 wt.% organic phase, indicating more stable liquid production over HPJ3. The degrees of deoxygenation achieved over SHF1 and HPJ3 were 46% and 25%, respectively. These changes were accompanied by clear shifts toward lower O/C ratios in the Van Krevelen diagram, indicating improved fuel-relevant properties and increased calorific value. In contrast, GT processed over HPJ3 formed a single liquid phase and achieved a DOD of approximately 22%, highlighting strong feed-dependent differences in upgrading behavior under identical steady-state operating conditions.

Continuous hydrodeoxygenation enabled stable pilot-scale upgrading of bio-derived oils, achieving significant oxygen removal and feed-dependent phase behavior. These results

highlight the relevance of continuous HDO as an upstream processing step toward marine fuel-oriented applications.

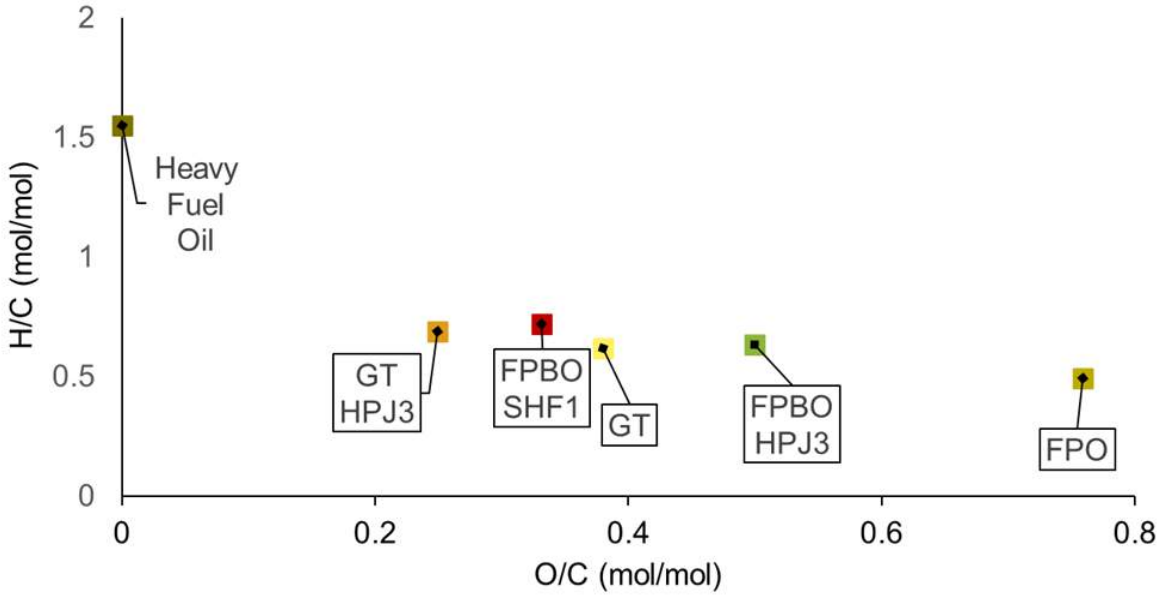

Figure. Van Krevelen diagram of upgraded oils and feedstocks

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HTT0103

Dinuclear Titanium on TS-1 for propylene epoxidation under alkaline conditions

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: TS-1, propylene epoxidation, alkaline condition, dinuclear titanium

Abstract Body.
Propylene oxide (PO) is widely utilized in the production of valuable chemicals such as polyurethanes, polyesters, and propylene glycol (PG). The current industrial methods of PO production rely on toxic reagents and generate substantial amounts of byproducts that need to be removed using additional purification steps. The synthesis of PO via titanium silicalite-1 (TS-1)-catalyzed epoxidation of propylene with H2O2 offers the advantages of a low environmental impact and high selectivity (>95%), although its reliance on H2O2, which is typically generated through the large-scale anthraquinone process. Previously, we reported an integrated photo-electro-heterogeneous catalytic system combining photoelectrochemical H2O2 production and propylene epoxidation. However, this system requires solar energy (which limits PO production to daytime hours) and a substantial amount of land because of the low efficiency of light-driven H2O2 production, which limits practical applications.
We developed an unassisted H2O2 production system requiring no solar or electrical energy by combining the two-electron O2 reduction reaction (2e– ORR) with the formaldehyde oxidation reaction (FOR). However, the above system is active in alkaline solutions and is therefore incompatible with the current propylene epoxidation process based on conventional TS-1, which is only active in neutral solutions.
To overcome the inhibitory effects of alkali metal ions and alkaline conditions on the propylene epoxidation, we modified TS-1 by treating it with tetrapropylammonium bromide (TPABr) and ethanolamine. This modification resulted in the formation of dinuclear titanium sites featuring Ti–O–Ti bonds. The presence of these sites was verified using X-ray absorption spectroscopy (XAS), ultraviolet-visible (UV-vis) spectroscopy, and Raman spectroscopy confirmed the presence of these dinuclear Ti sites. The results of density functional theory (DFT) calculations supported these findings, demonstrating that dinuclear Ti sites were active for propylene epoxidation and synergistically interacted with alkali metal ions to inhibit the hydrolysis of PO to PG. The modified TS-1 exhibited a high epoxidation activity even under alkaline conditions (pH 11), thus holding promise for efficient propylene epoxidation in challenging environments. By integrating the unassisted H2O2 production system with the modified TS-1–promoted propylene epoxidation system, we successfully demonstrated unassisted PO production with in situ H2 generation without the need for solar or electrical energy and achieved a PO productivity (1657 μmolPO cm−2 over 24 h) more than eight times that previously reported for a photoelectrochemical system relying on solar energy.

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HTT0270

Effective oxidative denitrogenation and desulfurization of liquid fuel with sulfonic acid functionalized porous carbon

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Metal-free catalysis, oxidative desulfurization, oxidative denitrogenation, sulfonated carbon

Abstract Body.
Crude fuels contain various sulfur-containing compounds (SCCs) and nitrogen-containing compounds (NCCs) that lead to catalyst poisoning and environmental issues such as acid rain and air pollution. While hydroprocessing is conventional, its high energy (due to high operation pressure/temperature) and hydrogen demands have made oxidative denitrogenation (ODN) and oxidative desulfurization (ODS) promising and more efficient alternatives. In this study, a poly-pyrrole-derived carbon (PDC) was prepared via high-temperature (800 °C) pyrolysis of poly-aniline under inert conditions, followed by modification to create a sulfonic acid functionalized porous carbon (S-PDC). The catalyst and relevant materials were comprehensively characterized using X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), N2 adsorption–desorption, scanning electron microscopy (SEM), transmission electron microscopy (TEM), Fourier transform infrared spectroscopy (FTIR), and Boehm titration.
The S-PDC material was utilized as a metal-free catalyst, for the ODN and ODS of model fuels using H2O2 as a green oxidant. Remarkable performance was confirmed in indole oxidation, achieving complete conversion of 1000 ppm indole within 60 min at 45 °C (with 98% conversion at 25 °C) and a low activation energy of 35.2 kJ mol-1. Additionally, dibenzothiophene (DBT), a representative SCC, was completely oxidized within 120 min at 45 °C, while quinoline could be fully oxidized with a slight optimization of the reaction conditions. This excellent performance is attributed to the well-dispersed sulfonic groups within the carbon matrix, which facilitate H2O2 activation following effective adsorption via electrostatic and hydrogen bonding interactions. Radical scavenger and electron spin resonance (ESR) spectrometry experiments detected no radical generation, indicating the non-radical-based catalysis or the formation of a peroxocomplexes over the catalyst. Based on the oxidation of methylindole isomers and density functional theory (DFT) calculations of H2O2 adsorption energy (Gaussian software), a mechanism involving H2O2 activation and nucleophilic attack from the nitrogen of NCCs onto the formed reactive oxygen species (like, peroxocomplex) could be suggested. Finally, the S-PDC catalyst demonstrated excellent reusability, maintaining high performance over five cycles, indicating its suitability for industrial oxidative purification processes like oxidative denitrogenation and desulfurization.

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HTT0328

Turning an Inert Binder into a Performance Lever: Transport-Driven Performance Gains in Shaped TS-1 for Propylene Epoxidation

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

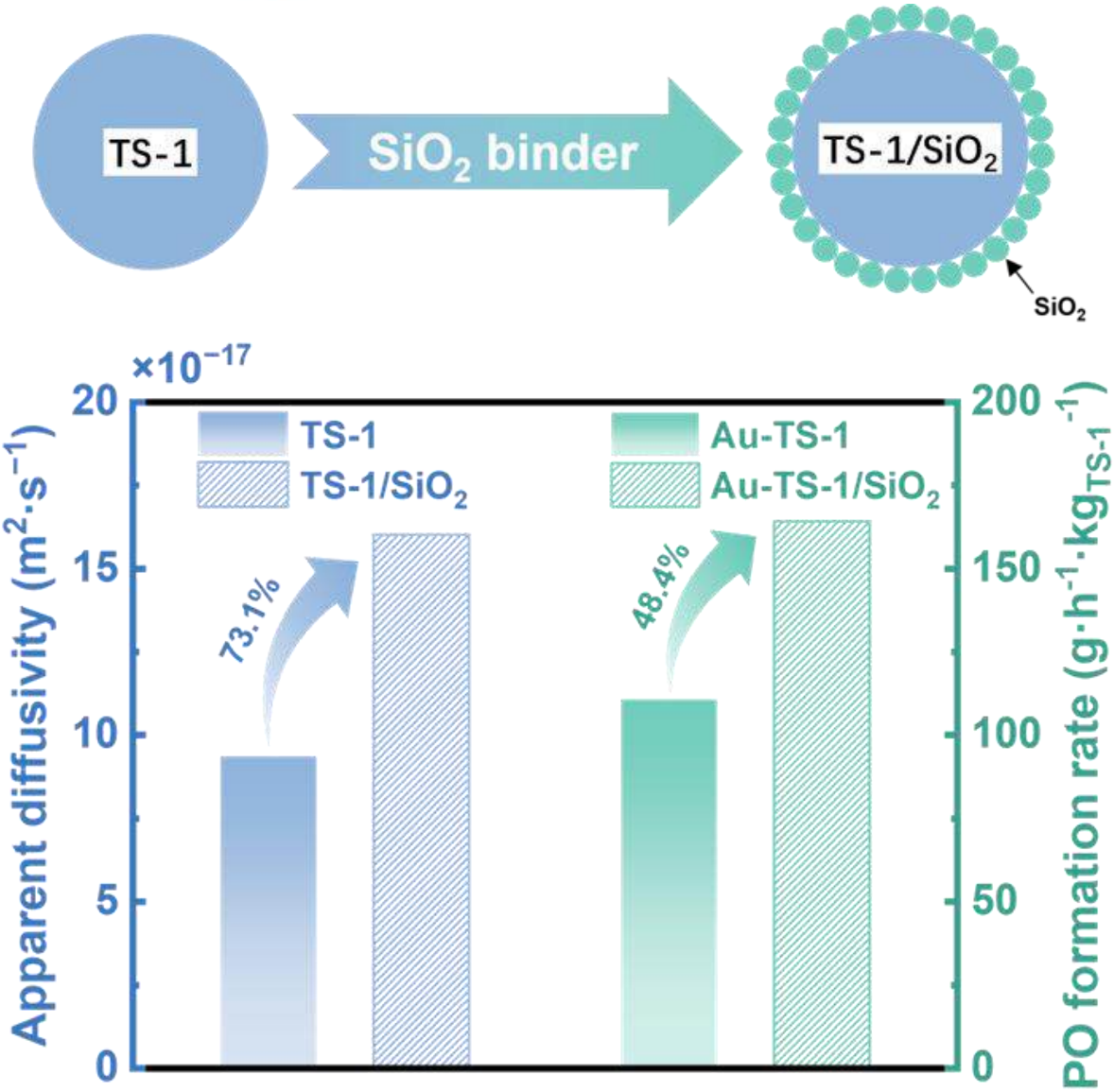
Keywords: TS-1, binder, mass-transfer, surface barrier, propylene epoxidation

Abstract Body.

Purpose. TS-1 is a representative heteroatom zeolite that catalyzes the selective oxidation of various substrates with H2O2 under mild conditions, making it attractive for greener chemical processes due to its high energy efficiency and low waste production. For industrial application, TS-1 powders are typically shaped into binder-containing pellets to enhance mechanical strength. Conventionally, inert binders are considered detrimental to catalytic performance, as they may block active sites and hinder mass transfer [1]. However, the specific influence of a binder on catalytic behavior, particularly in reactions such as propylene epoxidation with H2 and O2 (HOPO), remains unclear. This study examines how an inert binder alters TS-1 surface properties and mass transfer, and elucidates the underlying mechanism for its impact on catalytic performance.

Methods. Shaped TS-1 catalysts (TS-1/SiO2) were prepared by extrusion using SiO2 as a binder. Catalyst testing and kinetic measurements, together with in situ PO-DRIFTS, ZLC analysis, and complementary characterization techniques, were employed to elucidate how the SiO2 binder alters TS-1 surface properties and influences catalytic performance.

Results. Catalytic testing shows that introducing the binder increases both propylene conversion and PO selectivity on TS-1/SiO2, giving a 48.4% higher PO formation rate than binder-free TS-1 (Fig. 1). In situ PO-DRIFTS indicates weaker PO adsorption strength on TS-1/SiO2. ZLC measurements show a 73.1% increase in apparent PO diffusivity (Fig. 1), suggesting that PO retained in TS-1/SiO2 can desorb and diffuse out of the pores into the bulk gas phase more rapidly. Kinetic experiments show a lower apparent activation energy for the HOPO reaction on TS-1/SiO2 and a PO apparent reaction order closer to zero (−0.42), compared with −0.94 on TS-1. Collectively, these results indicate that the improved catalytic performance arises from enhanced mass transfer enabled by the introduced SiO2 binder. This binder partially covers the TS-1 surface, weakens the interaction between PO and TS-1 surface, reduces the surface barrier, and promotes PO desorption and diffusion. This re-exposes active sites and increases catalytic turnover, thereby enhancing catalytic performance.



Conclusions. Incorporating an SiO2 binder during TS-1 shaping not only provides mechanical integrity but also beneficially modifies surface properties, reducing the surface barrier and enhancing PO mass transfer to alleviate product inhibition in the HOPO reaction. As a result, the PO formation rate increases by 48.4%. This offers a rational strategy for designing high-performance shaped TS-1 catalysts and may be extended to other catalytic systems with strong product inhibition.

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HTT0385

Mechanistic Insights into Catalyst Deactivation during heterogenous Co-Oligomerization of C_2–C_4 Olefins to Fuels

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Heterogeneous catalysis, CO2 emissions, deactivation mechanism, co-oligomerization, sustainable aviation fuels (SAF).

Abstract Body.
Introduction: Aviation contributes 2-3% of global CO2 emissions. Sustainable Aviation Fuels (SAF) is one of the viable options for reduction of these emissions. The heterogeneously catalyzed co-oligomerization of lower olefins produced from methanol to SAF is successfully demonstrated.
Methods: A continuously operated lab plant with a fixed bed reactor is used to perform co-oligomerization experiments for 75 h to collect fuel and study the deactivation of catalyst. The feedstock is a mixture of ethylene, propylene and1-butylene (40/40/20 mol%) at 32 bar, 200 °C and space velocity of 4 h-1. 4 wt.% nickel/silica-alumina is employed as the catalyst. The products are in the range of gasoline, kerosene and diesel fuel. The mixture is distilled for kerosene cut and properties are evaluated.
Results and discussion: The initial conversions of ethylene, propylene and butylene are 60.7%, 80.1% and 54.5%, respectively. After 10 h, conversion dropped rapidly due to the deactivation of the catalyst. Extensive investigations are carried out on the fresh and spent catalysts to understand the mechanism of deactivation. The SEM images (Scanning Electron Microscopy) show that the size of nickel conglomerates is temperature dependent. The TEM (Transmission Electron Microscopy) studies show uniform dispersion of nickel particles and sintered nickel particles. Additionally, there is considerable reduction in the acidity of the catalyst measured from chemisorption resulting in a new spinel like nickel aluminate phase formation. The formation of this phase indicates metal-support interaction resulting in loss of active metal and acidity of the support.
In conclusion, the mechanism for deactivation could be nickel sintering as detected by TEM, nickel species migration to the support resulting in loss of Brønsted acid sites and formation of nickel aluminate phase as well as nickel leaching (<0.02 mg/kg). Nevertheless, the role of process temperature employed for the reaction in postulating deactivation mechanism is also noteworthy.

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HTT0467

Optimizing Metathesis-Dehydrogenation Catalysts Paring for Tandem Alkane Cross-Metathesis of Polyethylene

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Olefin metathesis, dehydrogenation, alkane cross-metathesis, plastic recycling, polyethylene

Abstract Body.

Chemical recycling of polyolefin waste into value-added products is increasingly important for carbon neutrality and mitigation of plastic pollution. Tandem alkane cross-metathesis (TACM) was emerged as a promising process for non-hydrogen route for polyethylene (PE) into saturated hydrocarbons at moderate temperatures (<300 °C). However, practical implementation remains challenging due to the intrinsic complexity arose form tandem catalytic system, in which dehydrogenation and olefin metathesis must operate in concert. Thus, TACM performance is highly sensitive to catalyst combinations, support effects, and pretreatment process.

Here, we systematically investigated heterogeneous metathesis active sites (MoOx, WO-x) supported on various supports (SiO2, Al2O3, mesostructured supports) and evaluated TACM performance in combination with robust dehydrogenation catalysts, including commercial Pt/Al2O3. Among the metathesis catalysts, MoOx/MCM-41 exhibits the highest activity, enabling TACM to overcome metathesis-limitation under our operating conditions. We identified the deactivation of tandem catalysis arose from the metal migration during high-temperature pretreatment, leading us to develop a two-step pretreatment protocol that suppresses the migration, resulting in markedly improved stability and reactivity. Utilizing the various combinations of dehydrogenation and metathesis catalysts, we revealed that the catalyst combination and support property strongly influence TACM efficacy, with mesostructured MCM-41 supported systems outperforming amorphous silica and alumina.

This comprehensive investigation provides valuable insights into catalyst design, pretreatment optimization, and thereby establishing a robust, hydrogen-independent pathway for polyolefin recycling. These advancements bring TACM closer to practical viability, offering a sustainable solution to the global plastic waste crisis.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

HTT0558

Scalable Olivine-Derived Catalysts for Non Oxidative Methane Coupling with Enhanced Ethylene Selectivity

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Non-oxidative methane coupling; Olivine-derived catalyst; Ethylene selectivity; Scalable catalyst synthesis; Sustainable catalysis

Abstract Body.

Purpose

Non-oxidative methane coupling (NMC) is a promising and sustainable route for the direct production of value-added hydrocarbons and H2 without CO2 emissions. The key challenge is achieving high ethylene selectivity alongside sufficient methane conversion. Low selectivity to ethylene often stems from side reactions forming aromatics, coke, or higher hydrocarbons, compounded by rapid catalyst deactivation under harsh conditions (>950°C). This study introduces a cost-effective and scalable catalyst synthesis strategy that utilizes olivine, an abundant Fe–Mg silicate. We evaluate the catalytic performance of the olivine-based catalyst, focusing on activity, ethylene selectivity, and stability during NMC reactions.

Methods

Olivine-derived catalysts were prepared by ball milling olivine with silica gel (SiO2–to–olivine mass ratios of 0:100, 5:95, 10:90, 20:80, and 30:70), followed by calcination at 1000 °C for 6 h. This treatment promotes in situ solid–solid interactions that disperse iron oxide species within the SiO_2 matrix, yielding highly dispersed iron oxide domains incorporated into the silica structure. This approach is intended to improve the stability of active iron sites and mitigate agglomeration and deactivation during high-temperature operation.

Results

Among the catalyst series, the sample with an olivine–to–silica gel mass ratio of 5:95 exhibited the best catalytic performance. Under identical operating conditions (1000 °C, 7% methane conversion), this catalyst achieved a higher C_2H_4 space–time yield (63 vs. 38 $\mu mol \cdot min^{-1} \cdot g^{-1}$, carbon-atom basis) and higher ethylene selectivity (22% vs. 13%) compared to the widely studied $0.5Fe/SiO_2$ catalyst in the literature (Liu et al). Although coke formed during the reaction, the catalyst fully recovered its activity after regeneration (Figure 1).

Conclusions

An effective NMC catalyst can be synthesized directly from a low-value natural mineral via a simplified, energy-efficient route. The olivine-derived catalyst delivers enhanced ethylene

selectivity and full regenerability. Systematic variation of the olivine-to-silica ratio identified an optimal composition, highlighting the role of controlled iron dispersion and physicochemical properties in governing catalytic performance. Overall, these results underscore the potential of mineral-derived catalysts for industrially viable, carbon-neutral methane conversion technologies.

Keywords
Non-oxidative methane coupling; Olivine-derived catalyst; Ethylene selectivity; Scalable catalyst synthesis; Sustainable catalysis

References:

Liu, Z.; Cheng, S.; Schulman, E.; Chen, W.; Vlachos, D. G.; Shu, Y.; Tran, D. T.; Liu, D. Direct non-oxidative methane coupling on vitreous silica supported iron catalysts. Catalysis Today 2023, 416, 113873. DOI:10.1016/j.cattod.2022.113873.

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HTE0581

Size-Dependent electrochemical CO_2 reduction on diverse bimetallic gold silver alloy nanoparticle morphologies: Synergistic effects on CO selectivity

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Electrochemical

Keywords: CO_2 reduction reaction (CO_2RR), Gold nanoparticles, Silver nanoparticles, Au-Ag alloy nanoparticles, Nanoporous gold, Size-dependent catalysis

Abstract Body.
Gold and silver-based nanoparticles are widely explored as catalysts for the electrochemical carbon dioxide reduction reaction (CO_2RR) due to their strong tendency to produce carbon monoxide (CO) with high selectivity. In this study, bimetallic Au-Ag alloy nanoparticles with controlled particle sizes in the 15-50 nm range were synthesized and compared to understand the influence of particle size, composition, and structure on catalytic performance. Electrochemical CO_2RR experiments were performed under identical conditions, and the results revealed a clear size-dependent trend for both Au and Ag nanoparticles, where smaller particles exhibited higher CO production than larger ones. Gold nanoparticles consistently delivered higher CO yield compared to silver, highlighting their superior intrinsic activity. The Au-Ag alloy nanoparticles showed improved performance relative to their individual metal counterparts, due to synergistic electronic and geometric effects that optimize intermediate binding and partially suppress the competing hydrogen evolution reaction (HER). Among all the catalysts investigated, nanoporous gold displayed particularly interesting behavior, showing the highest overall CO formation and distinct catalytic characteristics compared to the nanoparticle systems. This enhanced performance is broadly associated with its large electrochemically active surface area, interconnected porous framework, and abundance of defect-rich active sites. Overall, the comparative study demonstrates that catalyst size, composition, and structural design play a crucial role in tuning CO_2RR efficiency and selectivity, and that nanoporous architectures offer promising directions for developing more effective CO_2 reduction catalysts.

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HTT0310

Promotional Effect of Silica Shell Coated NiO Physically Mixed with Mo/HZSM-5 Catalyst on Methane Dehydroaromatization

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Methane dehydroaromatization, Mo/HZSM-5, NiO, Silica shell, Carbon nanotube.

Abstract Body.

The commercialization of methane dehydroaromatization (MDA) over Mo/HZSM-5 is significantly hindered by low catalytic activity and rapid catalyst deactivation. While physical mixing of NiO promoters can enhance activity and stability, their effectiveness is limited at smaller particle sizes because nano-sized Ni tends to react with MoOx to form inactive NiMoO4, which is detrimental to MoCx dispersion. This study aims to overcome this limitation by introducing a controlled silica shell on NiO particles of various sizes (5, 15, and 110 nm) to prevent unfavorable Ni-Mo interactions while maintaining the promotional effect of small-sized Ni.

Core-shell structured NiO@SiO2 particles were synthesized using a modified Stöber method and physically mixed with 12 wt.% Mo/HZSM-5 catalysts. To achieve a uniform coating on extremely small particles, NiO was supported on SiO2 nanospheres before shell introduction. Catalytic performance was evaluated in a fixed-bed quartz reactor at 700 °C under a 90 vol.% CH4 feed. The catalysts were characterized using XRD, CH4-TPSR, CO chemisorption, TEM-EDS, Raman spectroscopy, and TGA.

We found that the physical mixing of NiO with Mo/HZSM-5 leads to significant improvements in both BTX yield and catalytic stability. Ni facilitates the reduction of MoOx, which effectively enhances the dispersion of MoCx active sites within the zeolite channels and it promotes the growth of carbon nanotubes (CNTs) on itself rather than the accumulation of detrimental amorphous coke on the Mo active sites. The introduction of a silica shell on NiO plays a supplementary role by protecting nano-sized Ni from strong interactions with Mo, allowing the promotional effect of NiO to be maintained even at extremely nano-scale sizes. The MoOx activation temperature decreased proportionally with decreasing NiO size, from 652 °C (110 nm) to 589 °C (~5 nm). Correspondingly, CO uptake (an indicator of MoCx dispersion) increased from 0.19 cm^3/g for bare Mo/HZSM-5 to 0.91 cm^3/g for the (NiO/SiO2)@SiO2-Mo/HZSM-5 catalyst (~5 nm). This catalyst achieved the highest maximum BTX yield of 7.20%. Furthermore, the nano NiO@SiO2 catalyst (~15 nm) showed a significant improvement in both BTX yield (5.97%) and stability, as NiO particles effectively converted coke precursors into carbon nanotubes. This study demonstrates that the introduction of an appropriately designed silica shell maximizes the promotional effect of physically mixed NiO by protecting the Ni-Mo interaction. By enabling the use of smaller Ni particles without forming inactive phases, this

strategy enhances MoCx dispersion and provides a comprehensive approach for designing robust and high-performance catalysts for MDA.

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HTT0485

Structure-guided control of Al sites in MFI zeolites: Toward rational catalyst design for efficient methane dehydroaromatization

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Methane dehydroaromatization, Zeolite, Structural directing agents, Density functional theory

Abstract Body.

Purpose

Methane dehydroaromatization (MDA) offers a direct route to convert abundant methane into valuable aromatic hydrocarbons without syngas intermediates. However, catalyst deactivation by coke formation and limited BTX selectivity remain major challenges. In Mo/ZSM-5 catalysts, the interaction between molybdenum species and Brønsted acid sites associated with framework aluminum is critical, yet the influence of aluminum siting within the MFI framework has not been systematically clarified. This study aims to elucidate how precise control of aluminum distribution affects metal dispersion, reaction pathways, and catalyst stability in MDA.

Methods

MFI zeolites with controlled aluminum siting were synthesized using tailored combinations of structure-directing agents, including tetrapropylammonium cations, sodium ions, and pentaerythritol. Aluminum atoms were selectively positioned at channel intersections, within straight and sinusoidal channels, or distributed across both environments. Aluminum siting was characterized by high-field 27Al MQ MAS NMR spectroscopy, ion-exchange analysis, and ethylene aromatization as a probe reaction. After molybdenum impregnation, the dispersion, oxidation states, and reducibility of Mo species were investigated using X-ray photoelectron spectroscopy, H_2-temperature-programmed reduction, transmission electron microscopy, and X-ray absorption spectroscopy. Density functional theory calculations were performed to evaluate the stability of Mo2C2 species and benzene adsorption behavior in

different aluminum environments.

Results

Zeolites synthesized using the pentaerythritol–sodium combination exhibited a dominant population of channel-located aluminum sites, which generated stronger Brønsted acidity and provided robust anchoring sites for molybdenum species. This led to highly uniform Mo dispersion and a significantly higher surface Mo concentration compared to catalysts with intersection-dominant aluminum distribution. DFT results revealed that channel environments stabilized Mo_2C_2 species more effectively and reduced benzene adsorption energies, facilitating faster product desorption. Consequently, the optimized catalyst achieved the highest initial BTX yield and exhibited superior stability with substantially reduced coke formation, favoring the formation of more easily removable graphitic carbon.

Conclusions

This study demonstrates that aluminum siting within the MFI framework is a decisive parameter governing metal–support interactions, product desorption, and coke suppression in methane dehydroaromatization. Precise control of aluminum distribution provides a rational design strategy for developing highly active and stable zeolite-based catalysts for efficient methane upgrading.

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HTT0599

Screw-Extruder-Assisted Catalytic Upcycling of High-Viscosity Polyethylene Waste

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Zeolite Beta, Catalytic PE upcycling, Screw extrusion; Reactive extrusion

Abstract Body.
This study examines the role of catalyst particle size and screw-extrusion-assisted processing on the degradation reactivity of polyethylene during reactive extrusion. Two zeolite Beta catalysts with comparable framework compositions (Si/Al ≈ 13) but distinct particle sizes of micron-sized Beta-M and nano-sized Beta-N were systematically compared.
Quantitative kinetic analysis based on rheological degradation demonstrates that Beta-N exhibits significantly higher intrinsic reactivity than Beta-M. Under fresh-feed reactive extrusion conditions, the apparent degradation rate constant of Beta-N ($k = 24.1 \times 10^{-3}$ min^{-1}) is approximately two times higher than that of Beta-M ($k = 11.4 \times 10^{-3}$ min^{-1}), clearly indicating superior catalytic degradation performance. Transmission electron microscopy reveals that Beta-M consists of agglomerated particles with characteristic sizes of ~300 nm, whereas Beta-N is composed of nanosized primary particles with an average size of ~20 nm. These differences in particle size lead to pronounced contrasts in catalyst dispersion and accessible surface area within the polymer melt during extrusion. The improved dispersion of Beta-N enhances effective polymer–catalyst contact, thereby accelerating chain scission and molecular-weight reduction under identical processing conditions.
The screw extruder plays a critical role beyond serving as a thermal reactor by providing intense shear and continuous mixing. This processing environment disrupts polymer chain entanglements, improves melt homogeneity, and reduces mass-transfer limitations between the polymer and catalyst. As a result, catalyst-containing systems show a pronounced time-dependent reduction in shear stress and apparent viscosity, while catalyst-free samples exhibit only minor changes. When premixed-feed reactive re-extrusion is employed, degradation kinetics are further intensified. Rate constants increase dramatically, reaching up to 52.0×10^{-3} min^{-1} in Beta-N-rich systems, corresponding to nearly a 50-fold enhancement compared with catalyst-free reactive extrusion. This strong acceleration highlights the synergistic effect between nanoscale catalyst dispersion and extrusion-induced rheological pretreatment.
Overall, the results demonstrate that, even at similar Si/Al ratios, catalyst particle size and extrusion-driven dispersion critically govern degradation kinetics. Reactive re-extrusion combined with nano-sized catalysts offers an effective and scalable strategy for controlling molecular-weight reduction and enabling catalytic upcycling of high-viscosity polyethylene waste.

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HTT0622

Ammonia cracking activity assessment of PGM catalyst deposited on high surface carbon supports

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: ammonia cracking; catalysis; carbon xerogels; nitrogen-doped carbons; hydrogen production

Abstract Body.

Introduction.

Hydrogen is a sustainable and long-term energy carrier with the capacity to meet growing global energy demands.[1,2] It can be applied across sectors such as transportation, industry, and heating systems. However, the volatile and flammable nature of hydrogen poses significant challenges, particularly in distribution via pipelines due to the risk of leakage.[3] Ammonia offers a promising alternative as a hydrogen carrier, with a high hydrogen content (17.6 wt%), carbon-free properties, and ease of storage at low pressure (~7.5 atm at 300 K).[4,5] The endothermic NH_3 cracking process can reliably generate hydrogen for clean energy technologies like fuel cells.[6] Despite this potential, the cost and low energy efficiency of current NH_3 cracking catalysts hinder their large-scale adoption.[5,7] The performance of ruthenium-based catalysts is influenced by a number of factors, including the textural and structural properties of the catalyst support, the Ru particle size distribution, and the use of catalyst promoters.

Methods.

The samples 2Ru2Y/CX were synthesized through a wet impregnation method and a subsequent reductive deposition method. The carbon xerogels supports were synthetized by polycondensation of resorcinol and formaldehyde in aqueous solution. Porosity and electronic properties were tuned either by KOH activation or by nitrogen doping through a co-precursor route using urea as the nitrogen source. Fresh supports and catalysts were characterized using BET, XRD, CO-TPD, CO2-TPD, TPR, SEM, TEM and XPS techniques. Catalytic activity was evaluated for ammonia decomposition under controlled reactor conditions, and durability was assessed by extended time-on-stream operation and/or repeated thermal/operational cycling to quantify deactivation with time. After durability testing, post-mortem characterization of spent catalysts was performed, and the degradation mechanisms was investigated.

Results and discussion.

The ruthenium content was partially substituted with the secondary element yttrium, thereby allowing a reduction in the PGM usage. Synthesis of high surface areas carbon xerogels (SBET ≈ 1350 m2g-1) has been achieved, facilitating the uniform deposition of Ru nanoparticles (≤ 2 nm) and enhancing the catalytic performances. Current studies are focused on the identification of structural and chemical changes subsequent to durability testing, with a view to correlating degradation mechanisms with activity decay.

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HTT0652

Mixed zeolite system for catalytic cracking to enhance light olefin yield and selectivity

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Mixed zeolite system, light olefin, 10MR zeolites

Abstract Body.
Polyolefins, mostly used for packaging, take up about two-thirds of all plastic waste produced globally. Various methods to treat these wastes in a sustainable way are being researched, with catalytic cracking of WPPO being one of them. Zeolites are widely used in catalytic cracking due to their porosity and acidity. Among those, ZSM-5 (MFI), a 3-dimensional 10MR zeolite, is widely used. While the strong acidity of the 10-membered ring is advantageous, MFI also has a high shape selectivity for BTX, which is a loss in the light olefin yield point of view. In this research, we review the effects of mixed zeolite systems of zeolite Beta(*BEA) with several non-3-dimensional 10MR zeolites to enhance light olefin yield and selectivity in catalytic cracking of WPPO.
Zeolite Beta(*BEA) was selected for its large pore and high acidity, which are advantageous for treating bulky molecules. We prepared zeolite Beta with a Si/Al ratio of 11.5 and particle size of 450 nm, and physically mixed them with 10MR zeolites in a 1:2 ratio, which we found to be the optimum. We used dodecane as the model feed and MTT, FER, and TON of various Si/Al ratios and morphologies for the 10MR zeolites.
Cracking tests using these mixed zeolites showed that all three zeolite structures suppressed BTX formation while maintaining light olefin selectivity compared to MFI (Albemarle co.). In the case of the *BEA/MTT(Si/Al=25) system, it not only maintained the light olefin yield but also increased it by 13.2%. This was due to the increase in propylene yield, since ethylene yield decreased. Comparison with single zeolite systems using the same *BEA and MTT samples showed that the mixed system shows a synergistic effect on BTX suppression and propylene production. Results using MTT with the same Si/Al ratio with different particle size and morphology imply that these too play an important role.
These results imply that with optimization in Si/Al ratio, particle morphology, and mixing ratio, mixed zeolite systems using *BEA and 10MR zeolites can help enhance light olefin yield. Also, further research could help us understand the effect of mixed systems in terms of reaction mechanisms.

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HTT0667

Synergistic Co-pyrolysis of Coconut Husk and HDPE for CNT Synthesis: Catalyst and Process Optimization

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Carbon nanotubes, Co-pyrolysis, Coconut husk, High-density polyethylene, Bimetallic catalysts.

Abstract Body.
Introduction. This study aims to utilize coconut husks (CH) considered as one of the largest agro-industrial waste products in Thailand by co-pyrolyzing them, along with high-density polyethylene (HDPE) waste, into value-added carbon nanotubes (CNTs) via a catalytic chemical vapor deposition (CCVD) using metal catalysts. Incorporating HDPE with CH increases the carbon content and potentially creates a synergistic effect in CNT formation.

Methods. A two-stage fixed-bed reactor using nitrogen as a carrier gas was employed for co-pyrolysis and CCVD experiments. In the 1st stage, flash co-pyrolysis of CH and HDPE at various weight ratios occurred at 400–600 °C, while in the 2nd stage, CNT synthesis via CCVD was performed at 800 °C using bimetallic catalysts (2:1, w/w) of 30% CoMo, NiMo, or FeMo supported on MgO, SiO2, and Al2O3 as shown in a schematic diagram in Fig. 1.

Results and discussion. Among all catalysts, FeMo/SiO2 failed to produce CNTs when co-pyrolyzing 25 wt% CH blended with HDPE at 600 °C, while NiMo/Al2O3 demonstrated the best performance, achieving the highest carbon yield of ~16.2 wt%, exceeding the CNT yield obtained from pure HDPE (11.6 wt%) due to its synergistic effect during co-pyrolysis. By decreasing co-pyrolysis temperature to 450 °C, the highest carbon yield of ~51.7 wt% was achieved using 25 wt% of CH in HDPE. SEM images confirmed that uniform and small CNTs (14.5–15.3 nm) with a high graphitization degree (Ig/Id = 1.45 by Raman spectroscopy) could be obtained under the optimum condition. Further increasing biomass (CH) ratio in HDPE to 50 wt%, carbon yields slightly decreased to 48.7 wt% and drastically dropped to 20.2 wt% for 75 wt% CH in HDPE because of too high oxygen content in the mixed feedstock. These findings suggested that coconut husk can serve as a sustainable carbon source for CNT synthesis when combined with HDPE using the suitable catalyst and process conditions.

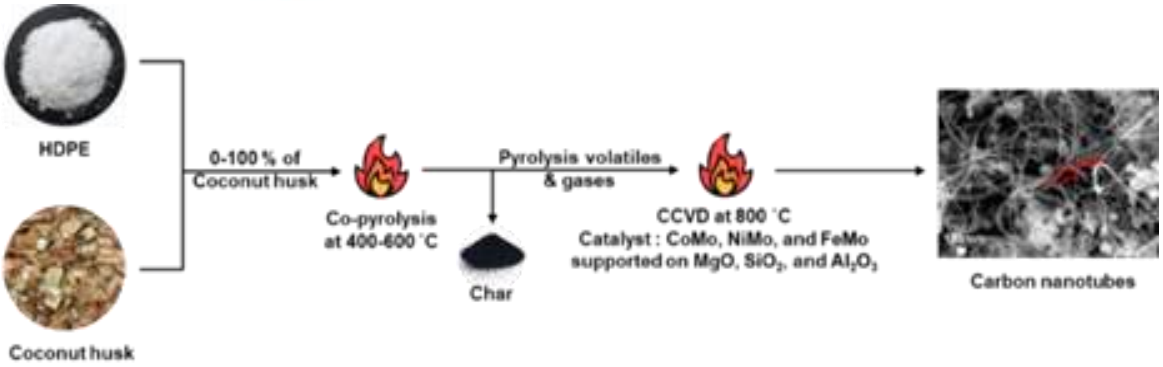

Fig. 1. Schematic diagram of CNT synthesis from co-pyrolysis of coconut husk and HDPE.

Acknowledgments: The authors express gratitude to the Mahidol University Frontier Research Facility (MU-FRF) and Catalysts & Carbon Nanotubes Reaction Process Prototyping Laboratory (CARP LAB), Mahidol University, for providing laboratory facilities and equipment.

Oral Presentation

Hydrogen

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HTE0326

Intrinsic Activity Enhancement of Iridium Oxide via a Modified Adams Fusion Route for Low-Ir Proton Exchange Membrane Water Electrolysis

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Electrochemical

Keywords: Iridium oxide, Oxygen evolution reaction, Adams fusion method, Low-Ir anode, Proton exchange membrane water electrolysis

Abstract Body.
Proton exchange membrane water electrolysis (PEMWE) is a key technology for sustainable hydrogen production amid decarbonization efforts. With high efficiency, rapid response to power inputs, and compact system design, PEMWE is well suited for integration with renewable electricity. However, the anode oxygen evolution reaction (OER) proceeds under acidic conditions and high current densities, necessitating iridium (Ir)-based catalysts. Ir is scarce and expensive, so catalysts with higher intrinsic activity are needed to reduce Ir loading. In practice, Ir is deployed as iridium oxide rather than metallic Ir due to superior anodic stability. The Adams fusion method is widely used because of its simplicity and scalability, typically yielding stable rutile-type IrO2. Nevertheless, conventional Adams-derived IrO2 often shows limited intrinsic activity, attributed to high crystallinity and a low density of electrochemically active sites. Therefore, tailoring the structure and electronic state of Adams-derived iridium oxide is a promising route to accelerate OER kinetics.
In this study, a modified Adams fusion method was systematically investigated to enhance intrinsic OER activity. Synthesis parameters—including alkaline additives during precursor mixing, calcination temperature, and post-synthesis acid-treatment procedures—were screened to identify conditions that maximize activity while retaining acid stability. The optimized catalyst (MA-IrOx) was characterized by electron microscopy, N2 adsorption–desorption, X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), and in situ Raman spectroscopy. OER activity was evaluated using a rotating disk electrode (RDE) in acidic electrolyte, followed by membrane electrode assembly (MEA) fabrication and PEMWE single-cell testing.
MA-IrOx exhibits a layered, platelet-like morphology with suppressed crystallinity (XRD) and an increased fraction of Ir(III) species relative to conventional Adams IrO2 (XPS). In half-cell measurements, MA-IrOx delivers an overpotential of 292 mV at 10 mA cm-2 and a mass activity of 73.63 A gIr-1 at 1.55 V_RHE. In an MEA with an ultralow Ir loading of 0.2 mg cm-2, the MA-IrOx anode achieves 1.744 V at 2.0 A cm-2 under PEMWE conditions, representing a

124 mV reduction versus Adams IrO2. In situ Raman spectroscopy reveals potential-dependent Ir–O stretching features for MA-IrOx, indicating a significant contribution from an oxide-pathway mechanism, whereas crystalline rutile Adams IrO2 predominantly follows the adsorbate evolution mechanism. In summary, MA-IrOx enables higher intrinsic OER activity and improved low-Ir PEMWE performance via a scalable modified Adams fusion route.

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HTE0361

Pulsing Towards High Selectivity Electrochemical Furfural Hydrogenation Over Multimetallic Sulfide Electrodes

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Electrochemical

Keywords: Pulse electrolysis, Furfural hydrogenation, elementary step optimization

Abstract Body.
Selective electrochemical hydrogenation (ECH) of furfural (FF) has the potential to produce several end products, such as furfuryl alcohol (FA) via aldehyde group hydrogenation, 2-methyl furan (2-MF) via aldehyde group deoxy hydrogenation, and 2-Methyl tetrahydrofuran (2-MTHF) through an additional ring hydrogenation process1. FF-ECH involves electrocatalytic water dissociation to generate adsorbed active hydrogen (H*) at particular sites, followed by interaction with co-adsorbed FF at adjacent catalytic sites to yield hydrogenation products. However, achieving specific site hydrogenation to control the selectivity and conversion of furfural is highly challenging as a result of lack of active H* and excessive HER in alkaline and acidic electrolytes, respectively. Hence, efficient electrocatalysts that balance active hydrogen (H*) generation and FF adsorption are crucial for selective FF-ECH. In addition, most systems exhibit conversion selectivity tradeoffs2, illustrating the highly challenging nature of the reaction. Accordingly, multimetallic electrocatalysts designed to preferentially interact with specific intermediates and starting materials are believed to steer selectivity while affording high conversion. Hence, in this work, to alleviate the challenges in conventional static ECH, a dynamic operation with periodic pulsing is introduced to maximize and assist in increasing surface coverage of intermediates impart simultaneously high conversion and selectivity. The electrocatalysts are synthesized via a sol-gel method followed by gelling, solvent exchange, and CO2 supercritical drying to obtain multimetallic oxide aerogels, which were exposed to sulfurization to get the final sulfide aerogels. The FF-ECH was performed in a 3-electrode, H-type electrochemical cell with 50mM FF+1M KOH as the catholyte and 1M KOH as the anolyte. Different pulse voltages were applied for 25ms every 20min while the rest of the reaction was conducted at a constant current of -50mA. As can be seen from Figure 1, static operation resulted in a significantly high conversion of 86% with a selectivity of 15% towards FA. Interestingly, the introduction of pulse resulted in a pronounced improvement in selectivity towards FA compared with the static operation. This improvement is attributed to the creation of abundant H* on the electrode surface during the pulsing intervals, which resulted in balanced FF and H* coverage. The successful identification and optimization of a unique pulse profile is expected to pave the way for accessing ring opening and complete hydrogenation products by electrocatalysis.
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KN0151

Polymer Syntheses Toward Carbon-Neutral Future

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Abstract Category: Invited Lecture - Keynote Lecture

Keywords: CO2/epoxide copolymerization, polyolefin catalyst, ethylene tetramerization catalyst, polyolefin-polystyrene block copolymer synthesis

Abstract Body.

Keywords: CO2/epoxide copolymerization; polyolefin catalyst; ethylene tetramerization catalyst; polyolefin-polystyrene block copolymer synthesis

Introduction. Currently, approximately 400 million tons of polymers are produced and used annually worldwide, leading some to define the present era as the “Polymer Age,” following the Iron Age. While polymers serve as indispensable materials that support modern civilization in numerous beneficial ways, they have also given rise to serious challenges, including carbon emissions, marine pollution, and microplastics. Addressing these issues is essential, and diverse efforts and strategies are actively being pursued globally to mitigate their impact.

Methods. Various efforts have been undertaken in my laboratory over the past two decades to address these challenges, with a particular focus on the development of efficient catalysts for CO2/epoxide copolymerization,1 polyolefin elastomer (POE) synthesis,2 ethylene tetramerization,3 and the synthesis of POE–polystyrene block copolymers.4

Results and discussion. CO2/epoxide copolymers are particularly attractive because they can incorporate up to 50 wt% of CO2 directly into the polymer backbone. My group developed a highly efficient catalyst that initiated commercialization efforts in industry; however, its large-scale industrial implementation was ultimately unsuccessful. In contrast, a catalyst developed by my group was successfully implemented in industry for the production of POE, which is now widely used as an encapsulation material for solar cell panels, thereby contributing to a carbon-neutral future. POE is a type of polyethylene containing a substantial amount of 1-octene. As demand for POE continues to grow, we have further developed an efficient catalyst capable of selectively producing 1-octene from ethylene. In addition, my group has developed a novel approach to the synthesis of POE–polystyrene block copolymers, which may offer significant advantages for polymer recycling. These latter two technologies are currently being actively pursued for commercialization within the Korean petrochemical industry.

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DER0775

Electrochemical Reactor Modeling for Sustainable Alkane Dehydrogenation

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Keywords: Alkane dehydrogenation; Reactor design, Electrochemistry, multiRegionFoam

Introduction. Electrochemical reactors employing selective proton/ ion conducting membranes have emerged as promising technologies for sustainable hydrogen production, CO_2 utilization etc at intermediate-to-high temperatures. The performance of such reactors is inherently governed by complex couplings among fluid flow, mass transfer, heat transfer, and electrochemical reaction kinetics[1]. Understanding these interactions is essential for guiding rational design and scale-up of electrochemical reactor system. Computational Fluid Dynamics (CFD) offers powerful framework to address these complex multi-physics phenomena by solving the coupled conservation equations for momentum, energy, species, and charge transport incorporating relevant rection kinetics. The present work aims to develop a CFD model for electrochemical membrane (proton conducting) reactors (ECR) within the open-source C++ library OpenFOAM, incorporating catalytic conversion of short chain alkanes to alkenes. Further, to validate the proposed model with existing experimental data under different operating conditions.

Methods. In the present work, a simplified 2D ECR consists of a porous solid electrolyte sandwiched between two porous electrodes which consist of electrolyte material (see **Fig 1(i)**) is considered. The catalytic conversion of alkane takes place in anode, followed by dissociation of H_2 into H^+ ions which migrates through the solid membrane to the cathode. The H^+ protons are electrochemically converted to H_2 gas at cathode and removed by purge gas. The CFD model of ECR is developed using multiRegionFoam platform proposed by Alkafri et al.[2] implemented in OpenFOAM extend 4.1.

Results and discussion. First, only the catalytic conversion reaction $(C_2H_6 \Leftrightarrow H_2 + C_2H_4;\ \Delta H = 137\ kkk/mol)$ is incorporated and simulations are performed (without electro-chemistry). In the beginning, the alkane dehydrogenation reaction proceeds in the reverse/backward direction i.e., alkene and hydrogen are consumed to produce alkane (see **Fig(ii)(b)**) followed by hydrogen diffuses from the reactive-region to membrane and finally to the purge region. At large time (t = 50 s), the reaction proceeds in the forward direction resulting in production of alkene and hydrogen (**Fig(ii)(a)**). The relevant physis of electrochemistry will be incorporated with the current solver and validation of model will be presented. In addition, effect of different parameters e.g., applied potential, flow rates, operating temperature on the alkane conversion, yield and different transport resistance (heat transfer, mass transfer. Electric potential) which becomes rate-limiting for alkane conversion will be discussed.

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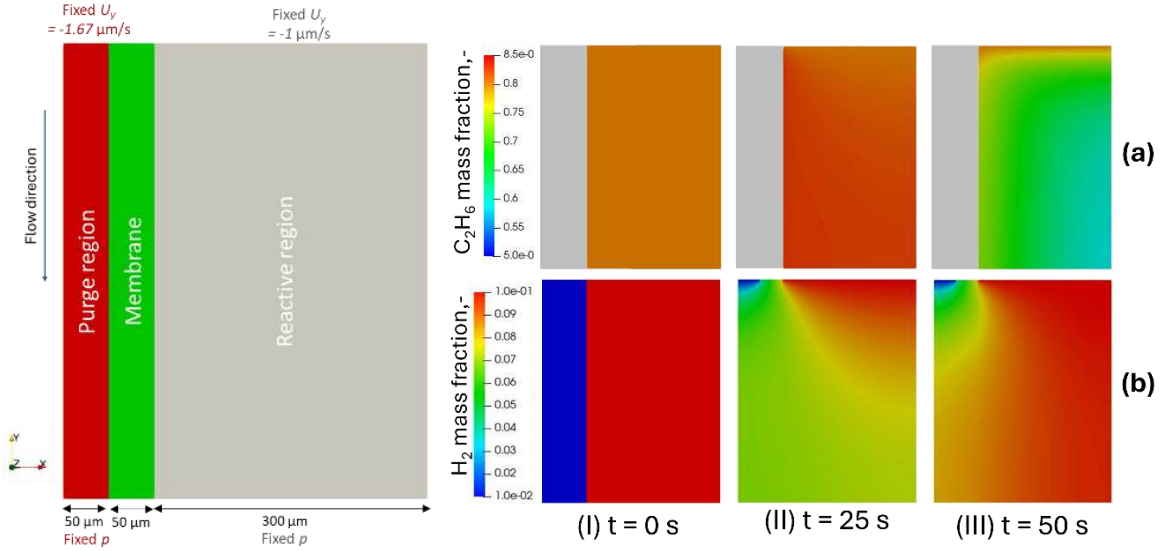

Fig 1. (i) details of computational domain, and (ii) distribution of H_2 and C_2H_6 mass fraction.

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HTP0365

Photoelectrode with Co-Catalyst-Embedded Ion-Conductive Polymer Layer for Solar-to-Chemical

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Photochemical

Keywords: photoelectrochemical cell, hydrogen, solar energy, passivation, Nafion

Abstract Body.
Solar-to-chemical energy conversion using photoelectrochemical (PEC) systems represents a direct approach to store intermittent solar energy in the form of chemical bonds. Despite this advantage, PEC cell remains limited by the instability of semiconductor photoelectrodes during operation. It is known that protection layer strategies based on ultrathin passivation layers or metal oxide layers often fail to maintain long-term stability. Therefore, a novel interfacial layer design that simultaneously preserves solar energy conversion efficiency and operational stability is required.

To achieve stable solar-driven hydrogen conversion, a cocatalyst-embedded polymer electrolyte membrane was introduced on photoelectrode surface, forming a composite layer with sufficient thickness to function as a solid electrolyte rather than a passive coating. The layers were deposited onto various photocathode materials (Si, CuInS2, and InP) using solution-based coating methods. Photoelectrochemical measurements were conducted under simulated solar illumination to evaluate solar-to-hydrogen conversion behavior, using linear sweep voltammetry and chronoamperometry in aqueous electrolytes in a three-electrode system. Long-term stability under continuous illumination was assessed at constant applied potentials.

The cocatalyst-embedded polymer electrolyte membrane significantly enhanced photocathode stability by physically decoupling the semiconductor surface from the liquid electrolyte while maintaining chemical interconnection through ion channels. As a result, cocatalyst detachment and photocorrosion were effectively suppressed. Simultaneously, cocatalysts embedded in the polymer matrix provided continuous charge-transfer pathways, enabling efficient extraction of photogenerated carriers for the hydrogen evolution reaction. Consequently, photoelectrodes incorporating the cocatalyst-embedded polymer layer exhibited higher photocurrent densities, more favorable onset potentials, and improved stability compared to bare electrodes.

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HTP0680

From Plasmons to Catalysis: Single particle correlative study of bimetallic Cu-Ag antenna-reactor nanowires

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Photochemical

Keywords: Bimetallic, Antenna-reactor, Single-particle Plasmonic, Catalysis, Surface Plasmon-Polariton (SPP), Nobel metals

Abstract Body.
Plasmonic catalysis, which combines plasmonic excitation with the activation of surface-adsorbed molecules, can facilitate catalytic reactions more effectively. By integrating plasmonic metals with traditional catalytic metals, both light conversion and molecular adsorption are improved, expanding the scope for photocatalytic reactions with greater efficiency and selectivity [1]. Correlating localized plasmonic properties and catalytic performance at nanoscale remains bottleneck in advancing plasmonic photocatalysis in bimetallic systems [2]. We synthesized Ag-Cu bimetallic nanowires with antenna-reactor morphology by galvanic replacement and characterized their structure-property relationship using single particle spectroscopy and operando catalytic monitoring techniques. Electron microscopy, X-ray techniques and optical spectroscopy confirmed Cu-Ag antenna-reactor architecture. Single-particle studies combining dark-field microscopy, photoluminescence and cathodoluminescence (SEM-CL) revealed distinct emission pathways from copper nanowires along with surface plasmon-polaritons (SPPs) propagation. Ag-Cu nanowires exhibit strong local field enhancement due to hot spot generation and effective plasmonic coupling in bimetallic system. Operando- SERS and UV-Visible absorption monitoring of photocatalytic conversion of 4-nitrobenzenethiol directly correlated plasmonic hotspots to single particle plasmonic resonance at sub 100 nm spatial resolution revealing reaction rate constant of 0.257±0.01 min-1 and reaction enthalpy of 16.4±0.1KJ/mol in bimetallic system. SEM-CL identified the field enhancement maxima at Ag nanoparticle interface while SERS confirmed higher reactivity at identical location demonstrating structure-property correlation in bimetallic systems. These findings provide quantitative framework for rational design of plasmonic-catalytic systems by resolving the interplay between electromagnetic field confinement and catalytic activity at nanoscale spatial resolution.

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HYP0096

Experimental investigation of green hydrogen production via Molten Carbonate Electrolysers directly coupled with PV

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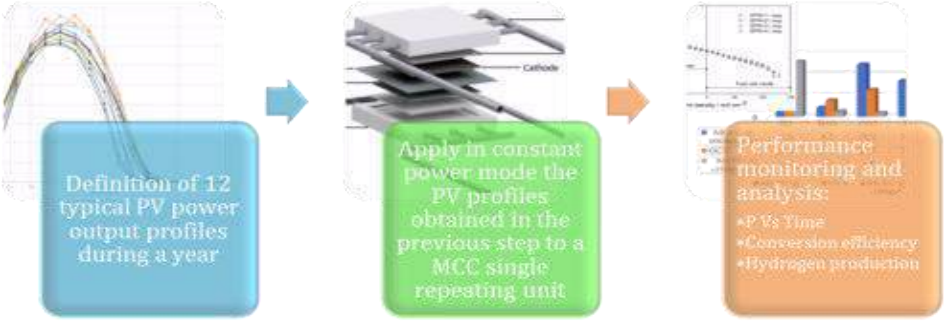
Abstract Category: Hydrogen - Hydrogen Production

Keywords: Low carbon hydrogen, Molten carbonate electrolysers, electrochemical characterization

Abstract Body.

Introduction

In green hydrogen production via electrolysis, several technologies have gained increasing attention in recent years. Among them, high temperature electrolysers, especially Solide Oxide Electrolysis Cells (SOEC), have emerged as one of the most efficient processes for hydrogen production. Alongside SOEC, Molten Carbonates Cells (MCCs) have been investigated as a promising alternative due to their high conversion efficiency and the absence of precious metals. MCCs differ significantly from SOCs in terms of operating conditions, such as reactants and operating temperature, and their performance has not yet been widely investigated. In particular, only one study has addressed the long-term degradation of MCCs [1], which was conducted on a lab-scale cell (3 cm2), while other studies on single repeating units (81 cm2) mainly focused on performance evaluation under different operating conditions [2,3]. The goal of this work is to perform a long-term test on an MCC single repeating unit simulating the direct coupling of the electrolyser with PV during a typical meteorological year. The experimental campaign carried out for this work aims to continuously monitor the electrochemical performance of a molten carbonate electrolyser operating in load-following mode, simulating twelve typical PV days distributed throughout the year. This approach will highlight the dynamic behaviour of molten carbonate electrolysis and identify degradation effects associated with progressive increases and decreases of power load.



Methods

To effectively tackle the aforementioned issues the first step was to quantify the solar radiation in a typical meteorological year using the opens source tool from EU Photovoltaic Geographical Information System (PVGIS) geolocated at ENEA Casaccia R.C..
Subsequently a typical day for each month has been extrapolated basing this choice on the maximum standard deviation in term of power produced. Finally, a MCC single repeating unit has been powered following the profiles previously obtained.

Conclusion

The direct coupling of a PV plant with an MCE is feasible, enabling the absorption of dynamically produced energy through a load-following strategy; maintaining a fixed gas composition while varying the power input appears to preserve optimal cell efficiency, whereas adjusting the gas composition according to power fluctuations negatively affects cell efficiency but may provide overall benefits when the entire balance of plant is considered.

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HYP0264

Interfacial engineering to boost photocatalytic hydrogen evolution via synergistic Z-scheme heterojunction in novel n-type metal free NiCoV-LDH/g-C3N4 Composite

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Abstract Category: Hydrogen - Hydrogen Production

Keywords: Hydrogen evolution, Z-scheme heterojunction, Graphitic carbon nitride, Layered double hydroxide, Photocatalysis, Electrocatalysis,

Abstract Body.
Fabrication of low cost, highly effective, noble metal free, thermally and chemically stable photocatalyst and alkaline water electrocatalyst with the wide pH range is posing a significant challenge in the hydrogen evolution reaction from water splitting to resolve the worldwide energy issues. In this study we have designed a novel n-type 2D semiconductor NiCoVLDH/g-C3N4 (LCN) composite with easy one-step hydrothermal method. Morphological results proved that in situ NiCoV-LDH lamellar sheets were deposited uniformly on g-C3N4 sup-port, resulting in larger electrochemical active surface area and enhanced photo/electrocatalytic hydrogen evolution rate (HER). Furthermore, the LCN with 15% loading of g-C3N4 (LCN-15) composite exhibited the highest photocatalytic hydrogen evolution rate of 1673.4 μmol/g, representing a 28-fold enhancement compared to that of bare CN at 59.9 μmol/g. The improved photocatalytic activity of LCN-15 composite was attributed to (1) enhanced surface area with a large number of active sites, (2) slow formation of NiCoV-LDH precipitates, leading to the fabrication of successful composite material with the g-C3N4, and (3) development of Z-scheme heterojunction, which effectively reduced the recombination rate of photogenerated charge carriers. Furthermore, the electrocatalytic HER performance for LCN-15 composite achieved a current density of -135.86 mA/cm2, which was about 10 times greater than that for bare CN. Moreover, LCN-15 composite exhibited excellent stability during repeated usage for both photocatalytic activities. Thus, this study presented a successful development of NiCoV-LDH/g-C3N4 (LCN) composite structures for enhanced photo/electrocatalytic hydrogen evolution.

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HYP0399

Aqueous phase reforming of methanol using copper-based catalysts: towards Pt-free hydrogen production

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Abstract Category: Hydrogen - Hydrogen Production

Keywords: Aqueous phase reforming, Hydrogen production, Methanol

Abstract Body.

Introduction. The transition to a hydrogen- based economy is constrained by hydrogen's high gravimetric but low volumetric energy density. Liquid hydrogen carriers, such as methanol, enable compact storage and on-demand H2 generation via aqueous-phase reforming (APR). This reaction is typically investigated on Pt-based catalysts, which show good activity and selectivity, but suffer from high price. This work evaluates Cu-based catalysts as a lower-cost alternative to conventional Pt catalysts, and targets improved stability through Ag alloying. Methods. Cu and Cu-Ag catalysts supported on Mg-Al mixed oxide (derived from a commercially available hydrotalcite) were synthesized by deposition-precipitation with urea using simultaneous or sequential deposition in case of bimetallic catalysts and varying the overall Cu loading and the Cu:Ag ratio. N2 physisorption, TEM, XPS, acidity measurements, and in situ DRIFTS were employed to elucidate structure–activity relationships. APR tests were carried out in a batch reactor; performance was assessed by hydrogen productivity and hydrogen turnover frequency (TOF). Apparent activation energies were obtained from temperature- dependent experiments.

Results and discussion. In screening experiments at 210 °C for 1 h with a 33 vol% methanol feed, the benchmark 1 wt.% Pt/Al2O3 exhibited higher H2 productivity than monometallic Cu catalysts, whether tested pre-reduced or not (Figure 1-left). Interestingly, the need for metallic Cu under APR conditions was underscored by the lowest activity obtained by the latter. Notably, introducing Ag produced a bimetallic Cu–Ag catalyst that delivered a 2.5-fold increase in H2 productivity relative to monometallic Cu. In Figure 1-right, HAADF-STEM/EDS map of the bimetallic catalyst demonstrates the interaction between Cu and Ag particles, together with small monometallic Ag nanoclusters. Overall, the results point out the positive outcome of the Cu-Ag system, and are therefore promising for the use of an innovative cheaper catalyst.

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HYP0518

Optimization of Anode Circulation Plate Parameters in Alkaline Water Electrolyzers for Enhanced Hydrogen Production

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Abstract Category: Hydrogen - Hydrogen Production

Keywords: Alkaline water electrolysis; Circulation plate; Gas-liquid flow; Energy consumption; Zero-gap; Hydrogen production

Abstract Body.
Introduction. Alkaline Water Electrolysis (AWE) is a mainstream technology for green hydrogen production, yet it suffers from uneven gas-liquid distribution and the "gas cushion effect" caused by bubble accumulation, leading to high cell voltage and energy consumption. Reducing cell voltage is fundamental to lowering operational costs. While zero-gap technology reduces ohmic losses, optimizing internal flow channels to regulate bubble dynamics remains a critical challenge. This study focuses on optimizing the anode circulation plate structure to accelerate bubble detachment via the "gas-lift" effect, aiming to enhance electrolytic efficiency and reduce energy consumption in laboratory-scale electrolyzers. Methods. Experiments were conducted in a transparent electrolytic cell to visualize gas-liquid two-phase flow patterns. An anode circulation plate was designed, and its parameters were systematically optimized, specifically the upper opening size (ranging from 2 to 10 mm) and electrode spacing. Current density-voltage (J-V) curves were analyzed to evaluate cell performance under current densities of 2000–5000 A/m². The actual hydrogen production energy consumption was calculated based on cell voltage variations. Comparative tests were also performed to assess the feasibility of a cathode circulation plate.
Results and discussion. Visualization results indicated that without circulation plates, bubbles accumulated significantly, increasing ohmic resistance. The introduction of an anode circulation plate successfully induced an upward circulating flow, accelerating bubble removal. Optimization tests revealed that an upper opening of 6 mm yielded the best performance. Smaller openings (2–4 mm) caused bubble stagnation, while larger openings (8–10 mm) failed to effectively accelerate flow.The optimal design parameters were determined as: 6 mm upper opening, 10.5 mm center distance, and 15 mm lower end distance from the electrode surface. Under these conditions, the cell operated stably at 5000 A/m² with a maximum voltage reduction of 0.60 V compared to the structure without plates. Consequently, hydrogen production energy consumption decreased from 64.3–96.5 kWh/kg H2 to 61.6–80.4 kWh/kg H2. Conversely, the cathode circulation plate showed negligible benefits due to the low solubility of hydrogen.

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HYP0624

Joule Heated Membrane Reformer for Ultrapure Hydrogen Generation

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Abstract Category: Hydrogen - Hydrogen Production

Keywords: Membrane Reformer; Hydrogen; Palladium membrane; Membrane separation

Abstract Body.

Introduction: The growing demand for ultrapure hydrogen in applications such as fuel cells, semiconductor manufacturing, and green ammonia synthesis necessitates compact, energyefficient, and low-carbon hydrogen production technologies. Most of the world's hydrogen is produced by steam reforming. Methanol is a liquid carrier that has the highest hydrogen content. In the steam reforming process, it produces CO, CO2, and H2. This hydrogen can be separated using pressure swing adsorption (PSA), temperature swing Adsorption (TSA), cryogenic separation, and membrane separation. Membrane separation can be integrated into a single unit that simultaneously generates and separates, thereby increasing process yield. In a conventional reformer, the catalysts are heated by conduction and convection. In this process, most of the heat loss occurs to the environment, reducing the thermal efficiency. In this work, Joule heating is used in membrane reformer to maintain the desirable temperature of catalyst and membranes targeting uniform heating of catalysts and membranes.

Methods: In a Joule-Heated Membrane Reformer, electrical current is passed through an electrically conductive catalyst support, generating heat internally via Joule heating. This heat directly drives endothermic methanol steam reforming. A hydrogen-selective membrane, PdAg membrane, is integrated within the reactor to continuously extract hydrogen from the reaction zone. Pd-Ag membranes were prepared on the porous alumina support (O.D. 10 mm, I.D. 7 mm) using the electroless pore plating method[1]. The Cu-Fe-AZZ catalyst was prepared by wet impregnation. The catalyst was coated on the conductive FeCrAl foam using the wash coating method[2]. The foam and the membranes were heated using direct joule heating by applying an external power source. The purity of the permeate and retentate was analyzed using gas chromatography.

Results and discussion: Joule-heated membrane reformers demonstrate significantly improved thermal efficiency compared to conventionally heated systems due to minimized heat losses and uniform temperature distribution. Pd-Ag membrane (8 μm thickness) was integrated into the reactor, exhibiting hydrogen permeances of 2 mol $m^{-2} s^{-1} Pa^{-0.5}$. Methanol steam reforming was performed using Cu-Fe-AZZ at 300-400 oC temperatures and 1-4 bar pressures. The pure hydrogen is simultaneously separated using the Pd-Ag membrane. The effects of temperature, pressure, WHSV, steam-to-methanol ratio, and metal loading are studied. The catalyst and membrane were characterized using the SEM-EDX, BET, and XRD.

Joule heated membrane reformer minimizes thermal losses and enables low start-up time, making the system well-suited for on-site hydrogen generation.

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HYP9698

Benefits of Piston Reactor-Based Autothermal Reforming for Hydrogen-Rich Synthetic Gas Conditioning from wet biomass: Modeling, Performance Evaluation and Benchmarking

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Abstract Category: Hydrogen - Hydrogen Production

Keywords: Piston reactor, Wet biomass processing, Hydrothermal Carbonization, Sorptionenhanced gasification, technoeconomic assessment

Abstract Body.
Hydrothermal carbonization (HTC) coupled with sorbent-enhanced gasification (SEG) offers a compelling pathway for converting wet biomass to hydrogen-rich synthetic gas without the energy penalty associated with feedstock drying. In this integrated concept, wet biomass is hydrothermally carbonized into carbon-rich hydrochar, which is subsequently turned into hydrogen-rich syngas through gasification assisted by calcium looping (in-situ CO_2 capture). Despite the high hydrogen content of the SEG-derived syngas, residual methane and tar compounds remain, posing a major coking challenge to downstream catalytic reforming due to catalyst deactivation.
This work investigates the feasibility and system-level performance of a piston reactor (PR) operated in autothermal reforming (ATR) mode as a conditioning technology for methane- and tar-containing, hydrogen-rich syngas, while assessing its potential contribution to power and heat cogeneration. The piston reactor was selected for its gas-phase operation, demonstrated tolerance to tar concentrations, and high methane conversion with strong hydrogen selectivity. A broad parametric space was explored, covering uptake temperatures of 300-600°C, H_2O/CH_4 ratios of 0.5-4, and O_2/CH_4 ratios of 0.1-0.8, with operating points screened based on methane conversion, hydrogen and carbon selectivity, reactant consumption, and opportunities for power and heat recovery from PR shaft work, hot exhaust gases, and thermal losses. A detailed process modeling framework combining Aspen Plus and MATLAB was developed to simulate the complete wet biomass-to-hydrogen chain, including HTC, SEG of hydrochar, PR-ATR, catalytic water gas shift (WGS), pressure swing hydrogen separation, and sorbent regeneration in the calciner. Two conditioning strategies were evaluated: direct PR-ATR conditioning of hydrogen-rich syngas and

conditioning after upstream hydrogen separation, with either natural gas or produced hydrogen supplying the energy demand for sorbent regeneration.
The results show that PR–ATR conditioning substantially increases hydrogen production capacity (+28 to 30% increase) from 16.17 to 29.75-ton H_2 per day for the same feedstock capacity. This improvement is achieved by reforming residual methane in the syngas, which directly translates into a lower hydrogen production cost. The levelized cost of hydrogen for the standalone plant decreases from 4.535 € kg^{-1} H_2 to 3.167 € kg^{-1} H_2 when the piston reactor is incorporated as shown in Figure 1. Overall, piston reactor-based ATR integrated with HTC-derived hydrochar sorbent-enhanced gasification and heat recovery provides an effective solution for wet biomass to hydrogen pathways that are otherwise limited by methane slip and tar contamination.

ISCRE29 & APCRE11
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HYP0253

A Two-Stage System for Enhanced Methane Pyrolysis using Activated Carbon Catalyst with Integrated Steam Regeneration

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Keywords: Methane pyrolysis; Two-stage reactor; Activated carbon; Turquoise hydrogen; Steam regeneration

Introduction. Methane pyrolysis is a carbon-neutral route for producing turquoise hydrogen and solid carbon; however, its industrial viability is influenced not only by reactor configuration but also by the effective regeneration of catalysts [1]. While previous studies have primarily focused on reactor design, they have often overlooked the critical role of catalyst regeneration, particularly for activated carbon (AC) catalysts [2]. In this study, the primary focus is on in-situ cyclic steam regeneration of the AC catalyst in a two-stage reactor system, aiming to improve methane conversion and catalyst lifespan.

Methods. The two-stage reactor included a thermal zone without any catalyst and an activated carbon catalytic zone. Experiments were performed at 700–1000 °C with methane flow rates of 0.1–1.0 L min^{-1}. Comparative tests determined the role of the catalyst, while stability and deactivation were assessed over multiple cycles. In-situ regeneration was carried out by supplying water (0.2 mL min^{-1} H_2O) to R-1 at 500–700 °C for 1 hour, to restore the activity of the AC in R-2. Methane pyrolysis experiments were conducted over regenerated AC catalysts to evaluate the catalyst's efficiency.

Results and discussion. The methane pyrolysis process achieved nearly complete methane conversion (~100%) at 1000 °C with a flow rate of 1.0 L min^{-1}. Lower flow rates significantly increased catalyst lifespan, while higher rates led to faster deactivation. Steam regeneration restored catalyst performance to about 60% methane conversion. Overall, this two-stage approach with integrated regeneration offers a scalable, energy-efficient solution for sustainable hydrogen production.

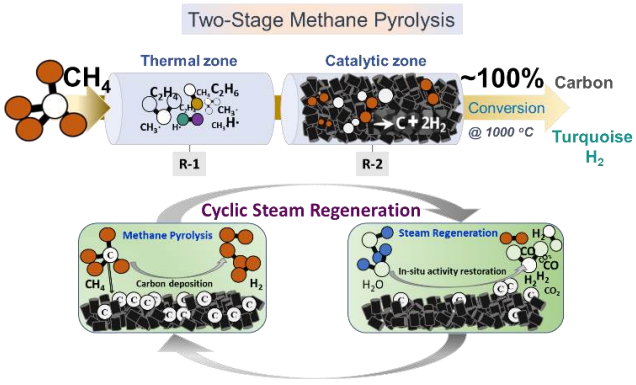

Figure 1: Two-stage methane pyrolysis over an activated carbon catalyst with in situ steam regeneration

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ISCRE29 & APCRE11
2026 / SEOUL, KOREA

HYP0102

Turquoise hydrogen (H2) production from methane pyrolysis using catalytic wire-mesh reactor system

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Abstract Category: Hydrogen - Hydrogen Production

Keywords: Wire-mesh reactor system, Catalytic stainless-steel mesh, Thermal and mass transport, Methane pyrolysis, Turquoise hydrogen (H2)

Abstract Body.

Purpose.

The global energy transition requires scalable, carbon-free hydrogen pathways, yet over 95% of hydrogen still comes from fossil fuels via steam methane reforming and coal gasification, both CO_2-intensive and economically constrained even with CCS [1]. Methane pyrolysis (CH_4) presents CO_2-free pathway, producing hydrogen alongside valuable carbon materials such as graphene, nanotubes, and fullerenes. This novel study focuses on methane pyrolysis for the production of turquoise hydrogen (H2) along with solid carbon (C) using stainless steel wire-mesh based reactor system.

Methods.

Two stainless steel wire-mesh of sizes, M-50 and M-30 were used as catalyst without any treatment for methane pyrolysis at a temperature across 800-1000 °C. Both the wire-mesh (M-50 and M-30) were cut into 2×2 cm and stacked vertically (16 pcs for each mesh size) to the flow of methane inside the reactor body. A total flow rate of 100 ml was employed comprising of 30 ml CH4 (99.999%) and 70 ml N2 (99.999%). The experiments were conducted at atmospheric pressure and the product gases were analyzed in real-time using non-dispersive infrared spectroscopy (NDIR; AO2000 Series, ABB, Switzerland).

Results and Conclusion.

Stainless steel wire-mesh based reactor system displayed some significant results for methane pyrolysis at a temperature across 800-1000 °C. CH4 conversion of 68% and 62% was achieved along with >90% H2 selectivity for mesh size M-50 and M-30, respectively. Mesh size M-50 with small pores resulted in higher CH4 conversion due to longer residence time contrary to M-30 with large pores and small residence time. Methane pyrolysis results revealed that stainless steel wire-mesh functioned as a catalyst, improving decomposition efficiency through its intrinsic heat and mass transfer properties [2].

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HYP0349

A detailed CFD investigation of bubble dynamics in molten metals for turquoise hydrogen production

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Abstract Category: Hydrogen - Hydrogen Production

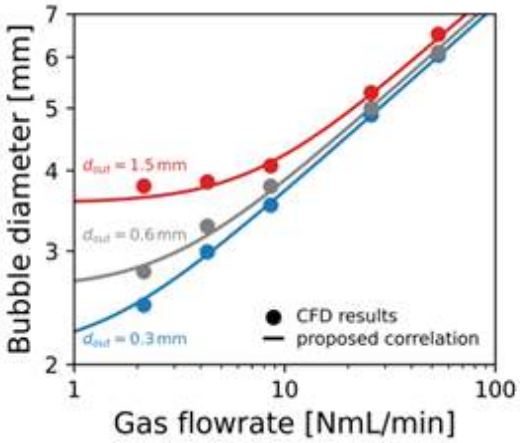
Keywords: Turquoise hydrogen production, Methane pyrolysis, Molten metal bubble column reactor, Bubble dynamics, Computational fluid dynamics (CFD)

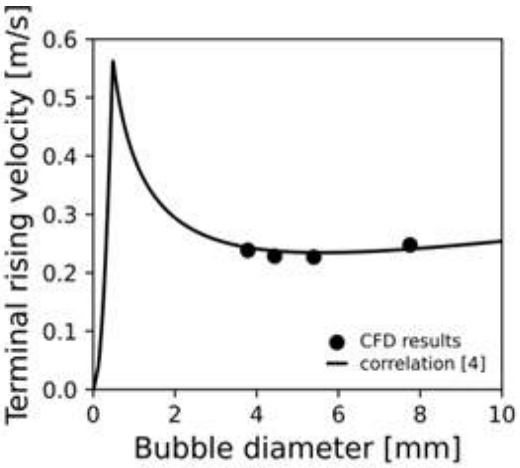
Abstract Body.

Introduction. Methane pyrolysis in molten metal bubble column reactors presents a promising pathway for clean hydrogen production, avoiding direct CO_2 emissions. The molten metal provides high heat-transfer rates and enables continuous separation of the solid carbon by-product, overcoming one of the main drawbacks of conventional pyrolysis reactors. Despite its potential, a mechanistic understanding of the interplay between fluid dynamics, transport, and chemistry relevant to reactor design is still missing. Bubble diameter and rising velocity play a critical role, as they directly influence the residence time and gas–liquid interfacial area, thereby affecting methane conversion and product distribution. However, these phenomena are difficult to experimentally investigate due to the harsh operating conditions and the opacity of the medium. Therefore, we investigate bubble dynamics in these systems through detailed CFD simulations and propose predictive engineering correlations that relate the injector geometry and gas flow rate to the bubble size and rising velocity, based on a hierarchical approach [1].

Methods. The formation of methane bubbles in molten tin from isolated micro-nozzles (dout = 0.18-1.5 mm) and their subsequent rise inside the liquid column are simulated using an algebraic volume-of-fluid (VOF) method, which allows tracing the shape and the position of the gas-liquid interface throughout the process. The computational approach has been assessed with experimental and numerical data from the literature (e.g. [2]).

Results and discussion. We investigated bubble formation from micro-nozzles. We identified a multistep bubble formation mechanism, where the specific wetting behavior of molten metals leads to growth around the injector. We observed a strong effect of the flowrate on the bubble diameter, combined with a secondary effect of the outer nozzle diameter relevant at small flowrates. We adapted the Mori correlation [3] to improve bubble size prediction across the investigated operating range (Fig 1, left). Further, we analyzed the bubble rise trajectory in the reactor. We observed that bubbles show a wobbling shape and follow a zigzagging/spiraling pathway. We also observed that their terminal rising velocity can be accurately described by the Tomiyama correlation [4] (Fig 1, right). Overall, this study provides a quantitative basis to estimate bubble hydrodynamic characteristics from injection conditions alone, supporting reactor-scale performance prediction and design for molten-metal methane pyrolysis.





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HYP0351

Kinetic and Deactivation Studies of Methane Pyrolysis on Waste-Based Biochars for Moving-Bed Reactor Modeling

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Abstract Category: Hydrogen - Hydrogen Production

Keywords: methane pyrolysis, biochar, kinetics, deactivation, reactor modeling

Abstract Body.
Introduction. Hydrogen is emerging as a key vector for decarbonization, but its conventional production is emission intensive. Thermo-catalytic methane decomposition (TMD) offers a cleaner alternative, yielding H2 and solid carbon without COx formation [1]. Carbon-based catalysts further enhance process sustainability while enabling carbon valorization in sectors such as steelmaking [2]. This study examines TMD over waste-based biochars as a route for co-producing hydrogen and carbon and develops a predictive model for a moving-bed reactor.
Methods. Samples derived from sewage sludge pyrolysis were upgraded through leaching, grinding, and activation, and characterized to evaluate their structural and compositional features. Ramp, time-on-stream, and kinetic tests enabled to evaluate catalyst deactivation and intrinsic reaction parameters. A MATLAB-based model was developed to simulate a moving-bed reactor, taking into account thermodynamic equilibrium, mass-transfer limitations, and thermal profile. Sensitivity analysis was performed to identify optimal operating conditions.
Results and discussion. Ramp tests revealed that upgrading treatments and particle size strongly affect long-term performance. Leaching improves pore structure by reducing ash content, while milling enhances activity and stability through increased surface area and reduced transport limitations. Kinetic analysis identified key reaction parameters, including reaction order (~0.5), pre-exponential factor, and activation energy of (~98 kJ mol-1). An innovative deactivation model showed that catalyst deactivation and carbon nature are independent from reaction temperature, unlike iron-based catalysts, as confirmed by spent catalyst characterization (Figure 1a). Kinetic and deactivation models were applied to design a moving-bed system for predicting reactor performance in different conditions. Sensitivity analysis indicated that performance is highly dependent on catalyst residence time (Figure 1b). Overall, this work shows an effective approach for lowering greenhouse gas emissions in H2 production sector, with potential implications for the steel industry and the energy transition.

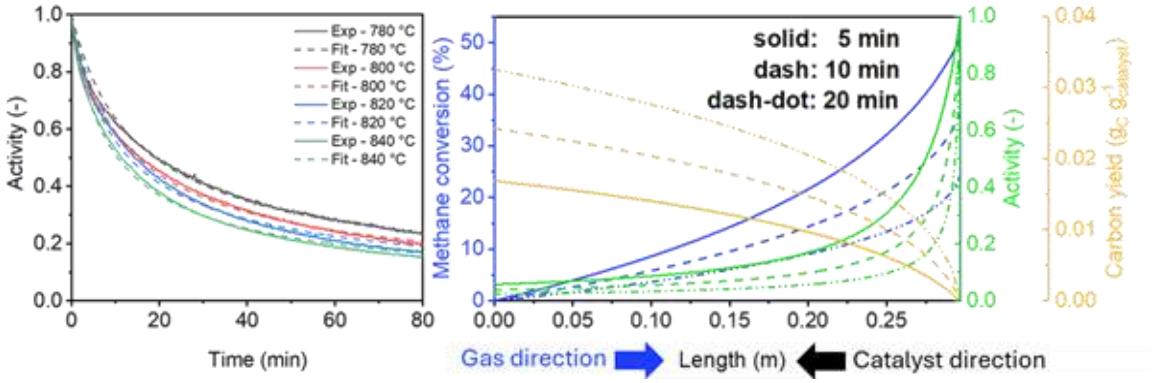

Figure 1. a) Experimental and model deactivation curves at various temperatures of sewage sludge biochar and b) sensitivity analysis on moving bed reactor model at different catalyst residence time.

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HYP0441

High-Performance Methane Pyrolysis using a Ni–Cu Spiral Structured Catalyst Prepared by Electroless Plating

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Abstract Category: Hydrogen - Hydrogen Production

Keywords: Electroless Plating, Spiral structured catalyst, Methane pyrolysis, Turquoise H2

Abstract Body.

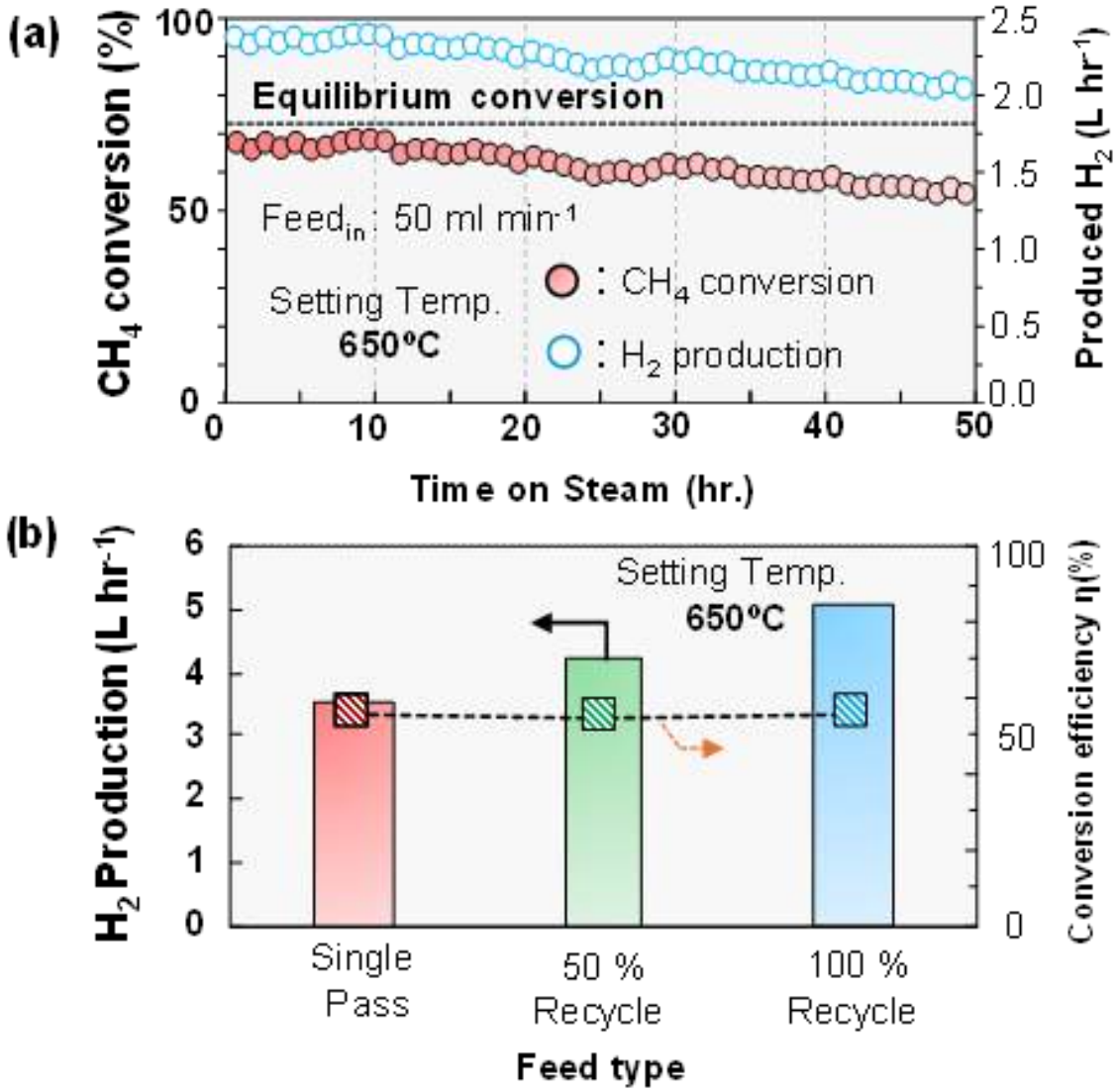

Fig 1. (a) Durability of ELP Ni–Cu spiral catalyst at 650 °C; (b) Effect of feed recycling on hydrogen production and methane conversion efficiency

Introduction. Methane pyrolysis ($CH_4 \rightarrow C + 2H_2$) is key technology for CO_2 -free hydrogen production. However, it typically requires high reaction temperatures 1000oC. While catalyst like Ni-Cu can lower the reaction temperature, carbon buildup often leads to reactor clogging and catalyst deactivation [1,2]. This study aims to lower the operating temperature and prevent carbon-induced blockage by developing spiral structured catalyst by electroless plating (ELP) method, achieving high conversion for lower temperature methane pyrolysis.

Methods. Ni–Cu catalysts were prepared by ELP on spiral substrates pre-coated with a sol–gel Al_2O_3 layer. After H_2 reduction (600°C), performance was evaluated in a fixed-bed reactor using CH_4 (50 mL/min) across 500oC-700°C temperature range and ambient pressure. For recycle study the unreacted CH_4 (50% and 100%) was mixed with original feed and evaluated.

Results and discussion. Fig. 1(a) shows the durability of the ELP Ni–Cu spiral catalyst at 650°C for 50 h. The catalyst maintained a stable, near-equilibrium methane conversion for the first 20 hours, with only a minor degradation afterward. Figure 1(b) shows how feed recycling—single pass, 50% recycle, and 100% recycle—affects hydrogen production and methane conversion. The higher recycle ratio greatly increased the total hydrogen production, reaching 5.36 liters per hour. This is 89.1% conversion of original feed. Importantly, the conversion efficiency stayed very stable. These findings demonstrated that the spiral structured catalyst has effectively intensified mass transfer, resulting in the powerful methane pyrolysis activity.

Conclusion: The combination of the ELP Ni–Cu alloy and the spiral substrate promotes the formation of filamentous carbon rather than amorphous carbon, which typically causes deactivation [2]. This carbon growth tendency, combined with the high mass transfer provided by the spiral structure, resulted in enhanced performance. Therefore, our approach offers a viable pathway for sustainable turquoise hydrogen production through mid-range temperature methane pyrolysis.

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HYP0635

Mitigating Catalyst Deactivation in Methane Pyrolysis via Controlled CO_2 Co-Feeding over Carbon Catalysts

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Abstract Category: Hydrogen - Hydrogen Production

Keywords: hydrogen production, methane pyrolysis, mesoporous carbon, CO2 co-feeding

Abstract Body.

Introduction.

Catalytic methane decomposition (CMD) is attractive for low-carbon hydrogen production, yielding H2 and solid carbon.[1] However, sustained production is constrained by catalyst deactivation driven by continuous carbon deposition. Under pyrolysis conditions, CO2 can react with deposited carbon to limit its accumulation and prolong the catalyst activity. Controlled CO2 co-feeding is therefore proposed to alleviate deactivation.

Methods.

Methane pyrolysis was performed in a fixed-bed quartz reactor at 850-900oC using three carbon catalysts: CB2000, CMK9, and SMC2.[1] The feed consisted of 50 vol% CH4 balanced with inert and co-fed CO2 at 0-3 vol% at constant total flow. Products were analyzed using RGA and MS. Fresh and spent catalysts were characterized by N2-sorption, XRD, and TPDRO.

Results and discussion.

Figures 1a and 1b show the evolution of the H2 space-time yield (STYH2) over the carbon materials during methane pyrolysis at 850oC, with and without CO2. Under CO2-free conditions, CMK9 and SMC2 exhibit the highest initial activity (~53μmolH2·gcat-1·s-1), whereas CB2000 yields a lower amount (~22μmolH2·gcat-1·s-1). With time-on-stream, CB2000 undergoes an early decline followed by a stable regime ~14μmolH2·gcat-1·s-1. SMC2 displays a continuous decrease, reaching ~12μmolH2·gcat-1·s-1 after 400min, while CMK9 deactivates rapidly after 140min, dropping to ~2μmolH2·gcat-1·s-1. CO2 co-feeding alters both activity and stability for CMK9 and SMC2, most pronouncedly for the latter. After a similar initial decay, SMC2 maintains a higher STYH2, reaching ~20μmolH2·gcat-1·s-1 after 400min, i.e. higher than without CO2 and remaining more active than CB2000. CB2000 retains its stable regime under CO2 co-feeding, while CMK9 deactivation gets slightly delayed.

Mesoporous carbons, SMC2 and CMK9, show in any case two deactivation regimes: a fast decline in 80min, followed by a slower regime. Based on characterization of fresh and (partially) spent samples, the former is governed by changes in surface oxygen functionalities (TPDRO), while the second is dominated by surface-area loss. For SMC2, CO2 co-feeding yields 4x more surface-retained oxygen after 20min time-on-stream and a 2.5x higher surface area after 400min compared to CO2-free operation. CMK9 responds less than SMC2, in line with its ~2x lower pore volume and oxygen content.[1,2] CB2000 shows limited response to CO2, due to

its higher degree of graphitization, which stabilizes the π-electron system within extended basal planes and limits interaction with CO2. Moreover, its low oxygen content reduces the density of defect-related active sites. Overall, CO2 co-feeding increases the cumulative H2 amount for SMC2 by ~20% at 850°C, which went up to ~50% at 900°C after 400min.

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HYP0669

CFD-DEM time-series (ML) investigation for advancing the Cu–Cl cycle hydrolysis process for hydrogen production

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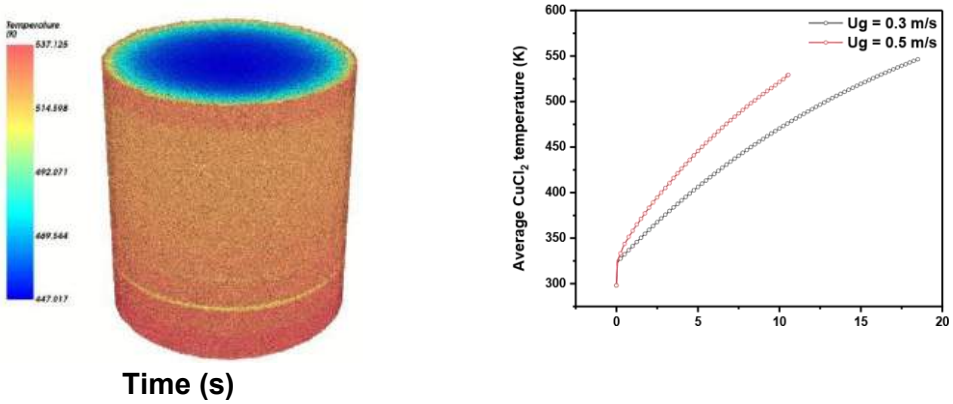
Keywords: ML; CFD; Discrete Element Method (DEM); Fluidized bed reactor; CuCl cycle; H_2 **Introduction.** The Cu-Cl cycle method to produce sustainable hydrogen synthesis is widely recognized for its low temperature requirement. The application of this approach is limited due to difficulties associated with multiphase reaction hydrolysis and thermolysis. In hydrolysis, solid $CuCl_2$ combines with steam in a gases phase; this slow kinetic reaction demands an efficient multiphase reactor to get a high product yield. The fluidized bed reactor has numerous advantages; yet, its complex multi-scale hydrodynamics limit the scaling up to industrial applications [1]. The current research incorporates the CFD-DEM methodology for the design and development of a hydrolysis fluidized bed reactor.

Methods. The CFD-DEM employs an Euler-Lagrangian methodology that delivers localized hydrodynamic data at the particle level, which is challenging to acquire using Euler-Euler simulations. The CFD-DEM model monitors each particle individually, offering critical data on collisions, various forces, particle trajectories, and the temperature of individual particles. The comprehensive heat transfer pathways (wall-particle, fluid-particle, and particle-particle) provide significant insights for the enhancement and optimization of heat transfer operating conditions. The hydrodynamic impact has been examined at different superficial gas velocities (Ug = 0.1-0.5 m/s). The CFD-DEM simulation has been carried out at 0.05 m reactor with 1.2 m height. The initial bed height is kept 0.027 m, 400 μm glass beads used as solid ($CuCl_2$ coating on glass bead) and steam is used as a gas phase [2]. The CFD-DEM simulation is highly computationally intensive as well as time-consuming. The kinetics of the hydrolysis is a slow process, requiring a minimum of 20 to 30 minutes for complete conversion. The current CFD-DEM simulation with 22,95,504 particles tracking for each instance took 28800 min (480 hr) to complete 10 s of the simulation. To reduce the computational time and cost for the CFDDEM model, this investigation proposed a time series Machine-Learning (ML) model.

Results and discussion. A lower superficial gas velocity results in a gradual increase in temperature, which subsequently lowers product yield, whereas a higher superficial gas velocity of 0.5 m/s raises the temperature by 18% more than at 0.3 m/s.



(a) (b)

Fig. 1: (a) $CuCl_2$ particle temperature after 10 s at Ug = 0.3 m/s, (b) average temperature variation of $CuCl_2$ particle for different time intervals

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HYP0692

Development of Ni-Based Catalysts and Their Application in a Fluidized-Bed Reactor for Turquoise Hydrogen Production

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Abstract Category: Hydrogen - Hydrogen Production

Keywords: Turquoise hydrogen, Carbon, Fluidized-bed reactor

Abstract Body.
Research Objectives and Background:
Turquoise hydrogen production via catalytic methane decomposition (CMD) is emerging as a promising low-carbon hydrogen pathway, as it enables the simultaneous production of hydrogen and solid carbon without direct CO_2 emissions. This study presents an integrated research framework combining the development of a highly efficient Ni-based catalyst with its performance evaluation in a fluidized-bed reactor (FBR) for CMD.

Methods:
Ni–Ce–La composite catalysts were developed to enhance catalytic activity and durability under severe carbon-forming conditions. Although nano-dispersed nickel catalysts are known to exhibit high activity for methane decomposition, they are vulnerable to rapid deactivation caused by coke formation. In this study, cerium and lanthanum were introduced as promoters to improve nickel dispersion, stabilize active phases, and suppress catalyst deactivation induced by carbon deposition. The physicochemical properties of the catalysts were systematically characterized using XRD, XPS, H_2-TPR, etc.
To bridge the gap between laboratory-scale catalyst synthesis and reactor-scale application, the effects of catalyst preparation parameters were evaluated and optimized, and the original recipe was modified for kg-scale catalyst production. This scalable approach is essential for continuous and long-term CMD operation in fluidized-bed systems. The physical properties of the synthesized catalyst particles, including bulk density and minimum fluidization velocity, were characterized to confirm their suitability for operating the FBR.
Catalytic performance was first evaluated through intrinsic activity tests using small quantities of catalyst to identify appropriate reaction temperature ranges. Subsequently, the catalysts were tested in a fluidized-bed reactor with an internal diameter of 3 inches. The effects of major operating parameters, including reaction temperature, system pressure, and superficial gas velocity, were systematically investigated to determine stable operating windows for turquoise hydrogen production.

Results:

Based on the parametric studies, continuous operation of the fluidized-bed reactor was successfully demonstrated under optimized conditions. Stable methane conversion and uniform bed temperature profiles were maintained for more than 6 hours through continuous catalyst injection and solid carbon discharge. In addition to hydrogen production, the graphitic carbon formed on the surface of the catalyst particles was also investigated by SEM, TEM and Raman spectroscopy.

Conclusions:
Accordingly, this study establishes a systematic research framework for the development of a catalytic turquoise hydrogen production process. The results highlight the potential of FBR systems for the continuous and simultaneous production of low-carbon hydrogen and solid graphitic carbon, providing valuable insights for future scale-up and industrial application.

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2026 / SEOUL, KOREA

DFL0302

Power Dense LOHC Reactors and Effective Hydrogen Purification for Railway Applications

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Abstract Category: Hydrogen - Hydrogen Storage (LOHC, NH3, MeOH etc)

Keywords: LOHC, dehydrogenation, benzyltoluene, inverse, purification, TSA

Abstract Body.
Purpose: Liquid Organic Hydrogen Carriers (LOHC), particularly the perhydro-benzyltoluene/benzyltoluene (H12-BT/H0-BT) system, show promise for hydrogen storage and transport, especially concerning future applications as fuels in heavy-duty vehicles. However, for onboard hydrogen release, the high volumetric power density of the hydrogen release unit and its compliance with hydrogen purity standards (ISO 14687) are crucial.
Methods: In order to address the limitation in power density, the "DehyMax" reactor concept was developed as shown in Figure 1. The apparatus under consideration consists of an inverted multi-tubular reactor with upstream H12-BT flow and hydrogen release, as well as crossflow heating through perpendicular heating tubes. In comparison with a classical multi-tubular reactor that utilizes vertical catalyst-filled tubes surrounded by a heat transfer fluid, the volumetric power density of hydrogen release can be doubled, relative to the total reactor housing volume.
The purity and purification of the released hydrogen were investigated in two steps: Initially, the gas was analyzed for critical impurities, including volatile organic compounds (VOCs), semi-volatile organic compounds (SVOCs), and carbon monoxide (CO), as released during the dehydrogenation. It has been demonstrated that by selecting optimized operating parameters, the CO content, can be reduced to meet ISO 14687 requirements. In addition, the possibility of adsorptive purification was examined, to remove VOCs and SVOCs in the released hydrogen below tolerable limit according to ISO 14687. A temperature swing adsorption (TSA) concept was developed and tested, incorporating a combination of silica- and carbon-based adsorbers. It has been demonstrated that the total time required for regeneration and cooling can be reduced to a shorter duration than the adsorption time. This allows for continuous operation on board with a two-vessel system.
Conclusion: The integration of the DehyMax reactor concept, characterized by its high power density, in conjunction with the effective TSA purification process, has been proved for significantly advance the technical feasibility of providing LOHC-bound hydrogen to fuel cells onboard heavy-duty vehicles. The new concept has been found to demonstrate considerable promise; consequently, it has been decided to expand its implementation to the railway demonstration unit called "LOHC-PowerPack".

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HYS0047

Reactor modelling and heat integration analysis of the hydrogen carriers 1,4 butanediol and perhydro-benzyl toluene for LOHC fueled vehicles

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Abstract Category: Hydrogen - Hydrogen Storage (LOHC, NH3, MeOH etc)

Keywords: LOHC; hydrogen storage; perhydro benzyl toluene; 1,4 butanediol

Abstract Body.

The transport sector remains one of the major global consumers of primary energy and thus represents a decisive lever on the pathway toward climate neutrality. In this context, hydrogen and hydrogen-based energy carriers constitute promising options.

Liquid Organic Hydrogen Carriers (LOHCs) are particularly attractive in this regard. They reversibly bind hydrogen to organic molecules that remain liquid in both hydrogen-lean and hydrogen-rich forms, thereby combining high storage capacity with straightforward handling. Among the established systems, perhydro-benzyl toluene (H12-BT)/ benzyl toluene (H0-BT) is widely regarded as a benchmark due to its favorable viscosity, high hydrogen content, and low vapor pressure. At the same time, the comparatively high reaction enthalpy of the dehydrogenation step reduces system efficiency and necessitates elevated reaction temperatures, which complicate thermal integration with hydrogen engines or fuel cells [1]. Recently, the 1,4-butanediol (BDO)/γ-butyrolactone (GBL) LOHC system has attracted substantial attention [2, 3]. Its significantly lower reaction enthalpy allows dehydrogenation at reduced temperatures and with improved thermal efficiency.

In this contribution, we present a reactor model for the multiphase dehydrogenation of both BDO and H12-BT, providing a robust framework for process development and scale-up. A reliable description of the multiphasic reaction environment requires the consistent coupling of correlations for the axially resolved liquid hold-up, heat transfer, and catalyst kinetics [4]. Based on this model, we examine a propulsion concept that couples a hydrogen engine with an onboard LOHC dehydrogenation unit. Particular attention is being paid to assessing the potential of engine exhaust gas as a heat source. For H12-BT, approximately two-thirds of the heat demand can be covered by the exhaust gas. The substantially lower heat demand and reaction temperature of BDO enable nearly complete thermal integration. As a result, despite its lower gravimetric storage density, BDO achieves a slightly higher usable energy density.

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2026 / SEOUL, KOREA

HYS0136

Reactor Stability for the Hydrogenation of Liquid Organic Hydrogen Carriers

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Abstract Category: Hydrogen - Hydrogen Storage (LOHC, NH3, MeOH etc)

Keywords: Liquid Organic Hydrogen Carriers, Catalytic hydrogenation, Reactor stability, Process scale-up

Abstract Body.
Purpose. The decarbonization of energy and industrial sectors is increasing interest in carbon-free fuels, particularly hydrogen, which introduces challenges in storage and transportation. Liquid organic hydrogen carriers (LOHCs) offer a promising solution for chemical hydrogen storage. To make this approach viable, hydrogenation and dehydrogenation processes must be thoroughly characterized and optimized in terms of catalytic formulation and process design. Preliminary sustainability analysis of LOHC candidates highlighted toluene-benzene-xylene systems as especially promising. This work aims to combine experimental and numerical approaches to analyze catalytic hydrogenation of aromatic species, supporting reactor design, stability assessment, and scale-up decisions.
Methods. A ruthenium-based catalyst was synthesized and characterized for structural distribution and integrity. Hydrogenation reactivity of toluene-based systems was experimentally measured to develop a quantitative kinetic model. The study integrates stability diagrams, bifurcation and continuation analysis, and sensitivity-based optimization to identify suitable operating conditions, evaluate intrinsic steady-state stability, detect potential runaway scenarios, and explore operating regimes beyond nominal design points. Numerical simulations were conducted for a reference single-jacketed continuous stirred reactor (internal diameter 0.7 m, height 3.6 m, gas hold-up 0.1, filling ratio 0.8, catalyst loading 10 kg), fed with a pure toluene stream at 0.3 kg/s and hydrogen at 30 bar, representing electrolyser-derived hydrogen.
Results. Under the specified conditions, a nominal reactant conversion of 44.8% is predicted. Stability analysis indicates no runaway at steady state or during conventional continuous start-up, though batch-type transients could lead to overheating. Continuation analysis using coolant-side inlet temperature as the bifurcation parameter shows no steady-state multiplicity; higher coolant temperatures decrease conversion due to gas–liquid mass transfer limitations. The integration of experimental kinetics with dynamic numerical predictions enables robust evaluation of reactor stability and operational limits.
Conclusions. The proposed methodology provides a structured framework for early-stage reactor design, enhancing insight into stability, controllability, and safety. By linking experimental and numerical analyses, the approach reduces experimental effort while

supporting reliable scale-up of hydrogenation processes in LOHC systems, facilitating the safe and efficient deployment of carbon-free energy carriers.

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HYS0148

Optimizing Pt Coordination for Enhanced Dehydrogenation: From Laboratory Insights to Practical Applications

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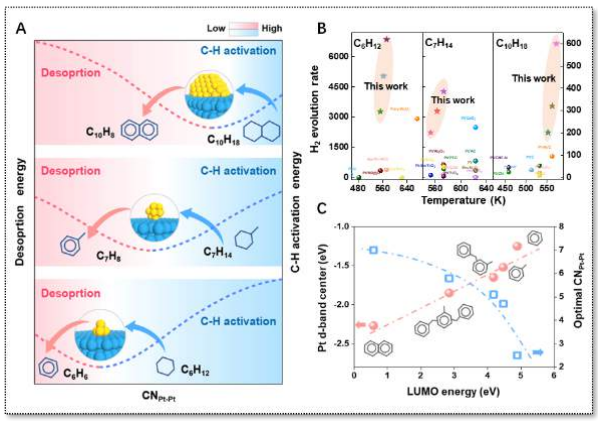
Abstract Category: Hydrogen - Hydrogen Storage (LOHC, NH3, MeOH etc)

Keywords: Cycloalkane dehydrogenation; Pt coordination number, Reactant-dependent volcano trends, LUMO energy, Adsorption-desorption balance

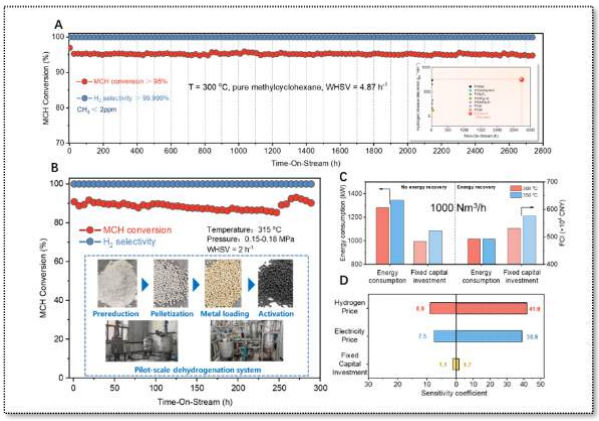
Abstract Body.
Catalyst design is often reaction-specific due to the lack of universal descriptors linking molecular structure to optimal active-site configurations. Here, we uncover reactant-dependent volcano relationships in Pt-catalyzed cycloalkane dehydrogenation and establish an orbital-hybridization-guided framework for rational active-site engineering. By constructing a coordination-tunable Pt/MgAl2O4 model system spanning isolated atoms, clusters, and nanoparticles, the Pt–Pt coordination number (CNPt–Pt) is identified as a quantitative descriptor governing intrinsic activity. Using cyclohexane, methylcyclohexane, and decalin as representative substrates, distinct volcano-type dependences of turnover frequency on CNPt–Pt are observed, with optimal coordination numbers of approximately 2.5, 4.7, and 7.0, respectively. Notably, the optimal coordination systematically increases with increasing molecular size of the cycloalkane.
Combined kinetic analysis, reaction-order measurements, and density functional theory calculations reveal that these volcano trends originate from a fundamental trade-off between C–H bond activation and product desorption. Low-coordinated Pt sites facilitate C–H activation but excessively stabilize unsaturated aromatic intermediates, leading to site blocking and inhibited turnover, whereas highly coordinated Pt sites suffer from weak reactant adsorption and elevated activation barriers. Intermediate coordination environments provide a balanced adsorption–desorption regime, thereby maximizing catalytic efficiency.
Electronic structure analysis further shows that this balance is dictated by orbital interactions between Pt d-states and the π* orbitals of dehydrogenated intermediates. Importantly, the LUMO energy of the aromatic products is identified as a universal molecular descriptor capturing the π* orbital energy. As the LUMO energy decreases with increasing aromatic conjugation and molecular size, metal–adsorbate interactions are strengthened, necessitating higher-coordinated Pt sites with a lower d-band center. A robust linear correlation is established between the LUMO energy of aromatic products and the optimal Pt d-band center (and thus CNPt–Pt), enabling predictive tuning of active-site electronic structure across different reactants and validated using perhydro-benzyltoluene and perhydro-dibenzyltoluene.
Guided by this principle, a next-generation embedded Pt/CeAl catalyst is developed. At 300 °C and a weight hourly space velocity of 4.87 h-1, the catalyst delivers hydrogen release rates

3–4 times higher than state-of-the-art Pt-based systems, while maintaining >99.999% selectivity and stable operation for over 2700 h. Kilogram-scale synthesis and pilot-scale operation in a 10 Nm3h-1 hydrogen production unit demonstrate its robustness and scalability. Process simulation and techno-economic analysis show that operation at 300 °C substantially reduces preheating energy demand and fixed capital investment relative to conventional 350 °C processes, lowering hydrogen production costs and improving economic resilience.

Mechanistic Insights and Catalytic Optimization



Pilot Testing and Demonstration



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HYS0181

Multi-Scale Hybrid Modeling of the Hydrogenation of Dibenzyltoluene in a Trickle-Bed Reactor

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Abstract Category: Hydrogen - Hydrogen Storage (LOHC, NH3, MeOH etc)

Keywords: LOHC, trickle-bed reactor, multiscale model, hybrid model

Abstract Body.
Introduction: Hydrogen storage in Liquid Organic Hydrogen Carriers (LOHCs) constitutes a promising alternative to physical storage [1]. It proceeds via strongly exothermic hydrogenation of H2-lean into H2-rich compounds, with subsequent dehydrogenation. Subject to intermittent operations, the reactors have to be resilient to hydrodynamic fluctuations. Within this framework, the EOLOHC project aims to develop an optimized electricity storage system based on LOHCs, supported by a dynamic model of the overall process. This work focuses on the dynamic modeling of a three-phase reactor (Figure). We compare a physical and a hybrid model where the fast phenomena were simulated with an Artificial Neural Network (ANN) to shorten computation time.

Methods: At the reactor scale, an axial dispersion model describes conversion profiles along the bed [2]. The model accounts for variations in phase densities and volume fractions, which are characteristic of LOHC processes. Dibenzyltoluene (DBT)/perhydro-DBT serves here as the reference LOHC, for which a kinetic model has been previously developed in Ji [3]. Since the three consecutive hydrogenation steps are limited by intraparticle mass transfer, a steady-state particle-scale model was developed and solved by collocation [4]. For the physical model, the two scales were coupled with a double PDE system. For the hybrid model, the steady-state particle-scale model was run 120,285 times to train an ANN, which was embedded in the reactor model to compute apparent reaction rates.

Results and discussion: A Python implementation simulates hydrogen-conversion profiles as a function of inlet flow rates over operating conditions spanning 10–50 bar and 100–250°C. Regarding the calculation speed, an equation system integration takes 1.37 s with the hybrid model instead of 462 s for the physical model. Combining physical equations and ANN in a hybrid model speeds up the calculations while keeping a good accuracy on the results. Our method can be generalized to other LOHCs and dehydrogenation reactors. Future work will focus on model-reduction strategies to optimize a full Power-to-H_2 energy chain.

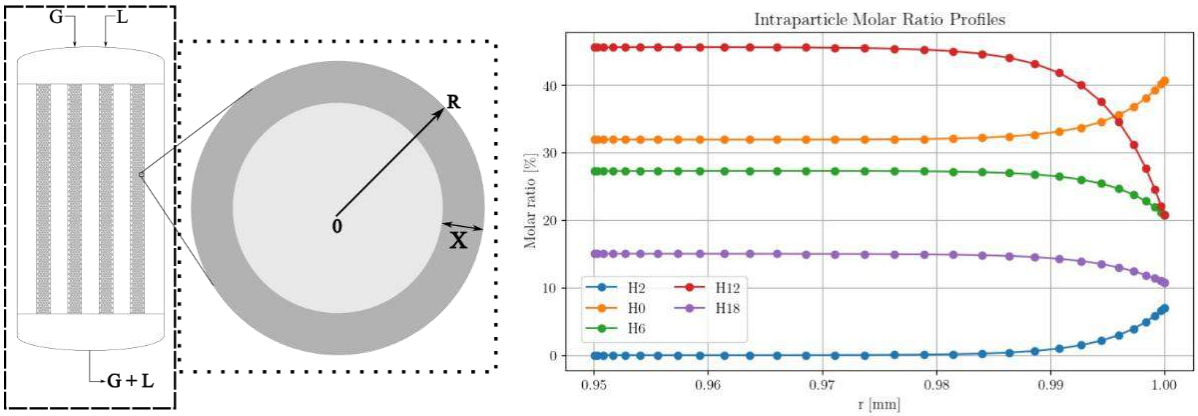

Figure. (a) Multi-tubular reactor; (b) Egg-shell catalyst (c) Simulated mole fractions in the active layer

Acknowledgments:
The EOLOHC project is supported by Institut Carnot Ingenierie@Lyon.

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HYS0182

Semi-batch reactor modelling for LOHC dehydrogenation

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Abstract Category: Hydrogen - Hydrogen Storage (LOHC, NH3, MeOH etc)

Keywords: Hydrogen Storage, LOHC, Alkycarbazoles, Dehydrogenation, Kinetics

Abstract Body.

Introduction. The global energy is undergoing significant challenges, prompting an urgent transition toward cleaner and low-carbon energy solutions. Hydrogen energy is emerging as a key in replacing conventional fossil fuels in this transition, but its storage and transportation remain major obstacles for large-scale industrial applications. One of the promising solutions is the use of Liquid Organic Hydrogen Carriers (LOHC). This technology promises to storage and transport the hydrogen through reversible hydrogenation and dehydrogenation cycles. Despite advances in identifying suitable molecules, catalytic activities and thermodynamic evaluations, comprehensive studies on reactor design and process optimization are still limited. Large number of experimental studies focus on reactive schemes without performing a reactor model. Our study establishes a semi batch catalytic reactor model for LOHC dehydrogenation, incorporating gas liquid properties and transport phenomena.

Methods. Because of its favorable dehydrogenation properties, including low reaction temperature and moderate reaction enthalpy, the N-ethylcarbazole (NEC) was selected. The NEC dehydrogenation was studied in a semi-batch reactor, using 5wt% Pd/Al2O3 at 1 bar with the temperature ranging from 160 to 200 °C. The kinetic model parameters were estimated by using our set of experimental data and previously published experimental data [1-4].

Results and discussion. Large number of reviewed studies are performed in semi batch system without accounting the gas stripping, the transfer limitations and the properties variation. For example, the experimental data analysis showed inconsistencies because lot of them did not consider the liquid density variation. The reaction scheme showed also discrepancies. Two studies required inclusion of the intermediate reaction of H12-NEC → H4-NEC, while another assumed a direct conversion of H12-NEC → NEC, excluding H4-NEC. These differences could indicate variability in the isomer composition of H12-NEC, which is likely to be due to differences in the hydrogenation methods used in different laboratories. The reaction scheme has to be amended by isomer addition. Our model accounts all these aspects. Besides, to enhance the accuracy, adsorption phenomena was incorporated into the kinetic model formulation. The final model fits published data.

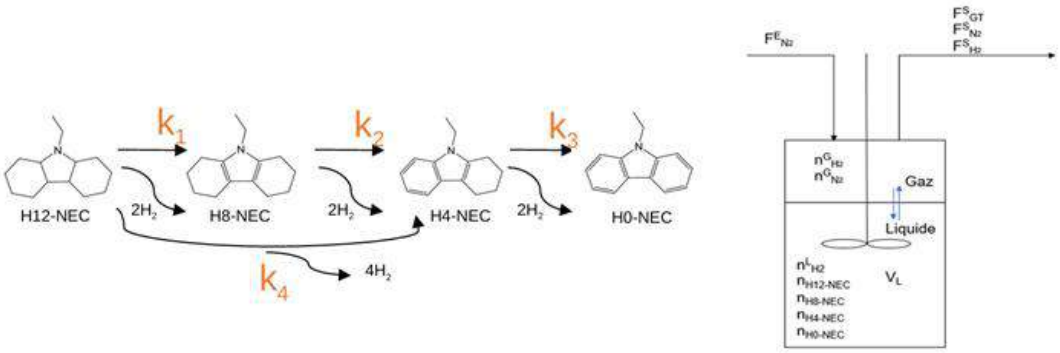

Figure: Semi batch Reactor and reaction models

Acknowledgments: This work has been partially supported by the ANR RID LOHC ANR-23-CE05-0007.

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HYS0534

Study of the hydrodynamic phenomena of three-phase packed bed reactors: hydrogenation and dehydrogenation of Liquid Organic H2 Carriers (LOHC)

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Abstract Category: Hydrogen - Hydrogen Storage (LOHC, NH3, MeOH etc)

Keywords: LOHC; hydrodynamics; reactors; γ -butyrolactone/butanediol;

Abstract Body.

Introduction. Liquid Organic Hydrogen Carriers (LOHCs) are high-potential compounds for efficient and safe hydrogen storage and transport. Based on previous research [1], this work focuses on the use of γ-butyrolactone (GBL) and 1,4-butanediol (BDO) as LOHC pair, due to their optimal properties and bio-based sourcing. The large hydrogen consumption and production in this technology significantly alter gas-to-liquid volumetric flow ratios within the three-phase reactor. Consequently, gas-phase kinetics cannot be neglected during hydrogenation and dehydrogenation. Moreover, the correlations of the literature to describe the hydrodynamics underestimate the gas volume fraction for our large particle-over-reactor diameter ratio. Thus, modelling and experimental characterization of the hydrodynamics are carried out in this work to validate the flows behaviours.

Methods. The dynamic model, computed with Comsol, takes into account the mass balances and the Navier-Stokes equations [2]. Experiments use an inert compound, ethyl acetate, at ambient conditions due to its properties (density, surface tension, and viscosity) comparable to those of GBL/BDO under process operating conditions [1]. Pilot set-up (Figure), with reactors of 16 and 30 mm ID, and the experimental procedures were designed to measure the fundamental hydrodynamic parameters. Tracers for gas (He, butane) and liquid (propyl acetate) phases are used for residence time distributions and analysed with on-line TCD and GC, respectively. Gas-to-liquid volumetric flow ratios range between 4 and 320. Pressure drops were measured via precise differential manometers.

Results and discussion. Measured pressure drops in the reactors are two orders of magnitude lower than estimations from literature correlations. Ergun's constants estimated in our reactors are lower than the classical values for spherical particles. Furthermore, measured liquid holdup ranges between 4 and 13%, whereas around the 20% was estimated via correlations, thus directly impacting wetting efficiency. Evaporation effects of ethyl acetate, as for GBL, are not to be neglected. The experimental axial dispersion, mass transfer coefficients and the particle wetting factor measured in our set-up have to be implemented in the computational model. Future work will include reaction and thermal aspects, to validate the simulations and obtain a complete description of both GBL hydrogenation and BDO dehydrogenation.

Acknowledgment: This work is financially supported by the CEA.

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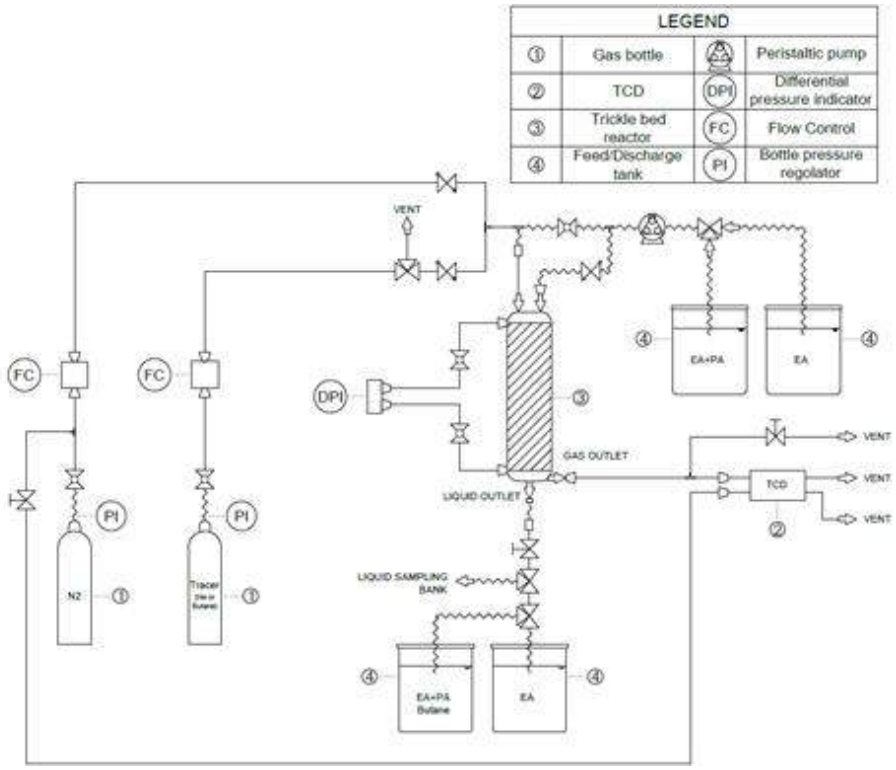

Figure: Schematic diagram of the set-up for the hydrodynamic study

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HYP0164

Cost-effective MgO-supported Ni Catalysts for COx-free Hydrogen Production from Ammonia

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Abstract Category: Hydrogen - Hydrogen Production
Keywords: Ammonia decomposition; Hydrogen; Heterogeneous catalyst; COx-free hydrogen production

Abstract Body.

Introduction. Addressing the global energy scarcity amid rapidly increasing energy demand remains a major challenge for the scientific community. Carbon-neutral energy vectors aligned with the Sustainable Development Goals (SDGs) have attracted significant attention. Hydrogen is regarded as a promising energy carrier due to its high energy density and clean combustion; however, challenges related to its transportation, storage, and safety [1]. Ammonia (NH3) is a promising hydrogen carrier for the H2-based energy transition due to its ease of handling, storage, and transportation, supported by well-established large-scale commercial production. Thermocatalytic decomposition of NH3 offers a carbon-neutral route for hydrogen production, yielding nitrogen as the sole by-product. Nevertheless, this process typically requires high operating temperatures due to its endothermic nature and relies on expensive noble metal catalysts [2]. Herein, a cost-effective MgO-based, alkali-promoted Ni catalyst was studied that enabled efficient hydrogen production via ammonia decomposition at relatively lower temperatures (~500-535°C).

Methods. The catalyst was synthesized by a co-precipitation method and evaluated for ammonia decomposition in a fixed-bed quartz reactor at a gas hourly space velocity (GHSV) of 6000 mL·h-1·gcat-1 for 5 h over a temperature range of 350-650°C. Comprehensive characterization was performed using N2 physisorption, XRD, XPS, TEM, SEM, TPR, and TPD.

Results and discussion. Various MgO-supported, K-doped Ni catalysts were synthesized and screened to achieve low-temperature thermocatalytic ammonia decomposition. Complete NH3 conversion was attained at 535°C, with the conversion trend increasing with metal loading. Catalysts featuring uniformly dispersed active sites and the formation of a NiO-MgO solid solution, combined with a high specific surface area and well-connected cylindrical mesoporous network, were found to be highly effective in enhancing catalytic performance by facilitating mass transfer. Furthermore, alkali-induced basic sites and loosely bound surface oxygen species, accompanied by electronic redistribution, played a crucial role in lowering the reaction temperature.

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HYP0337

Effective Hydrogen Production through Utilization of Hot Direct Reduced Iron in Ironmaking Processes

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Abstract Category: Hydrogen - Hydrogen Production
Keywords: Hydrogen, Direct reduced iron, Methane, Ammonia

Abstract Body.

Introduction.

Hydrogen is gaining significant attention as a carbon-free energy carrier to reduce fossil fuel consumption and mitigate carbon dioxide (CO2) emissions. POSCO is currently transitioning from traditional blast furnace operations to hydrogen-based iron-making, which is expected to create an annual demand for low-carbon hydrogen exceeding 3.5 million tons. To meet a portion of this massive demand, the development of efficient hydrogen production technologies is required. This study aims to develop a sustainable hydrogen production method within the steel industry by leveraging hot direct reduced iron (DRI) to drive the endothermic decomposition of methane (CH4) and ammonia (NH3) into hydrogen.

Methods.

The proposed approach uses hot DRI, produced through hydrogen reduction, as both a thermal heat source and a catalyst. In this process, NH3 is broken down into hydrogen and nitrogen, while CH4 is transformed through pyrolysis into hydrogen and solid carbon. Utilizing these fuels provides a significant opportunity to substantially minimize CO2 emissions during hydrogen production. This study focuses on thermally coupling these two reactions within an integrated system configuration. A key advantage of this process is that the metallic iron already present in the hot DRI serves as a natural catalyst. This eliminates the requirement for expensive or specialized materials such as Ruthenium (Ru) or Nickel (Ni), making the production more cost-effective material.

Results and discussion.

This innovative approach ensures high thermal efficiency and maximizes energy utilization by using the inherent sensible heat of the hot DRI as the thermal energy source. This process substantially reduces the requirement for external energy input. The study highlights that the catalytic properties of the metallic iron in DRI effectively support the chemical reactions, addressing critical issues such as catalyst activity and heat management. Finally, the produced hydrogen can be supplied back to the industries that require a stable hydrogen supply.

Conclusions.

In conclusion, this study plays a crucial role in achieving carbon-neutral steel production and advancing global efforts toward sustainable industrial practices. By harnessing the thermal and catalytic properties of hot DRI, this technology enhances hydrogen production efficiency and aligns with stringent CO2 reduction targets. This approach offers a promising pathway for economical hydrogen production within the iron and steel industry, in line with global decarbonization objectives and improved resource efficiency.

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HYS0166

Direct electrolysis of liquid anhydrous ammonia for high-purity hydrogen production at ambient temperature: Boosting kinetics of the hydrogen evolution reaction

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Abstract Category: Hydrogen - Hydrogen Storage (LOHC, NH3, MeOH etc)

Keywords: Ammonia (NH3), Hydrogen Production, Electrolysis, High-Purity and Pressurized Hydrogen, Ambient Temperature

Abstract Body.

Introduction. Ammonia (NH3) is a promising hydrogen (H2) carrier, but retrieving H2 typically involves energy-intensive thermal cracking at high temperatures (>600 °C) with complex purification/separation steps. This study demonstrates a proof-of-concept for the direct electrolysis of liquid anhydrous ammonia (NH3(l), >99.99% of NH3, free of water and solvent) at a temperature of 20 °C and a pressure of 9 bar, without requiring H2/N2 separation and compression processes. [1] In this electrolytic system, ammonium ions (NH4+) serve as the primary charge carriers. Consequently, the electrochemical NH3 splitting proceeds through the anodic Nitrogen Evolution Reaction (NER, Eq. 1) and the cathodic Hydrogen Evolution Reaction (HER, Eq. 2). Importantly, the theoretical reaction potential of this process is 0.059 V (Eq. 3), which is significantly lower than that of water electrolysis (1.23 V), indicating superior energy efficiency. [1,2]

Anode (NER): $4NH_3(l) \rightarrow 0.5N_2 + 3NH_4^+ + 3e^-$, E = 0.041 V vs. SHE (Eq. 1)
Cathode (HER): $3NH_4^+ + 3e^- \rightarrow 1.5H_2 + 3NH_3(l)$, E = -0.018 V vs. SHE (Eq. 2)
$NH_3(l) \rightarrow 0.5N_2 + 1.5H_2$, E = 0.059 V (Eq. 3)

Methods. Developed electrocatalyst were initially tested in a batch reactor to measure the electrocatalytic characteristics for the NER and HER. Based on these results, a continuous zero-gap electrolyzer was configured using a Ru-based anode and a bimetallic Pt-M cathode, separated by a cation exchange membrane. The system utilized NH_4PF_6 as a supporting electrolyte and operated at 20 °C and 9 bar to maintain NH3 in a liquid state.

Results and discussion. A Ru-based anode and Pt-M were used for the anode (NER) and cathode (HER), respectively. The Pt-M catalyst exhibits notably enhanced electrochemical properties compared to commercial Pt/C by facilitating N–H bond dissociation step, which is recognized as the rate-determining step of the HER in NH3(l) electrolysis. Notably, the overpotential of Pt-M catalyst is decreased from ca. 0.5 V (for Pt/C) to <0.1 V at 0.1 A cm-2. Consequently, the continuous electrolyzer achieved a current density of 0.1 A cm-2 at a cell potential of 0.9 V, which is significantly lower than that of theoretical potential of water electrolysis (1.23 V). In addition, the system successfully produced H2 with >99.99% purity and >8 bar pressure, achieving a Faradaic efficiency of >99%.

Acknowledgments
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HYS0186

Catalytic reversible hydrogen storage in aqueous formate solutions under mild conditions

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Abstract Category: Hydrogen - Hydrogen Storage (LOHC, NH3, MeOH etc)

Keywords: Hydrogen storage, Heterogeneous catalysis, Formate/bicarbonate system, Pd-based catalysts, Safety

Abstract Body.

Purpose

Hydrogen is expected to play a major role in the global energy transition, contributing significantly to long-term decarbonization targets. Despite the rapid expansion of green hydrogen production, storage and transportation remain major technological barriers to large-scale deployment. Conventional physical storage solutions, such as compressed and cryogenic hydrogen, require extreme operating conditions that negatively impact energy efficiency and safety. This work aims to provide an overview of hydrogen storage based on aqueous formate solutions as a viable chemical alternative, focusing on thermodynamics, kinetics, energy performance, and intrinsic safety.

Methods

The proposed storage concept relies on the reversible catalytic interconversion between aqueous formate and bicarbonate in the presence of hydrogen and water. Thermodynamic analysis was performed to assess equilibrium conditions and operating windows. Kinetic considerations were evaluated based on preliminary experimental data for representative catalytic systems. Energy density estimates were derived and compared with conventional pressurized hydrogen storage. Additionally, qualitative and quantitative safety and risk assessments were conducted to benchmark the proposed system against standard hydrogen storage technologies under normal and accidental conditions.

Results

Thermodynamic analysis shows that the formate–bicarbonate system operates close to equilibrium under mild conditions, with the Gibbs free energy approaching zero at temperatures around 50 °C, enabling efficient hydrogen uptake and release without extreme pressure or cooling requirements. Preliminary kinetic results indicate hydrogen release rates compatible with both mobile and stationary power applications. Depending on operating conditions, energy densities comparable to compressed hydrogen systems can be achieved while maintaining high overall energy efficiency. Safety analyses highlight a substantially reduced risk profile, due to the non-toxic, non-flammable, and highly stable nature of aqueous formate solutions.

Conclusions

Aqueous formate-based hydrogen storage combines favorable thermodynamics, promising kinetics, competitive energy density, and enhanced safety. These features make it a promising

alternative to conventional hydrogen storage technologies and a strong candidate for future hydrogen transport and utilization infrastructures.

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2026 / SEOUL, KOREA

HYS0188

Ni-supported LaCeAl mixed oxide catalysts for clean and efficient hydrogen production via ammonia decomposition

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Abstract Category: Hydrogen - Hydrogen Production

Keywords: Ammonia decomposition, Hydrogen production, La/Ce ratio, Ni dispersion, Electron density

Abstract Body.
Ammonia is a promising hydrogen carrier due to its high hydrogen storage density per unit volume and well-established transportation infrastructure. In this context, the ammonia decomposition reaction (ADR) enables the production of clean hydrogen without greenhouse gas emissions. Accordingly, Ni-based catalysts have attracted considerable attention for ADR owing to their cost-effectiveness and excellent activity.
In this study, Ni-supported La–Ce–Al mixed oxide catalysts (Ni/LaxCe1–xAl, x = 0, 0.1, 0.25, and 0.5) were prepared via a solvent-deficient precipitation method to investigate the effect of the La/Ce ratio on ADR performance. Al2O3 served as a structural framework providing a high surface area, while CeO2 and La2O3 were incorporated to introduce oxygen vacancies and surface basicity, respectively.
Among the prepared catalysts, NiLa0.25Ce0.75Al exhibited the highest NH3 conversion of 93.5% at 550 °C under a gas hourly space velocity (GHSV) of 30,000 mL gcat-1 h-1. Physicochemical characterization revealed that partial substitution of Ce with La gradually decreased the surface area and Ni dispersion, while simultaneously increasing the proportion of moderate and strong basic sites. Notably, the optimal catalyst possessed a higher electron density on Ni species compared with the other catalysts. This electronic modification is likely to facilitate associative N2 desorption, which is regarded as the rate-determining step in ADR. The optimal catalyst demonstrated stable performance over 100 h and achieved a superior hydrogen production rate of 136.6 mmol gcat-1 min-1 at 550 °C. These results demonstrate that tuning the La–Ce synergy is an effective strategy for designing high-performance catalysts for practical clean hydrogen production via ammonia decomposition.

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HYS0255

Decisive Role of Chlorine Removal in Activating Ru/Ce/Al2O3 Catalysts for Efficient Ammonia Decomposition

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Abstract Category: Hydrogen - Hydrogen Storage (LOHC, NH3, MeOH etc)

Keywords: ammonia decomposition, ruthenium catalyst, chloride poisoning, alkaline washing, Ru dispersion

Abstract Body.

Ammonia is a promising carbon-free hydrogen carrier due to its high hydrogen content and established infrastructure. Ruthenium catalysts exhibit superior activity for ammonia decomposition. However, the use of RuCl3 precursors often introduces residual chloride species that deactivate Ru catalysts by blocking active sites and suppressing hydrogen adsorption. To mitigate chloride poisoning, various strategies have been proposed, among which catalyst washing is one of the simplest and most practical approaches. Nevertheless, the impact of different washing treatments on industrial bead-type Ru/Ce/Al2O3 catalysts and their correlation with Ru accessibility and ammonia decomposition performance has not been clarified. Therefore, this study investigates chloride removal from bead-type Ru/Ce/Al2O3 catalysts using water and alkaline washing treatments and correlates chloride elimination with Ru dispersion and catalytic performance. Bead-type Ru/Ce/Al2O3 catalysts were prepared by sequential wet impregnation of Ce and Ru onto Al2O3 beads, followed by water (cold and hot) and alkaline (NaOH, KOH, NH4OH) washing treatments. Chlorine content, Ru dispersion,

hydrogen adsorption capacity, surface acidity, and textural properties were evaluated. Ammonia decomposition was tested at 450-550oC under a GHSV of 5,000 and 10,000 mL gcat-1 h-1. Alkaline washing effectively reduced residual chlorine from 0.82 wt% to 0.05 wt%, while water washing showed limited removal. This significant chloride elimination increased Ru dispersion from 11% to 29%, indicating enhanced Ru site accessibility. The improvement was further supported by recovered hydrogen adsorption capacity and suppressed chloride-associated acidity. Among the treatments, Ru/Ce/Al2O3-KOH exhibited the highest activity achieving 96% ammonia conversion at 500oC and maintaining over 95% conversion during a 100 h stability test. These results demonstrate that effective chloride removal via alkaline washing is a key factor governing Ru accessibility and sustained catalytic activity performance.

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2026 / SEOUL, KOREA

HYS0445

Design of cost-effective Ru-free perovskite derived catalysts with optimized Ni exsolution and electronic properties for high performance ammonia decomposition

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Abstract Category: Hydrogen - Hydrogen Storage (LOHC, NH3, MeOH etc)

Keywords: Ammonia decomposition, Ru-free, Perovskite-derived catalysts, Exsolution, Electronic density

Abstract Body.

Ammonia decomposition is a promising route for carbon-free hydrogen production; however, the development of highly active and cost-effective Ru-free catalysts remains a major challenge. In this study, we report the rational design of $LaNiO_3$-based perovskite-derived catalysts with optimized structural and electronic properties for efficient ammonia decomposition.

A series of perovskite oxides were synthesized via systematic A-site (La) and B-site (Ni) substitution combined with controlled thermal treatment to regulate Ni exsolution behavior. Ba incorporation at the La site enhanced surface basicity and increased the electronic density of Ni through electron donation, while partial Co substitution at the B-site destabilized the perovskite lattice, promoting the exsolution and dispersion of metallic Ni nanoparticles. Calcination and reduction parameters, including temperature and heating rate, were further optimized to maximize the formation of surface-accessible Ni active sites.

Comprehensive characterization using XRD, H_2-TPR, CO_2-TPD, H_2 chemisorption, XANES, and XPS revealed a strong correlation between Ni dispersion, electronic density, and catalytic performance. The optimally designed Ba- and Co-substituted catalyst with tailored thermal treatment (denoted optimal LBCN) exhibited superior ammonia decomposition activity, achieving 85.9% NH_3 conversion at 550 °C under a high gas hourly space velocity of 30,000 mL g_cat^{-1} h^{-1}. In addition, the catalyst demonstrated excellent thermal stability over 100 h of continuous operation.

These results highlight the synergistic role of structural accessibility and electronic tuning of Ni active sites in enhancing catalytic performance. This work provides a viable strategy for designing scalable, Ru-free perovskite-derived catalysts for hydrogen production from ammonia.

Oral Presentation

Net-zero CO_2 Technologies

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CDC0029

In-situ hydrothermal synthesis of b-axis oriented Si-MFI zeolite membranes with high binding strength and flue gas separation study

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Capture

Keywords: b-axis orientation, Si-MFI zeolite membrane, in-situ hydrothermal synthesis, APTES modification, flue gas separation

Abstract Body.

Capturing CO2 from flue gases in coal-fired power plants is essential for achieving carbon neutrality targets. To address the high energy consumption with conventional absorption methods, this study develops a b-axis oriented all-silica MFI zeolite membrane (Si-MFI) with high binding strength for CO2/N2 separation. By optimizing hydrothermal synthesis parameters, the b-axis growth of Si-MFI zeolite membrane has been successfully achieved, shortening the gas diffusion path and reducing grain boundary defects. Furthermore, the substrate is modified with the 3-aminopropyltriethoxysilane (APTES) to form a stable Si-O-Si-O-Al covalent bridge structure, improving interfacial binding strength significantly. Molecular simulations confirm that the straight channels along the b-axis (010) plane exhibit a higher binding energy for CO2 (0.38 eV) than for N2 (0.19 eV). The membrane demonstrates superior separation performance and thermal stability under simulating flue gas conditions (CO2/N2 = 1:5) which shows a separation factor of 15.8 for CO2/N2 separation at 90 ℃, surpassing the performance of the unmodified membrane. Aspen process simulation shows a CO2 product purity of 99.2%, while the specific energy consumption is 1.72 GJ/t CO2, which is 16.9% lower than traditional amine absorption. This method offers advantages such as low energy, high stability, and regeneration-free, showing a wide range of application.

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CDC0087

Experimental assessment of kinetics of co-adsorption for solid sorbents in sub-ambient DAC conditions

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Capture

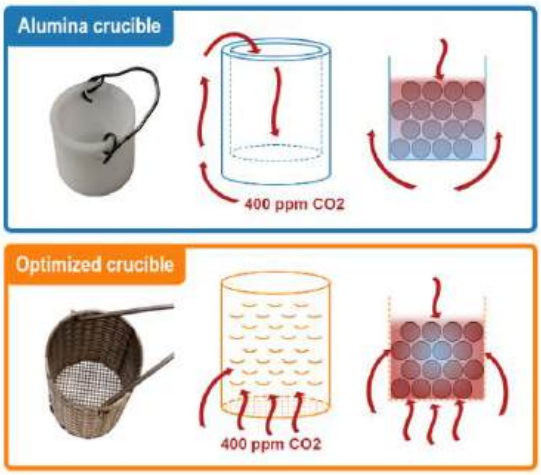
Keywords: Direct Air Capture, Lewatit VPOC 1065, kinetics, co-adsorption

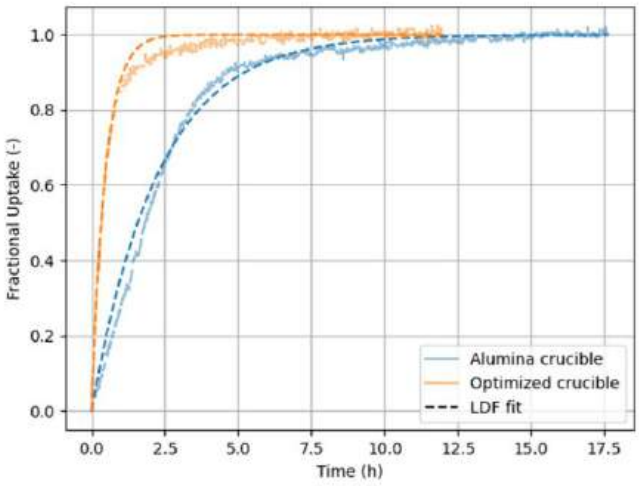
Abstract Body.
Direct Air Capture (DAC) is widely recognized as a promising technology for large-scale decarbonization, as it enables negative emissions by directly removing CO2 from the atmosphere. However, this approach faces significant challenges due to the very low atmospheric CO2 concentration and the presence of moisture. Amine-functionalized solid sorbents are particularly well-suited for DAC because their chemisorption properties give them high selectivity toward CO2. Moreover, they exhibit increased CO2 adsorption capacity in the presence of water vapor due to co-adsorption. To assess the economic feasibility of DAC through process modelling, extensive kinetic adsorption data under a wide range of operating conditions are essential. The Linear Driving Force (LDF) model is commonly used for this purpose because of its simplicity and broad applicability. However, such kinetic data remain scarce in the literature, particularly for co-adsorption scenarios.

For this reason, this study aims to provide additional kinetic and isotherm data for both unary and co-adsorption using thermogravimetric analysis (TGA) experiments. The TGA system is designed to accurately emulate DAC conditions by enabling atmospheric CO2 concentrations and maintaining stable relative humidity and reactor temperature. Furthermore, the crucible design was optimized to eliminate external mass transfer resistances – an issue often overlooked in the literature – resulting in an increase in the LDF constant (k-LDF) from 1.2e-4 to 5.9e-4 s-1 compared with a conventional alumina crucible. The resulting kinetic data are therefore more suitable for process modeling, as they reflect exclusively internal mass transfer and reaction kinetics. This improved TGA setup is then used to investigate the influence of relative humidity and temperature on the kinetics and thermodynamics of co-adsorption under DAC-relevant conditions.

Lowering the temperature from 20 to 0 °C reduced the k-LDF from 7.5e-4 to 3.4e-4, while increasing the adsorption capacity by 30%. This highlights the classic trade-off between kinetic performance and conversion commonly observed in exothermic reactions. In the presence of 30% relative humidity, the kinetics of CO2 adsorption decreased significantly. This effect was particularly pronounced for co-adsorption at 0 °C, where the adsorption curve showed additional diffusion limitations compared to higher temperatures. Overall, the results indicate that although the LDF model provides a reasonable approximation of adsorption behavior, more advanced kinetic models are needed to accurately describe adsorption dynamics in amine-functionalized sorbents.

This study thus provides much-needed kinetic data and insight into co-adsorption under DAC-relevant conditions, which can subsequently be used for process modeling and techno-economic evaluations for large-scale decarbonisation.





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CDC0231

Preliminary study of blu hydrogen production using MCFC as active CCS device

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Capture

Keywords: Molten carbonate fuel cells, CCS, blu hydrogen,

Abstract Body.

Purpose

This work aims to investigate the integration of Molten Carbonate Fuel Cell (MCFC) technology as a system for capturing carbon dioxide from the exhaust streams of a steam methane reforming plant located in Italy. MCFCs represent an active carbon capture solution, differing from conventional CCS systems by simultaneously producing electrical energy while capturing CO2 [1]. The study focuses on assessing the feasibility of using flue gases from the reformer as the cathode feed, and part of the off-gas from the PSA section as the anode feed, thereby avoiding the need for additional fuel input.

Methodology

A hybrid approach combining process modelling and experimental testing is adopted (Fig. 1). Process simulations based on real operational data from the reforming plant allow the identification of the fraction of off-gas suitable for feeding the MCFC anode. The experimental activity is conducted on a 100 cm2 laboratory-scale MCFC unit, where performance is monitored electrochemically and by analysing gas composition to determine the CO2 capture rate. Several anodic gas compositions are tested, investigating the effect of adding water to enhance internal steam reforming reactions and improve cell performance. Anodic-to-cathodic flow ratios are varied to explore the operational impact on both capture efficiency and power generation.

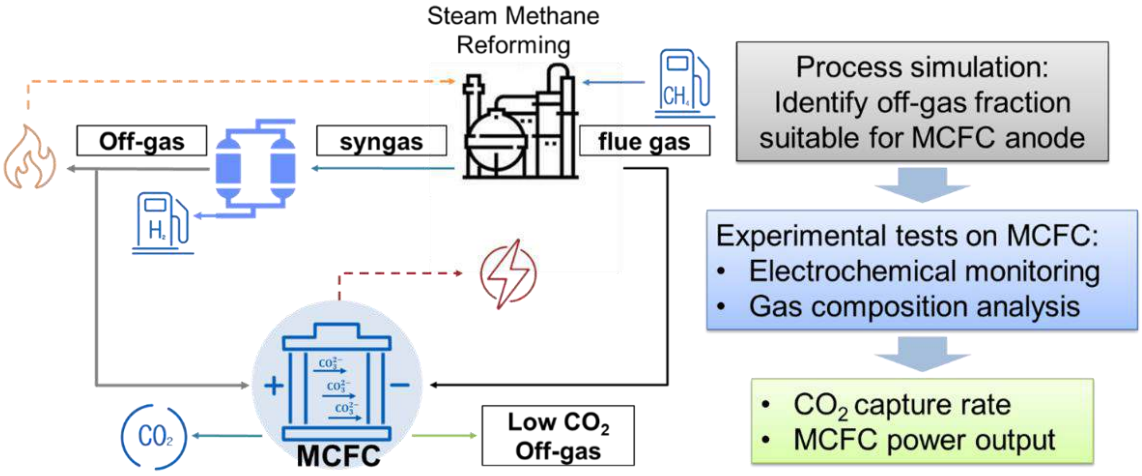

Figure 1. Schematic representation of the hybrid methodology adopted in this study.

Results

Experimental results indicate that increasing the water content in the anode feed improves electrochemical performance and enhances the CO2 capture rate. Under open-circuit conditions, the cathode composition remains largely unchanged, while the anode undergoes chemical transformations due to high-temperature reforming reactions. Higher flow rates tend to reduce CO2 capture and hydrogen utilization due to shorter residence times, highlighting the importance of optimizing gas flows to balance capture efficiency and energy production. Finally, an analytical estimate of the electrical power deliverable by the MCFC is carried out using the flow rates of the real system, comparing the results for different anodic gas compositions. This analysis provides a first evaluation of the potential power output achievable if the MCFC is integrated into the industrial plant.

Conclusion

This study demonstrates the feasibility of integrating MCFCs into a steam reforming plant as an active carbon capture system. Water content and flow conditions strongly influence both CO2 capture and electrical performance, suggesting that operational parameters can be tuned to maximize the benefits of MCFC technology as a dual-purpose solution for emission reduction and power generation.

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2026 / SEOUL, KOREA

CDC0287

Electrophoretic Dynamics in Electric Field-Assisted CO2 Capture over Molten Nitrate-Promoted MgO Sorbent

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Capture
Keywords: Electric Field; CO2 Capture; EM-MgO; Electrophoresis; Joule Heating Effect

Abstract Body.

Introduction. The concept of an electric field (EF)-controlled CO2 capture process was proposed, suggesting that applying an external EF on certain materials can activate CO2 adsorption on their surface.[1] However, research on EF-assisted CO2 adsorption has only been only conducted theoretically, with no experimental approaches reported. In this work, we conducted the first demonstration of EF-assisted CO2 capture process over molten nitrate-promoted MgO sorbent, in which adsorption performance was improved by Joule heating, electrophoresis of molten nitrates, and novel carbonate formation.

Methods. CO2 adsorption experiments were performed in a 6 mm I.D. quartz fixed-bed continuous-flow reactor connected to a GC-TCD. The sorbent bed was positioned between two stainless-steel electrodes at the reactor center for EF application. Adsorption tests were conducted at various temperatures using gas mixtures of 15% or 50% CO2/He at a total flow rate of 100 ml/min. A constant direct current of 5.0 mA was applied. Cyclic adsorption-regeneration tests were carried out with 50% CO2/He at 250 oC for adsorption and pure He at 350 oC for regeneration.

Results and discussion. Above the EM melting point, CO2 adsorption initially occurred at gas (CO2)-liquid (EM)-solid (MgO) triple-phase boundaries, followed by liquid-solid interfaces.[2] Under an applied EF, the adsorption capacity increased by 24.75%, primarily due to Joule heating, which elevated the sorbent bed temperature above the furnace input temperature and enabled CO2 uptake below the nominal EM melting temperature.

During EF-assisted adsorption, electrophoretic migration of EM was directly observed. SEM–EDS analyses confirmed EM enrichment at the negative side, enhancing EM–MgO contact and promoting MgCO3 formation. Nevertheless, depth-resolved XRD revealed layer-dependent formation of Li2CO3, K2CO3, K2Mg(CO3)2, and KLiCO3. NO formation during EF adsorption was also detected by NDIR and mass spectrometry.

These results demonstrate that the electric field facilitates CO2 adsorption and/or dissolution into EM while activating EM participation in carbonate formation, dynamically generating new carbonate phases absent under conventional conditions.

Acknowledgments

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (RS-2025-02306122) and the National Research Foundation of Korea (NRF) funded by the Ministry of Science and ICT (MSIT) (No. RS-2023-00261851).

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2026 / SEOUL, KOREA

CDC0161

Modelling approaches for sorption on solid sorbents

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Capture

Keywords: Adsorption, Intrinsic adsorption kinetics, Modelling, Direct Air Capture, Carbon capture, Amine sorbents

Abstract Body.
While adsorption is a promising approach for capturing CO_2 from low concentration streams and ambient air, efficient adsorbent-bed utilization remains an issue for which accurate prediction of breakthrough times and tailing behaviour are essential. These breakthrough characteristics are governed by external film resistance, intraparticle diffusion, and intrinsic adsorption kinetics. Conventional Linear Driving Force (LDF) model collapses these mechanisms into a single mass-transfer-coefficient, limiting mechanistic insight. To overcome this, Driessen et al. [1] proposed the Uniform Linear Approximation (ULA), which explicitly incorporates pore diffusion and kinetic resistances. Here, we further include film resistance to form a modified ULA (m-ULA). The aim of this study is to compare breakthrough behaviour predicted by both models, quantify how adsorbent properties influence model responses, and assess implications for column performance and design.

A one-dimensional pseudo-homogeneous packed-bed model for Direct Air Capture using Lewatit VP OC 1065 was solved using central finite difference MATLAB's ode15s solver. Particle properties (porosity, tortuosity, radius) and kinetic constant were varied to evaluate their impact on breakthrough time (tads, 5% inlet concentration) and pseudo-saturation time (tsat, 95% equilibrium loading). Analysis of Variance (ANOVA) quantified parameter sensitivity. Finally, both models were validated by fitting experimental CO_2/N_2 adsorption data on amine-functionalized SBA-15 [2].

The m-ULA and LDF models showed distinct breakthrough and uptake profiles when simulating the same adsorption column. The LDF model predicted pseudo-saturation at ~760 minutes, whereas the m-ULA model predicted it 60 minutes earlier. ANOVA revealed that the m-ULA model remained sensitive to selected parameters across temperatures, demonstrating diffusion-controlled trends without additional experiments. Particle radius had a notable influence on tads at all temperatures. At low temperatures, the intrinsic kinetic rate constant was dominant for tsat, while at higher temperatures, the particle radius became more influential due to reduced mass-transport limitations. In contrast, the LDF model's responses were primarily dominated by a single parameter. For the SBA-15 data, the m-ULA model provided a superior fit ($R^2 = 0.9972$) over the LDF model ($R^2 = 0.9927$) also generating particle-scale CO2 concentration profiles which showed minimal intraparticle diffusion limitations.

In conclusion, the m-ULA model offers a comprehensive and holistic approach to understanding adsorption processes compared to conventional models, yielding more accurate fit for the experimental data. This makes it a valuable tool for process design and optimization in carbon capture applications.

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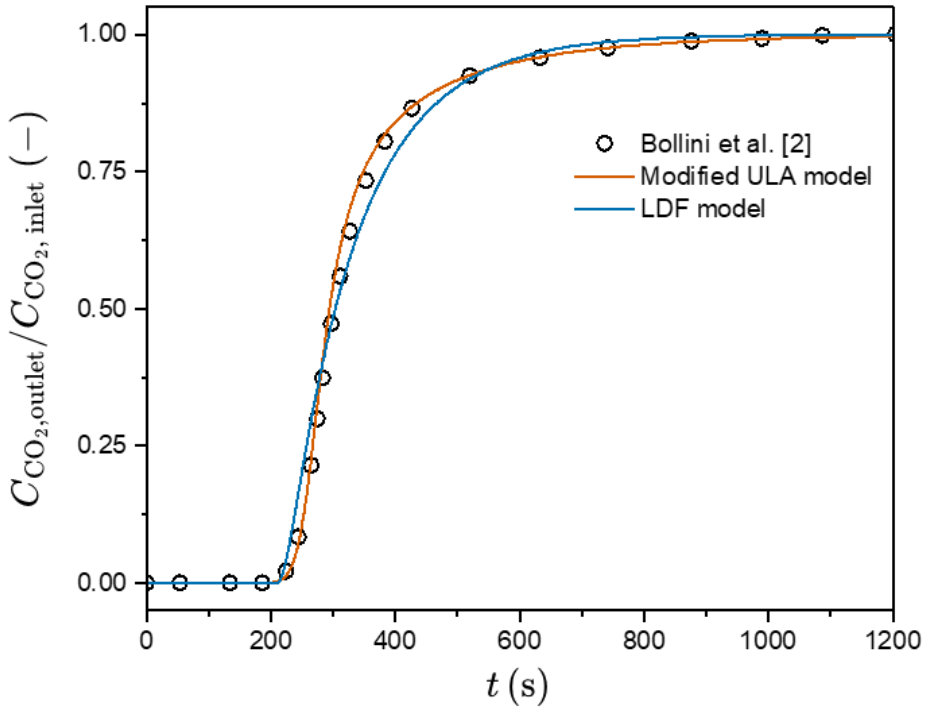

Figure 1: Numerical fitting of two models to the experimental breakthrough curves for post-combustion CO_2 adsorption on SBA-15 amine sorbent, obtained from *Bollini et al.* [2]

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CDC0666

Optimization of Operating Conditions in a Fluidized-Bed CO2 Capture System Using an Amine-based Solid Sorbent

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Capture
Keywords: Continuous CO2 capture, Process optimization, Fluidized bed reactor, Solid sorbent, CO2 adsorption

Abstract Body.
Introduction. To overcome the limitations of conventional amine scrubbing, specifically its toxicity and high energy penalties, this research investigates a commercial solid sorbent, called “Lewatit® VP OC 1065” (Lanxess, Germany) as a sustainable alternative for post-combustion CO2 capture. By evaluating this material under high-concentration industrial conditions, the study establishes the critical operating parameters, flow rate, concentration, and temperature, essential for engineering a cost-effective, circulating fluidized-bed system.
Methods. The experimental phase involved 81 runs using gas-solid dynamic adsorption system to evaluate the sorbent under various industrial conditions. The study tested CO2 concentrations of 6%, 12%, and 18%, representing different hydrocarbon sources. Flow rates ranged from 1 to 9 L/min, which were categorized into three distinct regimes: fixed (1–3 L/min), bubbling (4–6 L/min), and turbulent (7–9 L/min). Experiments were conducted at temperatures of 35°C, 45°C, and 55°C. Performance was measured using two key metrics: adsorption performance and exhaust gas composition.
Results and discussion. The results highlight a significant trade-off between uptake rate and total capacity, which is critical for system design. Lower flow rates allowed for maximum saturation, achieving a peak capacity of 522 mg/g at 18% CO2, 55°C, and 1 L/min. At this optimal saturation condition, the system achieved a maximum CO2 yield of 80% and a final yield of 29%. Conversely, higher flow rates, essential for fluidization, prioritized speed over total utilization. At 55°C and 18% CO2, increasing the flow rate to 8 L/min reduced the maximum yield to 16% and the final yield to 6%. However, these high-flow conditions significantly enhanced initial uptake; for instance, at 35°C, an 8 L/min flow rate yielded an immediate capture of 78 mg/g in the first minute, compared to only 2 mg/g at 1 L/min. These findings indicate that while low flows maximize total capacity, higher flow rates are necessary to maximize kinetic efficiency in a circular process. Utilizing Design of Experiments (DOE) and statistical analysis, this study characterizes adsorption behavior across distinct flow regimes to establish the kinetic baseline required for prototype modeling. These findings provide a critical benchmark for future research focused on substituting commercial media with sustainable, low-cost alternatives.
Acknowledgments: The Program Management Unit for Competitiveness (PMU-C), Office of National Higher Education Science Research and Innovation Policy Council (NXPO), Thailand, is acknowledged for partial financial supports to this project.

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CDC0684

Building-Integrated Direct Air Capture via HVAC Systems for Reduced Energy Demand and Cost

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Capture

Keywords: Direct Air Capture (DAC), Building integrated Direct Air Capture, Negative Emissions Technology (NET), Waste Heat Management

Abstract Body.
Introduction. Negative CO_2 emissions are considered essential for meeting climate targets, yet the deployment of direct air capture (DAC) remains constrained by high costs, centralized system designs, and public acceptance challenges. This study introduces an alternative DAC approach based on distributed, building-integrated capture, where compact, plug-and-play DAC units are embedded directly into existing HVAC ventilation systems. The proposed concept shifts DAC from isolated large-scale facilities to the built environment, enabling CO_2 capture from indoor air streams with elevated concentrations due to human occupancy.

Methods. A prototype building integration was engineered, and a physics-based MATLAB model was developed to investigate adsorption and regeneration processes within the DAC unit. The model resolves mass transfer in the adsorber bed using a linear driving force formulation and compares the performance of two amine-functionalized solid sorbents. System-level coupling with the HVAC infrastructure allows assessment of airflow conditions, CO_2 enrichment effects, and thermal integration. Regeneration energy is supplied via low-grade waste heat from an electrolyzer in combination with a heat pump and thermal storage.

Results and discussion. Results show that lower air temperatures and higher humidity enhance CO_2 uptake, while reduced humidity substantially decreases regeneration energy demand, achieving up to a 50 % reduction when relative humidity is lowered from 90 % to 10 %. The findings demonstrate that HVAC-integrated DAC systems can exploit building-specific synergies in airflow, waste heat, and thermal management. This work establishes distributed HVAC-DAC as a complementary pathway to centralized DAC plants, offering a scalable and potentially more socially acceptable route to negative emissions.
Conclusion.
This study shows that building-integrated, HVAC-coupled DAC systems can effectively leverage indoor CO_2 enrichment, existing ventilation infrastructure, and low-grade waste heat to reduce energy demand compared to centralized DAC approaches. As a distributed and modular concept, HVAC-integrated DAC offers a scalable and potentially more cost- and socially acceptable complement to large-scale DAC deployment.

Acknowledgments
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2026 / SEOUL, KOREA

CDU0051

Dual Upcycling CO2 and PET in an Integrated Electrolyzer

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: CO_2 Electrolysis, PET Valorisation, Electrolyzer Design, Gas-diffusion Electrode

Abstract Body.

Electrocatalytic CO_2 reduction (CO_2RR) offers a route to convert CO_2 into value-added products, but its viability depends strongly on the choice of anodic reaction. The conventional oxygen evolution reaction is energy-intensive and produces no co-product, often consuming >90% of the electrical input. Ethylene glycol (EG), obtained via PET hydrolysis, has emerged as an attractive alternative. PET consumption exceeds ~28.45 Mt yr^{-1} with only ~23% recycled, and hydrolysis enables true chemical recycling and upcycling [1]. Pairing CO_2RR with EG oxidation (EGOR) can lower cell voltage and add value at both electrodes [2], though current systems remain limited by modest current densities and stability.

We present a single, integrated electrolyser that co-processes hydrolysed PET and CO_2 to co-produce formate at ampere-scale rates. The anode employs a three-dimensional nickelfoam architecture to oxidise ethylene glycol (EG) obtained from PET hydrolysis [3]. By prioritizing mass transport and interfacial engineering rather than catalyst discovery alone, this anode delivers formate formation at 1.2 $A \cdot cm^{-2}$—to our knowledge, among the highest reported for non-noble metal systems. On the cathode, a $Bi_2O_2CO_3$-based gas-diffusion electrode (GDE) enables selective CO_2 electroreduction to formate, completing a closedcarbon valorisation loop within a single device.

The integrated design sustains 100 h of operation at 0.50 $A \cdot cm^{-2}$, maintaining Faradaic efficiencies of 93.7% at the anode (EG oxidation to formate) and 86.0% at the cathode ($CO_2$to-formate). Operating membrane-free, the cell achieves a 2.91 V full-cell voltage at 1.0 $A \cdot cm^{-2}$, corresponding to an energy input of ~0.10 $kWh \cdot mol^{-1}$, a ~65% reduction relative to conventional benchmarks. These outcomes arise from deliberate electrode structuring—high-surface-area current collectors, controlled wettability, and optimised gas–liquid pathways—that collectively minimise concentration polarisation and ohmic losses.

Beyond demonstrating a practical route for simultaneous PET upcycling and CO_2 utilisation, this work clarifies design rules for integrated electrolysers: (i) choosing anodic reactions that generate value while lowering overall cell energy; (ii) engineering transport-centric electrodes to sustain high current densities; and (iii) leveraging cathode GDEs that stabilise key intermediates for selective CO_2-to-formate conversion. The platform provides a blueprint for coupling waste-derived organics with CO_2 electroreduction to manufacture commodity chemicals efficiently, offering a scalable pathway toward circular-carbon manufacturing.

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CDU0091

Improving full energy efficiency in photoelectrochemical glycerol oxidation coupled with CO2 reduction using $BiVO_4$-based photoanodes

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: Photoelectrochemical co-valorisation; glycerol oxidation; CO2 reduction; process optimisation

Abstract Body.

Introduction. Photoelectrochemical (PEC) processes driven by photoanodes represent a more sustainable approach than conventional electroreduction methods. In particular, coupling relevant anodic oxidation reactions with cathodic CO2 reduction enables a more efficient use of photogenerated charges while lowering the overall energy demand of the PEC cell. This work focuses on maximizing the Full Energy Efficiency (FEE) of CO_2 and glycerol co-valorisation by evaluating multi-layered $BiVO_4$-based photoanodes, optimising both photoanode structure and operational conditions.

Methods. The study covers the application of different substrates (FTO and carbon paper), introduction of multi-layered architectures (WO_3/$BiVO_4$, $CaTiO_3$/$BiVO_4$, and $CaTiO_3$/WO_3/$BiVO_4$), photoanode thickness, and surface decoration (e.g., Ni) [1]. Beyond photoanode design, operating conditions are systematically optimised by tuning electrolyte pH, anolyte flow rate, and glycerol concentration (0.5–1.5 M) to assess viscosity-related effects on charge-transfer resistance. In parallel, incident light intensity is increased using a solar concentrator (>1 sun) to evaluate its impact on photocurrent generation and FEE. PEC characterization includes galvanostatic (CA) and potentiostatic (CP) measurements through LSV (to determine the effective operational windows) and EIS (to analyse resistive and charge-transfer limitations of the photoanode and the overall system). Besides, a detailed spectral analysis is conducted using a monochromator to determine IPCE across various wavelengths. The production of high-value compounds, particularly dihydroxyacetone (DHA) and formate ($HCOO^-$), is quantified to evaluate the selectivity of the different photoanodes and to identify the operating conditions that maximize the FEE.

Results and discussion. The results show that the $BiVO_4$/$CaTiO_3$ (3:1) configuration, corresponding to the lowest $CaTiO_3$ loading, exhibits the highest and most stable photocurrent [2]. In addition, LSV analyses indicate that the $BiVO_4$/WO_3 (80:20) photoanode delivers the best photocurrent response, confirming this ratio as the most favourable [3]. Finally, water splitting and glycerol oxidation are investigated using a Ni-decorated $CaTiO_3$/WO_3/$BiVO_4$ photoanode, highlighting the advantages of glycerol oxidation in terms of energy demand, a key factor for improving the FEE of the process. The analysis demonstrates that the synergistic optimisation of photoanode design and operating conditions significantly reduces the required

external bias while enhancing performance, paving the way toward PEC systems with an improved FEE.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

CDU0137

Na-Doped Ru/Mg-Al Dual-Function Material for Isothermal Integrated CO2 Capture and Methanation

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization
Keywords: CO2 Capture and Utilization (CCU); Chemical Looping; CO2 methanation; insitu DRIFTS

Abstract Body.

Introduction. Integrated CO2 capture and methanation (ICCM) using dual-function materials (DFMs) represents a promising strategy for flexible power-to-gas processes and CO2 utilization [1]. For practical implementation, DFMs must simultaneously ensure high CO2 storage capacity and rapid, selective methane formation under cyclic operation, particularly when realistic feeds containing H2O and O2 are employed [2].

In this study, a Ru-based DFM supported on a hydrotalcite-derived Mg-Al oxide and promoted with Na (Ru/Na-Mg-Al) is investigated for isothermal ICCM in a fixed-bed reactor. This formulation, not previously explored for this operating mode, is compared with unpromoted and K-promoted analogues to elucidate the role of alkali metals on CO2 adsorption, hydrogenation kinetics and cyclic performances under both ideal conditions (5% CO2/N2) and simulated realistic flue-gas compositions including H2O and O2 during the capture stage.

Methods. DFMs were prepared by dispersing Ru (1 wt%) via incipient wetness impregnation on the alkali-doped and undoped supported followed by calcination and reduction at 400°C. A multitechnique approach is adopted, combining catalysts' chemical-physical characterization, H2-TPSR in TG-MS, fixed-bed methanation tests, and operando DRIFTS, to correlate surface chemistry with macroscopic performance.

Results and discussion. The Ru/Na-Mg-Al system exhibits a favourable balance between CO2 uptake and methane productivity, outperforming the reference materials (i.e., Ru/Mg-Al and Ru/K-Mg-Al). While Ru/Mg-Al displays faster intrinsic methanation but limited CO2 storage, and K promotion favours the formation of stable surface intermediates with enhanced CO formation, Na doping leads to the accumulation of reactive carbonate, formate and carbonyl species. These intermediates persist after isothermal purging and are progressively converted to CH4, showing an initial fast methanation regime followed by a diffusion-limited stage associated with transport towards Ru active sites. Parametric ICCM experiments indicate that the presence of O2 during the capture step reduces cyclic CH4 production by 10-15%, mainly by delaying the availability of metallic Ru at the onset of hydrogenation. Water shows a dual effect: it enhances CO2 storage through activation of MgO adsorption sites, while moderating early-stage methanation kinetics and promoting CH4 selectivity, resulting in a temperature- and cycle-dependent effect.

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CDC0050

Data-driven DeepONet surrogate modelling for Direct Air Capture applications

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Abstract Category: *Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Capture*

Keywords: Direct Air Capture, DeepONet, Machine Learning, Optimization, TVSA modeling.

Abstract Body.

Introduction. Direct Air Capture removes CO_2 directly from ambient air and is increasingly considered essential for climate mitigation and for supplying CO_2 to downstream processes, such as green hydrogenation. Temperature Vacuum Swing Adsorption (TVSA) is one of the most promising DAC technologies, yet its simulation remains computationally expensive due to the nonlinear, tightly coupled PDEs governing heat and mass transfer in adsorption beds, limiting rapid optimization, sensitivity analysis, and real-time control [1]. Among all TVSA steps, the adsorption step is the dominant computational bottleneck, and it must begin from arbitrary spatial profiles inherited from the previous step. To overcome this, we develop a Deep Operator Network (DeepONet) surrogate that learns the adsorption operator conditioned on any admissible initial condition. This enables fast, differentiable, high-fidelity adsorption simulations suitable for optimization, inverse design, and cycle acceleration.

Methods .DeepONets consist of a branch network encoding the initial-condition function and a trunk network encoding spatial–temporal coordinates, whose outputs combine to approximate the operator [2]. We focus on an isothermal adsorption model with local thermal equilibrium, negligible axial dispersion, and film-controlled mass transfer. A dataset of 10 000 initial conditions (gaussians, sigmoids, exponentials, and straight lines) is generated, and high-fidelity PDE solutions (at a given initial condition) serve as training data. An extrapolation dataset with sinusoidal functions and unseen parameter ranges assesses robustness under atypical TVSA conditions.

Results and discussion. DeepONet achieves excellent interpolation accuracy across all initial-condition classes. Parity plots show near-perfect agreement between predicted and numerical fields for both gas-phase and solid-phase concentrations. Importantly, the model correctly handles both monotone and non-monotone shapes, indicating operator learning rather than memorization. Under extrapolation (sinusoidal and parameter-shifted inputs) the model retains strong predictive capability and physical consistency, with expected accuracy loss outside the training range. Even for completely unseen sinusoidal initial conditions, it generates meaningful spatio-temporal fields, confirming robust operator-level generalization. The key novelty is that the surrogate can start adsorption from any arbitrary initial condition, enabling significant computational savings: the DeepONet simulates adsorption in milliseconds, compared to the seconds–minutes range of PDE solvers. Such speed unlocks rapid CSS

detection, multi-objective optimization, uncertainty propagation, and the integration of adsorption surrogates into real-time digital twins.

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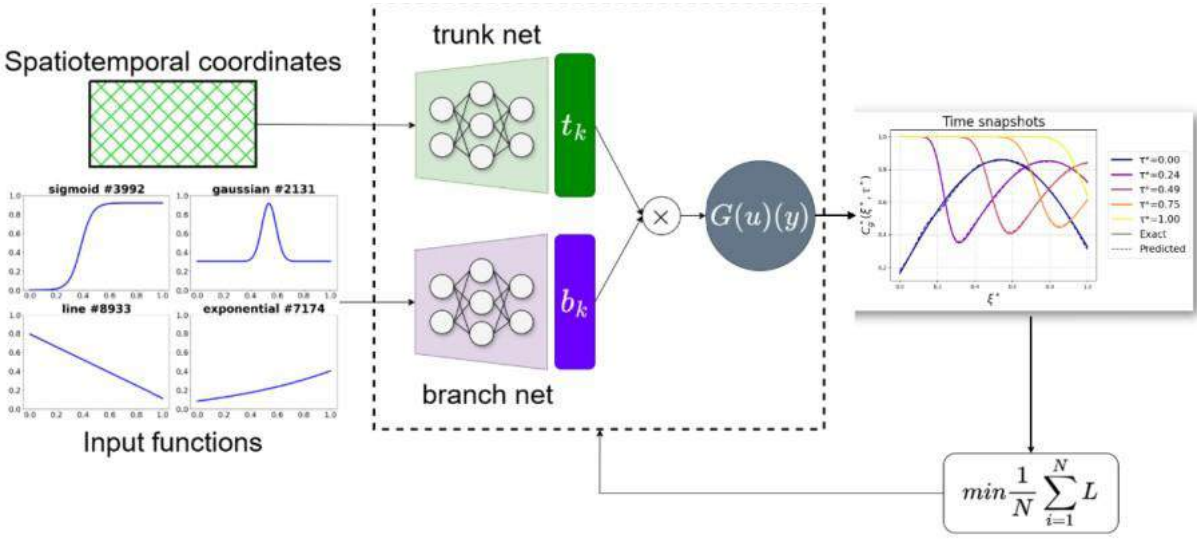

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CDU0184

Analysis of an Electricity-Price Optimized Operating Strategy of a Carbon Capture and Power-to-Methanol Pilot Plant

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: Power-to-Methanol, Dynamic operation, Control strategies, Load fluctuation

Abstract Body.

The electricity-based production of methanol is considered a potential key technology for the long-term storage and utilization of CO_2 captured from unavoidable point sources such as waste incineration plants or other industrial facilities with process-related emissions. By converting captured CO2 into valuable chemical energy carriers like methanol, a reduction of greenhouse gas emissions can be achieved while simultaneously supporting sector coupling between the electricity, chemical, and fuel sectors. However, due to the explicitly higher energy demand associated with both the CO_2 capture process and the subsequent methanol synthesis, e-methanol is currently far from being economically competitive with conventional fossil-based methanol production.

In this work, the potential reduction of operating costs is investigated by optimizing the operating modes of two coupled pilot plants that are dynamically operated and connected via intermittent storage systems. One plant is dedicated to CO_2 capture, while the second plant performs methanol synthesis. The coupling of both systems introduces additional operational constraints and interdependencies, which increase the complexity of flexible operation and limit the degree of operational freedom compared to independently operated plants.

Based on hourly electricity price forecasts over the span of a reference year, a Python-based optimization model determines which operating mode is financially favored at each point in time under the coupling-induced constraints. The model accounts for key parameters, including emitted and captured CO_2, produced methanol, electricity consumption, and additional utility requirements.

As both pilot plants were designed following comprehensive basic and detailed engineering studies, the assumptions implemented in the model provide realistic and reliable estimations of operating costs. The results indicate that adapting the operating strategy to fluctuating electricity prices and switching between multiple operating modes can reduce total operating costs by approximately 30% compared to a static operation strategy. Furthermore, a sensitivity analysis shows that increasing CO_2 certificate prices significantly enhance the economic

benefits of flexible operation. Cost savings increase by more than a factor of five due to avoided CO_2 emissions. These findings suggest that the economic viability of carbon capture and power-to-X processes at unavoidable point sources can be substantially enhanced, thereby strengthening the case for their large-scale application under future energy market conditions characterized by volatile electricity prices and increasing carbon pricing.

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CDU0248

Mitigating Ni Catalyst Oxidation in ICCU-Methanation via a Dual-Temperature Fluidized-Bed Chemical Looping Strategy

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: Chemical looping, Carbon capture, CO2 utilization, Methanation

Abstract Body.

Introduction. Integrated CO_2 capture and methanation is limited by severe oxidation of Ni catalysts under O_2-containing flue gas [1]. We propose a dual-temperature chemical-looping strategy using physically separated Ni/γ-Al_2O_3 and Na_2O/γ-Al_2O_3 circulated in interconnected fluidized-bed reactors, enabling suppressed Ni oxidation, rapid in-situ reactivation, and stable low-cost CO_2-to-CH_4 conversion.

Methods. Adsorbent and catalyst were circulated in a dual-interconnected fluidized-bed system [2] under alternating CO_2 capture (O_2-containing gas) and methanation conditions.

Results and discussion. Fluidized-bed redox cycling experiments using only the Ni catalyst demonstrated that oxidation at 120 °C preserved most catalytic activity, whereas higher oxidation temperatures caused progressive deactivation. Increasing the methanation temperature significantly accelerated in-situ NiO reduction; at 400 °C the catalyst was fully reactivated within ~30-35 s and even exceeded its fresh activity due to surface renewal during redox cycling (Fig. 1). When both catalyst and adsorbent were circulated in the dualinterconnected bubbling fluidized-bed system under O_2-containing CO_2 capture and H_2based methanation, stable and reproducible CH_4 production was achieved over multiple cycles. The rapid and repeatable CH_4 response confirmed effective CO_2 release, Ni reactivation, and robust dual-temperature chemical-looping operation.

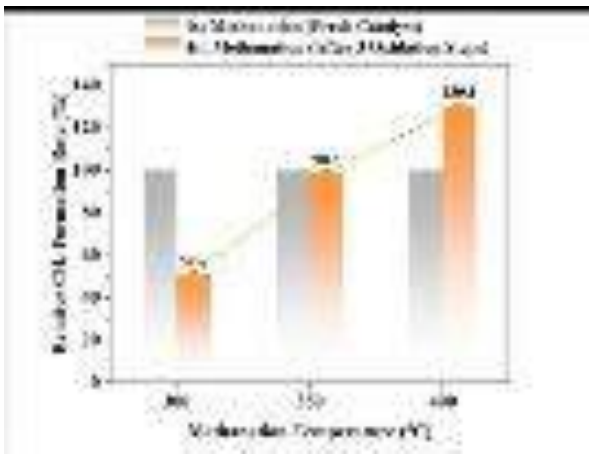

Fig. 1: Suppressed Ni oxidation at 120 °C and rapid Ni reactivation at elevated temperature using dual-temperature strategy.

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CDU0347

Engineering PFAS-Free Gas Diffusion Electrodes for Electrochemical CO_2 Reduction

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: Gas diffusion electrode, PFAS-Substitution, Sustainable electrocatalysis, Electrochemical CO2 reduction

Abstract Body.

Electrochemical CO_2 reduction (eCO_2R) represents a promising technology for mitigating CO_2 emissions and closing the carbon cycle. By selecting an appropriate catalyst, eCO_2R enables the direct conversion of CO_2 into valuable products. In this study, silver is used as the catalyst, showing high selectivity toward CO formation. [1]

To achieve current densities suitable for industrial applications, a gas diffusion electrode (GDE) is employed. The GDE overcomes mass transport limitations arising from the low solubility of CO_2 in aqueous solutions and enables direct transport of gaseous CO_2 to catalytically active sites. Typically, polytetrafluoroethylene (PTFE) is utilized as a mechanical binder and hydrophobicity agent. Its hydrophobic properties not only support the electrode function but also serve as a porous separator between gas and electrolyte compartments. [2]

Given concerns about the hazardous nature of polyfluorinated alkyl substances (PFAS) used in PTFE synthesis, and the prospect of European Union restrictions on PFAS, the development of environmentally friendly alternatives to PTFE is of growing importance [3]. In preliminary experiments, polyether ether ketone (PEEK) was evaluated as a fluorine-free binder, replacing PTFE in the GDE at various mass fractions. However, the lower hydrophobicity of PEEK resulted in a loss of separator function and significant electrolyte penetration, thereby precluding successful GDE operation.

To increase hydrophobicity, SiO_2 nanoparticles coated with highly hydrophobic methyl MQ silicone resin ($MeMQ/SiO_2$) a co-hydrolysis product of tetraalkoxysilane and trimethylalkoxysilane—were embedded in the PEEK-based GDE. It was demonstrated that incorporating $MeMQ/SiO_2$ particles could yield sufficient hydrophobicity to enable normal operation. Nonetheless, a side reaction was detected during operation, leading to rapid electrode degradation as can be seen in figure 1. However, the non-degraded $MeMQ/SiO_2$/PEEK GDE displayed an initial performance comparable to the PTFE-based GDE as shown in figure 2. These findings suggest that the integration of hydrophobic particles into silver-based GDEs is a promising strategy for PFAS substitution and the future development of PFAS-free electrodes. Ongoing research focuses on evaluating other hydrophobic particles for embedding in the GDE, with the aim of mitigating rapid degradation and enhancing long-term electrode stability.

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2026 / SEOUL, KOREA

CDU0419

Tuning e-fuel properties using zeolites in CO2-modified Fischer-Tropsch Synthesis

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: CO2 hydrogenation; Modified Fischer-Tropsch; E-fuel; Fe-based catalyst; Zeolite

Abstract Body.
Introduction. The increasing demand for sustainable fuels has accelerated research in the CO2-modified Fischer-Tropsch Synthesis (FTS) for obtaining liquid hydrocarbons (HCs). This study investigates the impact of zeolite structure and acidity on the performance of a Na-Fe3O4 catalyst, offering new insights into the optimization of the CO2-to-HC pathway.
Methods. The Na-Fe3O4 catalyst was synthetized according to the protocol reported by Tauro et al. [1], pelletized and then physically mixed with zeolite pellets with a mass ratio of 1:1. MFI- and BEA-type zeolites with SiO2/Al2O3 molar ratio ranging from 23 to 360 were employed. According to our previous work [1], the samples were first reduced and then carburized at 400 °C before testing them at 360 °C, 23 bar and 7 NL/gFe3O4/h of H2/CO2/N2 gas mixture. The gas phase was analyzed by means of an in-line GC system, while the two oil phases, separated at 150 °C and 5 °C, were analyzed according to ASTM D6352 and ASTM D6730, respectively. In addition, each catalyst was characterized using Mössbauer spectroscopy to identify all iron species and correlate them to their performance. Lastly, zeolites' acidity was measured using NH3-TPD and FT-IR spectroscopy using d3-acetonitrile as probe molecule.
Results and discussion. The addition of zeolites shifted the oil product distribution from olefin/naphthene-rich to iso-paraffin/aromatic-rich compositions and increased the C6+ yield by at least 25% [2]. On the one hand, DHA quantified more than 200 HC species, clarifying the influence of zeolites on the reaction mechanism and oils' properties (EN-228 regulation). On the other hand, structural characterizations revealed that iron carbides are preserved during pretreatment, but their oxidation is promoted under reaction conditions due to water retention. In addition, alkali migration from the Fe-based catalyst to the zeolite was observed by comparing TEM-EDS elemental maps of fresh and spent catalysts. The zeolite structure significantly affected the HC distribution. MFI-type zeolites narrowed the HC distribution in the gasoline-like range (C6 – C12); while BEA-type zeolites, that have larger pores, reduced the heavy HCs (C14+) fraction from 54% [1] to 26% of the total oil, promisingly rising the kerosene-like cut yield.

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CDU0498

Direct utilization of ambient carbon dioxide by reactive carbon capture

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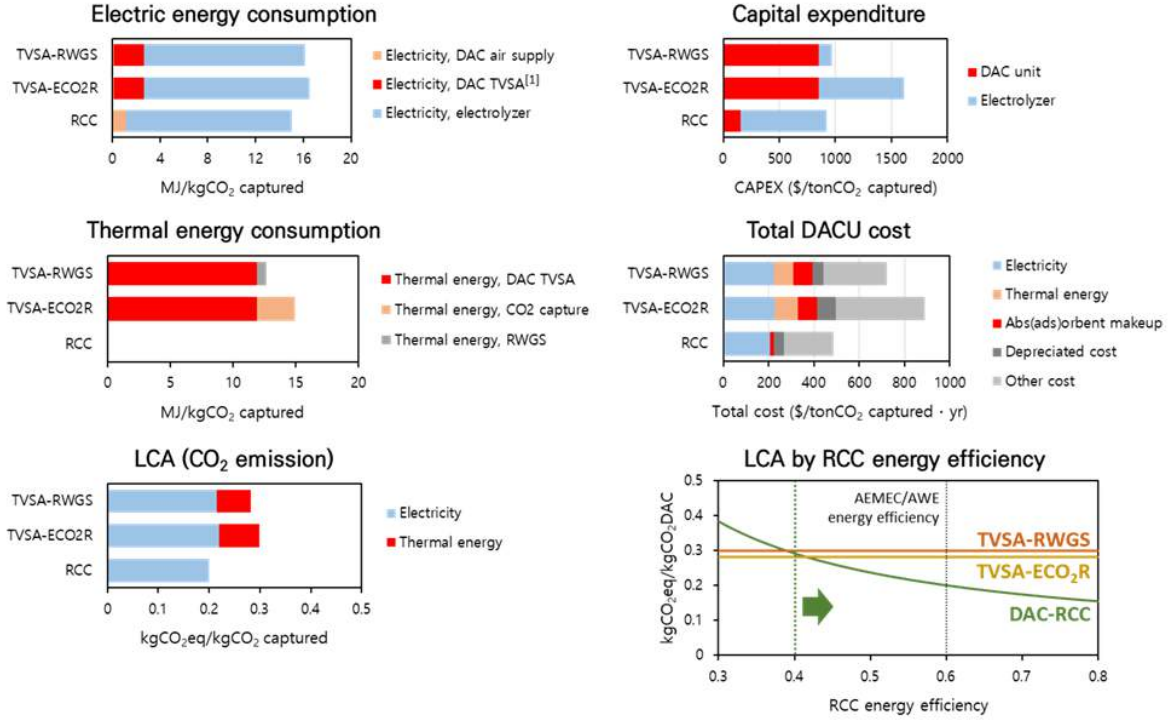
Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: Direct air capture, CO2 utilization, reactive carbon capture, sustainability, technoeconomic assessment, life cycle assessment

Abstract Body.
Amidst the steadily increasing global CO2 level, direct air capture (DAC) is considered as a solution to mitigate the CO2 level to below 400 ppm. Carbon utilization combined with DAC will bring true net-zero CO2 technology. Reactive carbon capture (RCC) has recently been proposed to avoid carbon regeneration energy from the carbon capture side and utilize the CO2 in aqueous phase directly, allowing more efficient pathway. Herein, we examine the potential of DAC-RCC systems in terms of energy consumption, technoeconomic assessment (TEA), and CO2 life cycle assessment (LCA). The multiple aqueous solvents are analyzed for the capture stage and thermochemical and electrochemical RCC are both considered. We compare the evaluation results of the DAC-RCC systems with three-stage systems (DAC – CO2 regeneration – CO2 utilization), and finally provide perspectives on DAC-RCC process, providing the required performance level that DAC and RCC should achieve.



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2026 / SEOUL, KOREA

CDU0548

Experimental and Modelling Assessment of Intraporous Mass Transport in Highly Active CO_2 Methanation Catalysts

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Keywords: CO_2 methanation; internal diffusion limitations; Ru/γ-Al_2O_3

Introduction. This study investigates the feasibility of developing highly active Ru-based catalysts suitable for intensified PtX applications by assessing intraporous mass transport limitations. Indeed, while methanation catalysts with conventional activity exhibit minor internal diffusion limitations effects [1-3], this can change in the case of highly active catalysts.

Methods. 4 wt.% Ru/Al_2O_3 catalysts were prepared by dry impregnation of γ-Al_2O_3 pellets (Sasol Puralox, 100 – 2300 μm) with an aqueous solution of Ru(NO)$(NO_3)_3$ (Alfa Aesar, 31.3 wt.% Ru). Textural properties were characterized by N_2 physisorption, while Ru loading and distribution were verified by SEM-EDX. Catalytic tests were performed in fixed-bed reactor from 0 barg up to 20 barg in a temperature range of 250 – 330 °C. Intraparticle diffusion and reaction phenomena were interpreted using a 1D pore model developed in gPROMS®.

Results and discussion. When working at constant GHSV, the increase of the catalyst pellet diameter from 100 to 2300 μm leads to a progressive decline in CO_2 conversion and CH_4 selectivity, with a marked performance decrease beyond 800 μm (Fig. 1A) (characteristic diffusion length of 130 μm). Interestingly, when operating at constant CO_2 conversion, a decrease in CO selectivity is observed in the pellet size range between 300 and 1000 μm compared to the 100 μm catalyst operating under kinetic regime (Fig. 1B). This phenomenon is attributed to CO_2 diffusion limitations within the catalyst pores, which locally increase the H_2/CO_2 ratio inside the pellet and favor CH_4 formation at the expense of CO. Operating under pressure (up to 20 barg) also partially mitigates the activity losses associated with internal diffusion limitations. The developed diffusion model accurately predicts the experimentally observed diffusion effects on CO_2 conversion for pellet diameters up to 2300 μm (e.g., Fig. 1A), relying solely on three adaptive parameters of a simplified kinetic rate expression [4], refitted with data from the 100 μm catalyst working in kinetically controlled regime (Fig. 1C).

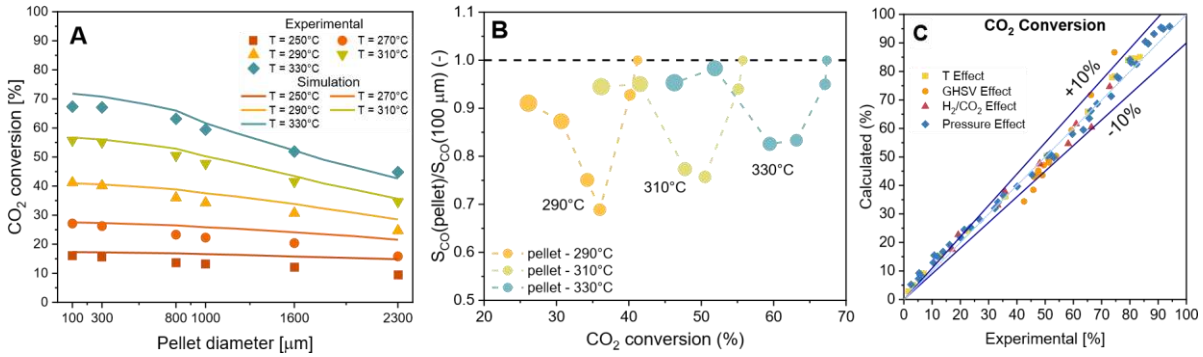

Figure 1. (A) Simulation and experimental results of CO_2 conversion at different pellet diameter and temperature. (B) CO selectivity measured on the 300 – 2300 μm samples (increasing point size corresponds to increasing pellet size) normalized to that of the 100 μm sample working at same CO_2 conversion. (C) Parity-plot of CO_2 conversion.

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2026 / SEOUL, KOREA

CDU0568

Highly Dispersed ZnZrOx Species on Zeolites Enabling CO2 Hydrogenation to Hydrocarbons

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: CO2 hydrogenation; Methanol-mediated pathway; Methanol-to-hydrocarbons; ZnZrOx/ZSM-5 catalyst

Abstract Body.

Introduction.

CO2 hydrogenation to hydrocarbons via a methanol-mediated pathway requires the effective integration of CO2-to-methanol synthesis and the methanol-to-hydrocarbons (MTH) reaction [1]. ZnZrOx catalysts exhibit high methanol selectivity at ~350 oC, enabling direct coupling with zeolitic MTH catalysts. This study reveals that highly dispersed ZnZrOx species positioned adjacent to zeolitic acid sites enable highly selective CO2-to-hydrocarbon conversion through the integration of methanol synthesis and the MTH reaction.

Methods.

Zn–Al-incorporated MFI zeolite was synthesized via hydrothermal treatment, followed by ZrO2 deposition using an impregnation method and calcination in air at 500 oC to obtain ZnZrOx/Al–MFI (Si/Al = 200, 400). As a reference, a physically mixed catalyst consisting of ZnZrOx and Al-MFI (ZnZrOx+Al-MFI) was also prepared. CO2 hydrogenation reactions were conducted at 350 oC and 2 MPa after H2 pretreatment, with a GHSV of 3600 mL h−1 gcat−1. The methanol synthesis reaction was evaluated in the absence of acid sites.

Results and discussion.

Nitrogen adsorption–desorption and XRD analyses confirmed the formation of well-developed micropores and the MFI-type zeolite structure for all samples. XRD patterns further revealed diffraction peaks assigned to tetragonal ZrO2 (t-ZrO2), indicating that incorporation of Zn into ZrO2 promoted stabilization of the tetragonal phase at <500 oC. XPS analysis of Zn 2p showed a progressive shift to lower binding energy in the order of ZnZrOx/MFI and sequentially impregnated ZrO2/ZnO/MFI, suggesting electron transfer from Zr to Zn and the preferential formation of Zn–O–Zr linkages in ZnZrOx/MFI.

Catalytically, ZnZrOx/MFI without acid sites exhibited high methanol selectivity, whereas the presence of acid sites promoted methanol conversion to hydrocarbons. While reducing acid

site density decreased CO2 conversion, it enhanced hydrocarbon yield, especially aromatics. This demonstrates that optimized acidity allows simultaneous methanol synthesis and MTH reactions, highlighting the importance of spatially proximate ZnZrOx species and appropriately tuned acid sites. Overall, spatially proximate ZnZrOx species and optimized zeolitic acid sites are essential for efficient CO_2-to-hydrocarbon conversion.

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CDU0594

Advancing CO2 Hydrogenation to Liquid Fuels via Spatial Proximity Control and Exsolution Engineering

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: CO2 Hydrogenation, Exsolution, Spatial Proximity, Sustainable Aviation Fuel

Abstract Body.

Introduction. The direct hydrogenation of CO2 into carbon-neutral liquid hydrocarbons offers a sustainable alternative to fossil-based fuels. However, precise control over product selectivity, particularly toward gasoline-range hydrocarbons (C5-11) and specific aromatics for sustainable aviation fuel (SAF), remains a significant challenge. This research aims to develop highly efficient multifunctional catalysts and elucidate the mechanistic roles of structural restructuration and catalyst spatial arrangement in governing reaction pathways.

Methods. We synthesized K-promoted Fe-supported CuAl2O4 (FeK/CAO) catalysts via co-precipitation and wet impregnation[1,2]. Exsolution-driven restructuration was systematically tailored by controlling reduction temperatures (350–500°C)[2]. A bifunctional system was developed by integrating FeK/CAO with a hierarchical nanosheet MFI zeolite (NS-HMFI)[3]. Four integration methods–physical mixture (PM), granule mixture (GM), dual-bed (DB), and multi–bed (MB)–were employed to investigate the impact of spatial proximity on catalytic performance.

Results and discussion. Optimization of FeK/CAO through 450°C reduction induced Cu exsolution and the formation of abundant oxygen vacancies, facilitating a cascade mechanism of CO2 activation and hydrogen spillover. This catalyst achieved a C5-11 productivity of 290.7 mLCO2 g cat -1 h-1 at 36.4% CO2 conversion. In the zeolite-integrate systems, the GM configuration yielded the highest CO2 conversion (39.2%) and lowest CO selectivity (13.0%) due to potassium migration and increased surface basicity. Conversely, the DB system maximized aromatic distribution by selectively converting light olefins into C8-10 aromatics. Notably, all NS-HMFI systems exhibited > 95% selectivity for C8-10 aromatics within the total aromatic fraction, highlighting the critical role of external acid sites on mesoporous zeolite walls. This study establishes a quantitative relationship between catalyst structure, spatial proximity, and performance. By engineering exsolution features and spatial arrangement, we demonstrated efficient CO2 conversion into SAF-range hydrocarbons.

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CDU0664

On the optimal design of cooled fixed-bed reactors for the direct methanation of biogas and syngas via 2-D modelling

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: COx methanation, cooled reactor, 2D model, thermal management, radial profiles.

Abstract Body.

Introduction

Biogas and syngas can be exploited to produce synthetic natural gas (SNG) through CO and CO2 methanation, to partially replace fossil natural gas. Since hydrogenation reactions are strongly exothermic, thermal management throughout the reactor is crucial to avoid hot spots that may lead to catalyst deactivation (e.g., via sintering). The main purpose of this work is to assess the role of strategies to control the temperature increase within the reactor, such as reactant staging and product recycling.

Methods

A two-dimensional model for multi-tubular, cooled, fixed-bed reactors was developed, solving a set of partial differential equations (PDEs) from the species and energy balances. Kinetics for COx methanation is obtained from the open literature [1]. Inlet temperature is set equal to 250 °C, and the reacting gas pressure is fed to the unit at 15 bar. The effectiveness factor for a catalyst pellet was calculated through the Thiele modulus [2]. A series of reactors was considered to achieve high conversion, enabling the production of a synthetic gas that potentially fulfills the natural gas prescriptions for the injection into the distribution grid [3].

Results and discussion

Even though the reactors are cooled, thermal management challenges result from two-dimensional modeling. If once-through methanation is carried out without staging, the maximum temperature exceeds the fixed threshold of 550 °C. This is due to the strong radial temperature gradient resulting from the model, which is caused by low heat transfer in the central zone of a tube section. A methanation unit with recirculation was thus adopted and modelled to control the temperature increase. Figure 1 shows the temperature profiles along the reactors when 30% of the gas exiting the first reactor is recirculated.

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CDU0676

Impact of Catalyst Preparation Routes on Structural Properties and CO2 Methanation Performance of Ni/CeO2 Catalyst

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: CO_2 methanation, Ni/CeO_2 catalyst, Pechini-derived synthesis, Sabatier reaction

Abstract Body.

Introduction

The catalytic hydrogenation of carbon dioxide to methane (CO_2 methanation) is a promising route for carbon capture and utilization (CCU), enabling the conversion of CO_2 into synthetic natural gas while facilitating renewable energy storage. Nickel-based catalysts supported on ceria have attracted significant attention due to their high activity, oxygen storage capacity, and strong metal–support interactions. However, the catalytic performance of Ni/CeO_2 systems is strongly influenced by the catalyst preparation method, which governs metal dispersion, reducibility, and surface properties. In this study, the effect of different synthesis routes on the structural characteristics and CO_2 methanation performance of Ni/CeO_2 catalysts is systematically investigated.

Methods

Ni/CeO_2 catalysts with identical nickel loading were synthesized using co-precipitation, impregnation, urea hydrolysis, and Pechini-derived sol–gel methods. The prepared catalysts were characterized using XRD, BET surface area analysis, H_2-TPR, and Raman spectroscopy to elucidate crystallinity, textural properties, reducibility, and oxygen vacancy concentration. Catalytic performance was evaluated in a high-pressure fixed-bed reactor over a temperature range of 200–550 °C at 5 bar using H_2/CO_2 feed, and product analysis was carried out by online gas chromatography.

Results and discussion

The preparation route markedly influenced the physicochemical properties and catalytic behavior of Ni/CeO_2 catalysts. Among all samples, the Pechini sol–gel derived catalyst exhibited superior nickel dispersion, enhanced metal–support interaction, and higher concentration of surface oxygen vacancies, leading to improved reducibility. As a result, this catalyst achieved a maximum CO_2 conversion of 84% with CH_4 selectivity of 93% under optimized reaction conditions. Catalysts prepared by conventional impregnation and co-precipitation showed comparatively lower activity and selectivity due to larger Ni particle sizes and weaker metal–support interactions. The results clearly demonstrate that controlled synthesis via the Pechini sol–gel route plays a crucial role in optimizing the structure–performance relationship for CO_2 methanation.

Acknowledgments
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CDU0283

Advancing CO2-Derived e-Fuels through Fischer–Tropsch Synthesis

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: CO2 Utilization, e-Fuel, Fischer-Tropsch, Syngas

Abstract Body.
CO2-derived e-fuels have recently attracted worldwide attention as a promising solution for decarbonizing hard-to-abate sectors such as aviation, marine transportation, and heavy-duty applications. In this context, Fischer–Tropsch synthesis (FTS) has re-emerged as a core technology for converting CO2 into synthetic fuels via syngas (CO + H2). Among various process configurations, the combination of precipitated iron-based catalysts and slurry-phase reactors is one of the commercially proven approaches for producing C5+ hydrocarbons through low-temperature FTS (LT-FTS). Conventional precipitated iron-based catalysts are typically obtained in oxide phases, such as α-Fe2O3, which are inactive for FTS and therefore require activation pretreatment in a CO-containing reducing atmosphere to form catalytically active iron carbide phases. However, such oxide catalysts are scarcely carburized under conventional high-pressure syngas FTS conditions. Recently, we have developed a novel class of precipitated iron-based catalysts that can be spontaneously activated under FTS reaction conditions without extra pretreatment, referred to as SponCat. In this presentation, we report our recent advances in SponCat technology and demonstrate its applicability and performance in slurry-phase Fischer–Tropsch reactors.
The SponCat efficiently promoted LT-FTS, exhibiting exceptionally high wax selectivity (SponCat-Wax). The maximum wax selectivity reached approximately 70 wt% of total hydrocarbons, corresponding to C5+ selectivity exceeding 90 wt%. This enhanced performance is attributed to enriched surface carbon species and increased surface basicity induced by electron donation from highly dispersed potassium species. Notably, SponCat-Wax demonstrated excellent applicability in slurry-phase reactors, maintaining stable catalytic performance without significant deactivation. Furthermore, a physical mixture of SponCat and zeolites enabled a tandem process integrating LT-FTS with downstream cracking reactions, achieving a high liquid-range (C5–C20) hydrocarbon selectivity of up to 80 wt% of total hydrocarbons. The cracking rate was found to be linearly correlated with the concentration of Brønsted acid sites, highlighting the critical role of zeolite acidity in tailoring product distributions. Overall, the SponCat technology offers a robust and scalable catalytic platform for efficient CO2-derived e-fuel production through simplified activation, high wax selectivity, and flexible integration with slurry-phase and tandem reactor systems.
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of Energy Research (KIER) (No. C6–2406-21) and the Next-generation CCU technology advancement project through the National Research Foundation of Korea (NRF) funded by the Ministry of Science and ICT (RS-2025–02219162).

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CDU0279

La-based perovskite mixed metal oxide for CO2 removal via direct air capture and in situ conversion

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: Direct Air Capture and Conversion; Dual Functional Materials; CO Selectivity; Lanthanum Perovskite; La2CoO4

Abstract Body.
Introduction. Negative emission technologies are critical for removing CO2 from air, with direct air capture and in situ conversion (DACC) offering a promising route for simultaneous CO2 capture and conversion into value-added products. The performance of DACC relies on advanced dual functional materials, particularly those enabling isothermal and modular operation.
Methods. Herein, we report a La-based DFM for isothermal DACC synthesized via a solvothermal route followed by annealing. The materials were in situ reduced in 5% H2 at 500 °C and evaluated for CO2 capture (400 ppm CO2) and subsequent hydrogenation. La-based perovskite (Co/LCO) and its individual components, La2O3 and Co/CoOx, were used as control DFMs for comparison.
Results and discussion. In (Fig. 1(a)), Co/CoOx break-through curve increased almost immediately to 400 ppm indicating negligible CO2 uptake at 400 °C. In contrast, La2O3 exhibited breakthrough before 5 min and a gradual increase toward 400 ppm. Moreover, Co/LCO displayed breakthrough at 16 min (delayed by 700% relative to Co/CoOx) and showed a much less pronounced rise with the effluent concentration remaining around 0.002 µmol mL-1. Fig. 1(b) compares CO2 capture and product formation at 400 °C. Co/CoOx showed negligible CO2 capture (1.1 µmol g-1) and trace CO/CH4, while La2O3 exhibited moderate capture (14.5 µmol g-1) with CO as the only product. In contrast, Co/LCO achieved a much higher CO2 capture of 48.9 µmol g-1 and produced 20.9 µmol g-1 of CO. Co/LCO delivered ~3.4 times higher CO2 capture and ~4 times higher CO production than La2O3.

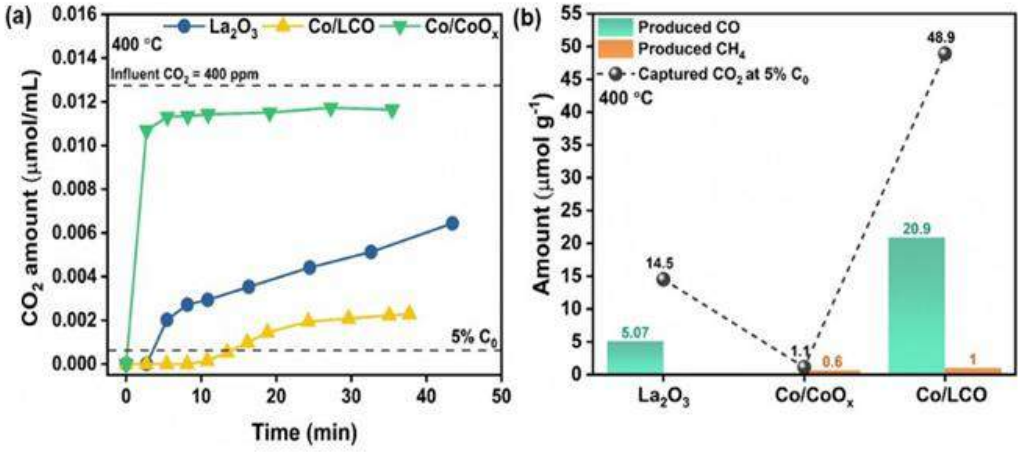

Fig. 1. (a) Breakthrough curves of 400 ppm CO2 at 400 °C for La2O3, Co/CoOx, and Co/LCO. (b) Initial CO2 capture capacity (μmol g-1) determined at the breakthrough point (5% of inlet CO2 concentration) and CO/CH4 production performance during the subsequent hydrogenation stage at an isothermal temperature of 400 °C under 5% H2.

Acknowledgments
This work was supported by the Korea Institute of Science and Technology Institutional Program (2E33952 and 2E33954) and DACU Project (No. RS-2023-0025992) through the National Research Foundation of Korea (NRF) grant funded by the Ministry of Science and ICT (MSIT), Republic of Korea.

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CDU0299

Low-content Ru/TiO2 catalysts for efficient CO_2 methanation: catalyst development and reactor design

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: CO2 methanation, reactor design, Ru catalyst, Titania

Abstract Body.
Introduction. This study aimed to compare different supported low-content Ru-based catalysts for CO2 methanation, identify and carry out an in-depth analysis of the most performant one, and employ it in a real-case scenario.
Methods. A series of low-content Ru-based catalysts supported on Al2O3, TiO2, CeO2, MgO, and ZrO2 were synthesized via incipient wet impregnation and evaluated for CO2 methanation. Among them, Ru/TiO2 exhibited the highest activity in terms of turnover frequency (TOF = 3.35 s-1) and selectivity toward CH4 (> 95%). To elucidate the underlying reaction mechanism, operando Diffuse Reflectance Infrared Fourier Transform Spectroscopy (DRIFTS) analyses were performed, revealing the presence of key surface intermediates. Based on these observations, several power-law and Langmuir–Hinshelwood–Hougen–Watson (LHHW) kinetic models were formulated and fitted to experimental data, to design an industrial reactor minimizing catalyst cost and ensuring wide operating conditions flexibility.
Results and discussion. The characterizations revealed a dispersion of Ru atoms above 40 % and a TOF of 3.35 s-1. In particular, operando DRIFTS measurements (Fig.1-up) revealed the presence of bidentate carbonate species at low temperatures (T < 300 °C), that disappeared at higher temperatures (T ≥ 300 °C), where C–H bands appeared confirming the production of CH4. Bridge-bonded CO* species were detectable only in stoichiometric H2/CO2 conditions. Those pieces of information were used to derive different kinetic models, corroborating the idea that the reaction mechanism follows the dissociative formyl route. Lastly, the kinetic results were employed in a real-case scenario to show the advantages of using Ru-based catalyst to manage the thermal issues of the CO2 methanation reactors (Fig.1-right): the proposed scenario exemplifies the effective integration of a Ru-based catalyst with a Ni-based one to reduce costs while ensuring proper thermal management: within 2.7 m of tube length a near-equilibrium CO2 conversion is reached, with 1/3 of the catalytic bed length with undiluted Ru/TiO2 and 2/3 using 24 wt.% Ni/Al2O3 with a catalyst-to-inert ratio of 1:7.

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CDU0320

Kinetic and Experimental Investigation of CO2 Methanation in a Bubbling Fluidized Bed

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: CO2-methanation, Fluidized-bed reactor, Kinetic-modelling, Sorption-enhanced-methanation, Carbon Capture and Utilization

Abstract Body.

Introduction. Limiting the annual emissions of carbon dioxide into the atmosphere represents a major challenge that could be addressed through carbon capture and utilization (CCU) technologies, wherein green or blue hydrogen is employed to convert captured CO2 into chemicals or synthetic fuels. In this work we have focused on the production of synthetic natural gas (SNG) in a fluidized bed reactor, a topic largely overlooked in the literature.

Methods. A kinetic study was performed using data obtained from purposely designed methanation experiments conducted in a lab-scale bubbling fluidized bed reactor, under traditional and sorption-enhanced methanation (SEM) conditions. A one-dimensional model of the catalytic fluidized bed reactor was developed and implemented in MATLAB. Finally, mass balances were derived including the possible presence of a selective water adsorbent to shift the equilibrium towards methane production (SEM) [1].

Results and discussion. Based on experimental data, kinetic parameters were estimated and benchmarked against reference literature values [2], achieving Mean Absolute Percentage Errors below 10%. The validated model was then used to analyze reactor behavior, with predicted concentration profiles revealing reaction zone distributions under different operating conditions (e.g. Figure 1). Overall, the model showed excellent agreement with experiments and accurately described both conventional methanation and SEM conditions.

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CDU0407

Decoupling the Role of Exsolved Ni and Active Support in Dry Reforming of Methane: Enhanced CO2 Dissociation over Ni-doped La2Ti2O7

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: Dry reforming of methane, Exsolution, Layered Perovskite, La2Ti2O7, CO2 activation, Ni nanoparticle

Abstract Body.
Introduction. Developing coke-resistant catalysts for dry reforming of methane (DRM) requires a fundamental understanding of the synergy between active metal and support. While exsolution is a promising strategy to anchor metal nanoparticles, the distinct contributions of exsolved particles versus support-mediated activation have remained elusive. Herein, we decouple the roles of exsolved Ni and the La2Ti2O7 support by precisely controlling the non-stoichiometry (A-site (La) vs. B-site excess (Ti)) of Ni-doped layered perovskites, aiming to establish a robust design principle for coking-resistant catalysts.[1]
Methods. A series of Ni-doped layered perovskite catalysts (La2Ti2-xNixO7-δ) were synthesized with varying Ti contents to induce specific non-stoichiometric environments: A-site excess (La2Ti1.8Ni0.1O7-δ, LT-Ae), stoichiometric (La2Ti1.9Ni0.1O7-δ, LT), and B-site excess (La2Ti2Ni0.1O7-δ, LT-Be). The local coordination structure and exsolution behavior of Ni were characterized using STEM-EDS and EXAFS. To elucidate the reaction mechanism and the role of the support, comprehensive kinetic studies, including reaction order analysis and transient CO2-and C18O2 isotope pulse experiments, were conducted alongside catalytic performance tests at 500-800 °C.
Results and discussion. Structural analysis revealed that the host lattice stoichiometry dictates the Ni coordination environment: B-site excess promoted the formation of metallic Ni ensembles (Ni-Ni dominance), driving high initial conversion but suffering from severe carbon deposition. In contrast, the stoichiometric LT catalyst maintained a balanced Ni dispersion. Crucially, kinetic studies uncovered a paradigm shift in the reaction mechanism; the LT catalyst exhibited a high positive CO2 reaction order (1.8), whereas the B-site excess counterpart showed a near-zero order (-0.1). Coupled with CO2 pulse experiments, these results demonstrate that the stoichiometric support (LTO) actively participates in CO2 dissociation, effectively gasifying surface carbon deposited on adjacent Ni sites. This reveals a critical trade-off between promoting Ni exsolution and maintaining the support capability. While B-site excess enhances metallic sites, it compromises the support ability to participate in the Mars-van Krevelen mechanism (CO2 activation). Therefore, the stoichiometric catalyst represents the optimal design point, effectively balancing active Ni sites for methane activation

with sufficient oxygen vacancies for coke gasification. This work offers a distinct guideline for designing perovskite catalysts: maximizing exsolution is not solely sufficient; preserving the support active role is equally vital for long-term stability.

Acknowledgments
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CDU0409

Green syngas production via eRWGS: an in-depth analysis of an electrified packed foam reactor.

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Keywords: Electrified reactor; Reverse Water Gas Shift; Joule-heating; CO_2 valorization.

Introduction. In a world committed to reducing CO_2 emissions, the production of green syngas via Reverse Water Gas Shift (RWGS) is expected to play an important role. Given the endothermic nature of the RWGS reaction, an electrified reactor that uses renewable electricity to provide high-temperature heat completely eliminates CO_2 emissions from combustion processes. In this work we provide an in-depth experimental and modelling analysis of a directly Joule-heated Silicon infiltrated Silicon Carbide (SiSiC) foam packed with Rh catalysts for syngas production, shedding light, for the first time, on the thermal effects of competitive methanation.

Methods. Experimental activities were conducted using a lab-scale reactor where a SiSiC open cell foam (L=100 mm, d = 35mm) was packed with 56 g of Rh-Al_2O_3 catalyst pellets (dp=1mm) by Heraeus. As illustrated in Figure 1a, the SiSiC structure (purchased from Engicer SA) was connected to an AC power supply via two stainless steel electrodes in contact with flat surfaces of the cylindrical foam. Being characterized by a high resistivity, this structure acts as a heating element that, by Joule effect, generates thermal power directly inside the catalytic bed, in intimate contact with the catalyst [1]. The effects of GHSV, temperature and pressure were investigated operating the system up to 750°C, 5 bar and 18 $Nm^3/kg_{cat}/h$, corresponding to a total inlet flow rate of 1 Nm^3/h. A H_2:CO_2 feed ratio equal to 3:1 was set to obtain a syngas composition suitable for methanol production. A 2D mathematical model of the packed foam reactor was applied to data analysis and scale up, employing a C1 kinetic scheme independently developed for the same catalyst.

Results and discussion. Experimental data demonstrated that our reactor was able to achieve equilibrium CO_2 conversion and CO-selectivity throughout the whole set of conditions while ensuring thermal efficiencies up to 76%. Measured axial temperature profiles (Figure 1b) showed the effect of methanation on the temperature distribution inside the catalytic bed; indeed an increase of 300°C occurred in the first section of the reactor, for the combined action of Joule heating and methanation exothermicity, enhanced at higher pressure. These data were used to validate a mathematical model of the e-reactor, currently the packed foam.

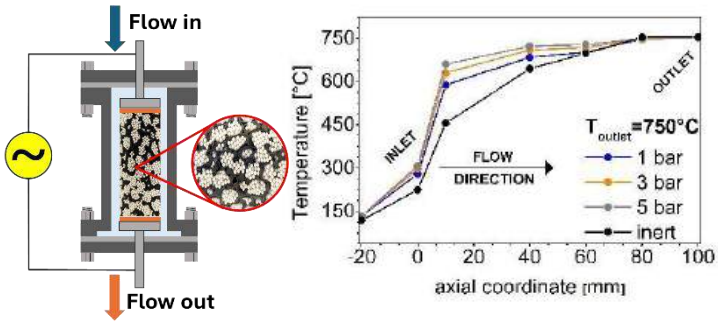

Figure 1 a) scheme of the electrified reactor and highlight on the e-reactor, b) effect of pressure on the axial

temperature being used to design an industrial profiles. GHSV=12 $Nm^3/kg_{cat}/h$. scale unit.

Acknowledgments
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CDC0511

A Novel DMEA-based Tri-Amine Solvent for Efficient CO_2 Capture: Performance, Kinetics, Spectroscopic and Toxicity Assessment

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Capture

Keywords: CO2 capture; DMEA/PZEA/DETA blend; CO2 solubility; kinetics; KE model; 13C NMR and FTIR

Abstract Body.

Introduction: Anthropogenic CO2 emissions from fossil fuels, industry, and deforestation are major drivers of climate change. Post-combustion carbon capture via chemical absorption is preferred due to ease of integration and industrial feasibility. Conventional amines such as MEA and DEA offer fast CO2 uptake but require high regeneration energy.1 Polyamines (DETA, TETA) provide fast kinetics and high cyclic capacity, but a higher heat of absorption and moderate energy demand, while tertiary amines (DMEA, MDEA) form bicarbonates with lower heat of absorption and lower energy demand but slower kinetics.1,2 Cyclic amines (PZ, PZEA) combine rapid kinetics, high loading, and steric advantages for regeneration.1,2

This study investigates a tri-amine aqueous blend of N,N-dimethylethanolamine (DMEA), 2(1-piperazinyl)ethylamine (PZEA), and diethylenetriamine (DETA) for post-combustion CO2 capture, aiming to synergize fast kinetics, high loading, and low energy requirements. Methods: Certified chemicals were used to prepare the tri-amine blend. CO2 absorptiondesorption performance was evaluated under varying operating conditions using a lab-scale setup, and CO2 loading was determined using a Chittick apparatus. Key physicochemical properties (pH, density, viscosity, and refractive index) were measured over relevant operating conditions. Experimental data were correlated using KE and empirical models, and performance parameters, including the heat of absorption, cyclic loading, cyclic capacity, heat duty, and regeneration efficiency, were calculated using established relations.2 Molecular interactions and structural changes were investigated using ^{13}C NMR and FTIR spectroscopy, while toxicity was assessed using reported LD50 (oral, rat) data.

Results and discussion: The effects of key operating parameters-including temperature, CO2 partial pressure, total amine concentration, and activator (DETA and PZEA) weight fractions- on CO2 loading were systematically studied. The novel tri-amine blend exhibited outstanding performance, achieving CO2 loadings above 1 mol CO2/mol amine. Compared to conventional 30 wt% MEA, it showed a lower heat of absorption (>20% reduction), higher cyclic capacity (>30% increase), reduced regeneration energy (>30% reduction), improved regeneration efficiency (>60% increase), and faster absorption-desorption kinetics. CO2 solubility predictions from empirical and modified Kent–Eisenberg models matched experimental data within <5% deviation. Reversible carbamate and bicarbonate formation was confirmed via ^{13}C NMR and FTIR, while measured physicochemical properties indicated favorable solvent stability. Toxicity analysis further highlighted a safer solvent profile. These results demonstrate that the proposed

tri-amine blend is a scalable, energy-efficient, and cost-effective alternative for post-combustion CO2 capture.

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CDC0659

Breakthrough in Direct Air Capture: High-Performance CO2 Adsorption Tower Design and Optimization

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Capture

Keywords: Direct air CO2 Capture; Solid sorbents; Optimization; Breakthrough curve.

Abstract Body.
Introduction. The current atmospheric carbon dioxide (CO2) level has increased to 420–425 ppm by 2024, which is close to the critical value of 580 ppm. Furthermore, the continued use of coal for electricity generation contributes significantly to global CO2 emissions. CO2 has the ability to trap heat, causing the global temperature to rise. In large industries, liquid amines are used to absorb CO2 from the power generation process. However, liquid amines are expensive, toxic to humans, and require high energy for regeneration.
Methods. This study presents a high-performance Direct Air CO2 Capture (DAC) system utilizing Lewatit® VP OC 1065 (Lanxess, Germany), a commercial solid sorbent for CO2 adsorption. The system's architecture and performance were evaluated through a multivariable optimization involving (1) loading amount of solid sorbents, (2) CO2 flow rate, and (3) adsorption temperature. The experimental setup and the resulting adsorption profiles are illustrated in Fig. 1, which details the innovative structural schematic of the adsorption tower and the corresponding breakthrough curve analysis. A factorial design and ANOVA were employed to quantify the influence of operational parameters and their interactions. Results and discussion. The results showed that all three variables significantly influence CO2 adsorption capacity, with CO2 flow rate being the most dominant factor. Notable interaction effects were observed between solid sorbent loading and CO2 flow rate, as well as the temperature and CO2 flow rate. The highest adsorption capacity achieved was 84.43 mg CO2/g sorbent, using 18 g of the sorbent, at 20 °C, and 10 LPM of airflow. This innovation generates a novel approach to implementing proactive policies aimed at reducing atmospheric CO2 concentration from the current level of 420 ppm to pre-industrial levels of 280 ppm. This paradigm shift establishes a new framework for environmental improvement technology, enhancing capabilities to advance carbon-neutral and net-zero initiatives beyond mere emission reduction to active atmospheric carbon removal.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

CDU0097

Autothermal Reactor Design for CO2 Hydrogenation to Methanol

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: CO2 Utilization, Alternative Fuel, Methanol Synthesis, Autothermal Reactor

Abstract Body.

Introduction

Catalytic conversion of CO2 into methanol using renewable H2 represents a promising pathway for mitigating atmospheric CO2 while producing a sustainable alternative fuel [1].

For the exothermic CO2 hydrogenation reaction, conventional reactors often exhibit low CO2 conversion and limited selectivity towards methanol due to thermodynamic and kinetic limitations. In such cases autothermal reactors, utilizing the heat of reaction to preheat the feed and operating in the region of multiple steady states, can increase per pass conversion of CO2 while operating at low feed temperatures.

Methods

In this work, a pseudo-homogeneous model of catalytic tubular reactor with external heat exchanger is developed (Fig.1a) assuming no temperature and concentration gradients between fluid and catalyst phase. Bussche and Froment kinetic model [2] for Cu/ZnO/Al2O3 catalyst is used and the particle size of catalyst is selected such that the pressure drop along the reactor length is negligible and pore diffusion in the catalyst particle is minimum. Pseudo arc-length continuation algorithm is used to solve the model equations and capture the multiplicity features of reactor – heat exchanger configuration in autothermal operation. The results obtained are compared with that of adiabatic and isothermal PFR configurations.

Results and Discussion

Results indicated that, with similar inlet conditions (40 bar and 0.2:1:3 CO:CO2:H2 feed), CO2 conversion achieved in autothermal reactor at the extinction point was fourfold higher than that obtained in PFR (Fig. 1b). It was further observed that, the space-time necessary to attain methanol selectivity greater than 80% is reduced by a factor 10 in the autothermal reactor (Fig. 1c). For optimal autothermal reactor design, the heat transfer area was determined under various operating conditions to achieve maximum methanol selectivity. This is the first report of multiple steady states and feasibility of autothermal operation in CO2 hydrogenation to methanol.

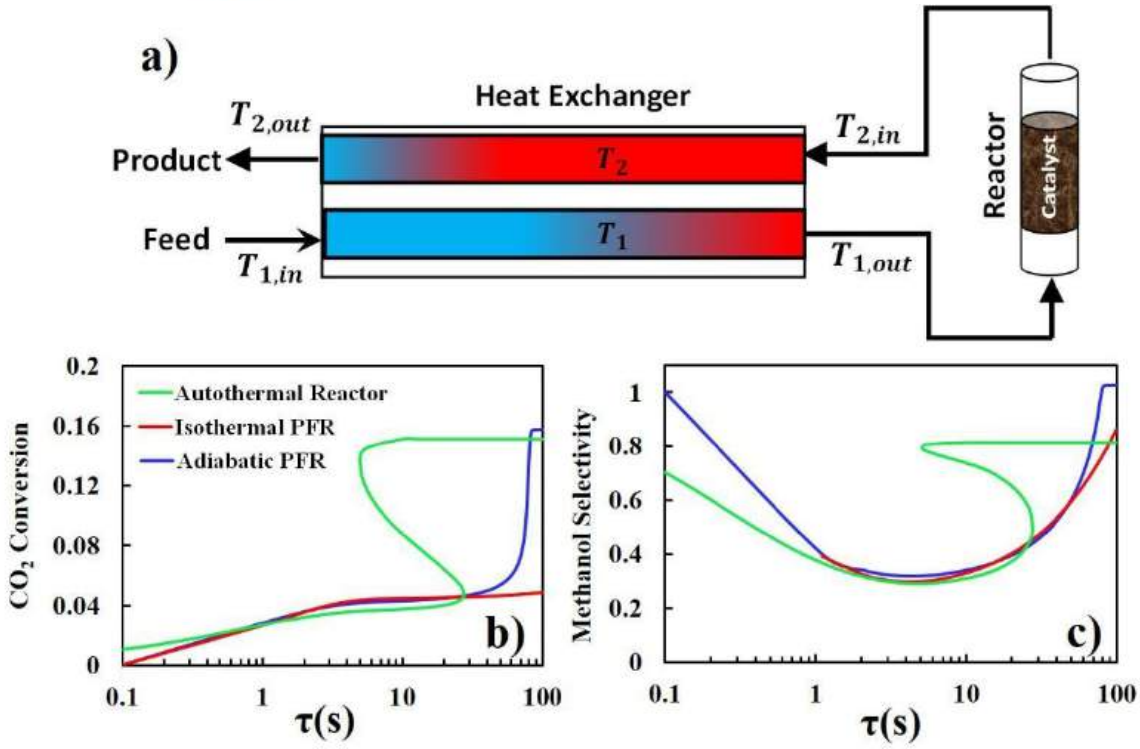

Fig 1. a) Schematic of autothermal reactor (tubular reactor with external heat exchanger) . Comparison of CO_2 conversion (b) and methanol selectivity (c) of three different reactor configurations with space-time (τ).

Acknowledgments

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Legal Disclaimer: The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

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CDU0113

Pilot-Scale Assessment of Fe2O3-MgAl2O4 Extrudates in Chemical Looping Reverse Water-Gas Shift: Performance and Structural Stability

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: CO2 capture and utilization, Iron oxide oxygen carrier, Upscaling.

Abstract Body.
This study investigates the chemical looping reverse water-gas shift (CL-rWGS) process using Fe2O3-MgAl2O4 oxygen carrier extrudates in a pilot-scale packed-bed reactor. The research aims to quantify the effects of operating parameters, including reduction duration, bed dilution, temperature, and flow configuration, on CO2 conversion, CO productivity, oxygen carrier stability, and reactor pressure drop, addressing challenges in upscaling CLrWGS for continuous CO production.

Three oxygen carrier beds were operated in countercurrent under cyclic reduction and oxidation at 923 K and 1073 K, 2.0 bara, active gas concentrations of 84 %, and oxygen carrier loadings between 0.8 and 3.5 kg. Activity testing was performed in both cocurrent and countercurrent, with reduction durations ranging from 5 to 40 min. Temperature-programmed reduction (TPR) and oxidation (TPO) on used samples characterized the chemical changes that occurred. Mechanical stability was assessed through single-pellet crushing, bed compression tests, and X-ray micro-computed tomography (µCT).

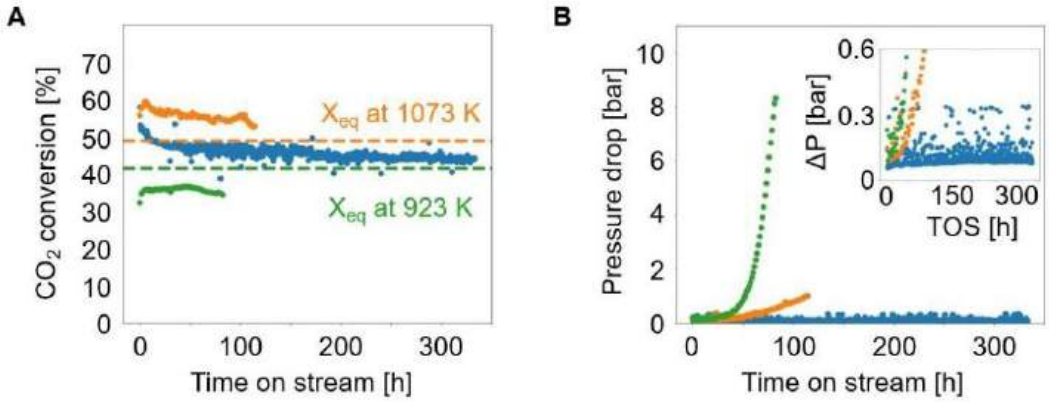

Figure 1. (A) CO_2 conversion [%] as a function of time on stream [h]. (B) Pressure drop [bar] over the reactor as a function of time on stream [h]. Experiment at 923 K (green), 1073 K (orange), and 1073 K with diluted bed (blue). Solid lines in (A): equilibrium conversion at 923 and 1073 K. Inset in (B): zoom in for the region between 0 and 0.6 bar pressure drop.

Countercurrent operation achieved the highest CO2 conversion of 54 % at 1073 K, which exceeds gas-phase equilibrium, while a diluted bed (inert to oxygen carrier ratio of 3:1) stabilized at 44 % conversion over 330 hours of operation (Figure 1A). Space-time yields (STYCO,avg) exceeded 100 kg product/m3/h. In contrast, catalytic rWGS at 923 K yielded only 23 % CO2 conversion and 1 % CH4, highlighting the enhanced performance of CLrWGS. Operation at both 923 and 1073 K showed significant pressure drop rises from 40 h onwards (Figure 1B). Testing the mechanical strength of used extrudates from the first oxygen carrier bed, revealed top-bed weakening due to carbon formation and sintering, with crushing strength dropping from 118 N (fresh) to 27 N (after 370 h). µCT revealed morphological changes in the materials, including the formation of surface cracks and a reduction in internal porosity at the microscale, following extended redox cycling. However, increasing the oxygen carrier calcination temperature to 1173 K and adding bed dilution prevented the pressure drop rise observed in the other experiments (Figure 1B).

Fe2O3-MgAl2O4 oxygen carriers exhibit excellent chemical stability and high CO productivity under cyclic CL-rWGS in a pilot-scale packed bed reactor. Performance is improved through countercurrent operation and optimization of the reduction step duration, while high-temperature calcination and bed dilution help to control pressure drop. The findings provide quantitative guidance for scaling CL-rWGS reactors, demonstrating that carefully considering redox and regeneration conditions enables efficient, long-term CO2 conversion to CO, supporting pilot- and industrial-scale chemical looping CO2 utilization.

ISCRE29 & APCRE11
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CDU0449

Effect of Ni loading method on the deactivation behavior of Ni/Al2O3 catalysts prepared via mechanochemical synthesis for Dry reforming of methane

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: Dry reforming of methane, Deactivation, Mechanochemical synthesis, Nickel on alumina

Abstract Body.

Introduction.

Catalyst deactivation is primarily caused by two mechanisms: sintering of active metal particles and carbon deposition. To mitigate deactivation, strategies such as reducing metal particle size, enhancing metal-support interactions (MSI) to prevent sintering [1], or incorporating promoters to suppress carbon deposition have been widely adopted [2]. Onepot synthesis, where active metal precursors are integrated during the support preparation stage, is frequently employed to strengthen MSI and has been reported to exhibit superior catalytic performance compared to conventional impregnation [3]. However, comparative studies between one-pot synthesized and impregnated catalysts with similar morphologies prepared via the same synthesis route remain limited in the literature. This study aims to elucidate the influence of Ni loading methods on the deactivation of Ni/Al2O3 catalysts with similar support morphology through mechanochemical synthesis. The synthesized catalysts were evaluated via dry reforming of methane (DRM), a harsh reaction operation at high temperature with facile coke formation. Catalyst deactivation behavior and deactivation mechanisms were compared through long-term reaction tests.

Methods.

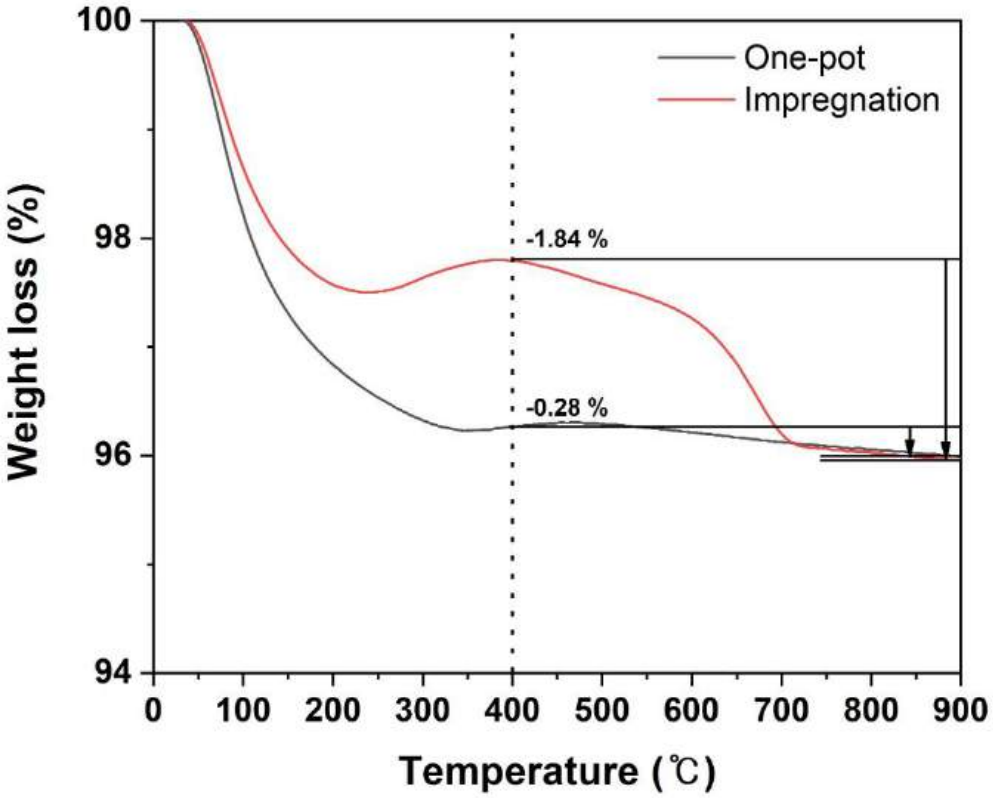
One-pot Ni/Al2O3 was synthesized following the procedure described in previous work [4], with a H2O/AlP molar ratio of 3. Impregnation Ni/Al2O3 was prepared using same procedure as one-pot Ni/Al2O3, except that the Ni precursor was added via incipient wetness impregnation method onto the pre-synthesized pristine Al2O3.

Results and discussion.

To evaluate the deactivation factors, catalysts were subjected to a 100-h reaction test. Postreaction coke deposition on one-pot and impregnation catalysts was quantified via thermogravimetric analysis (TGA), and changes in Ni crystallite size before and after reaction were compared using X-ray diffraction (XRD). TGA analysis revealed a significant difference in weight loss attributed to coke, with the impregnation catalyst producing over 6 times more coke than one-pot catalyst. This suggests that the

impregnation catalyst suffers more severe deactivation from coke formation. XRD analysis further revealed that the onepot catalyst maintained a stable Ni crystalline size of 6.4 nm even

after 100 h of reaction, while the impregnation catalyst experienced notable sintering with crystalline size increasing from 9 nm to 11 nm.



Acknowledgments
This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (Ministry of Science and ICT, MSIT) (RS-2025-00557069)

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CDU0510

Application of model predictive control in a methanol synthesis miniplant under fluctuating conditions

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: CCU; methanol synthesis; fluctuating conditions; model predictive control

Abstract Body.

Capturing and utilizing carbon content from flue gases of the steelmaking industry is an important step to reduce their carbon footprint [1]. Methanol is a promising target product since it has a wide variety of applications and is already among the quantitatively largest chemicals with a worldwide capacity of about 100 Mt [2, 3]. However, fluctuating gas streams, catalyst poisons and a high inert content pose significant challenges [4]. This work presents the application of model predictive control (MPC) to optimize the process under realistic industrial fluctuations in a miniplant setup.

The miniplant with a production capacity of about 0.75 kg d-1 raw methanol was operated with all industrially relevant steps: commercially available Cu/ZnO/Al2O3 catalyst, jacket cooled tube reactor, synthesis gas compressor, product condensation and gas recycle to optimize the overall process yield.

The process control was carried out with a SIMATIC PCS 7 system. The model and design of the controller were derived via experimental data taking real world data from the steelmaking industry into account. Afterwards it was transferred to the PLC. The controller ran autonomously on the PLC, eliminating the need for external computing infrastructure. In total 3 controlled, 3 manipulated and 2 disturbance variables were taken into account. Due to the limited memory available in the PLC the controller was split into two parts: One calculating faster dynamics with a shorter time horizon and one slower controller with a longer horizon.

Running both controllers in parallel resulted in stable behavior under random induced disturbances as well as with step changes of ±10 % which reflect the expected fluctuations from real world data. The maximum hotspot temperature could be kept well within specifications of ±1 K. Furthermore, the amount of hydrogen needed could be minimized automatically without crossing boundary conditions which ensure catalyst lifetime.

The successful application of the MPC in the industrial like synthesis process is a promising step towards dynamically operated CCU plants. It overcomes the limitations of PIDcontrollers in systems with several manipulated and disturbance variables and provides stable operation in the optimum operating range.

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ISCRE29 & APCRE11
2026 / SEOUL, KOREA

CDU0614

Spillover effects between Ru and CO2 sorbent for integrated CO2 capture and methanation

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: Reactive Carbon Capture; CO2 capture and methanation; DFM;

Abstract Body.

Introduction. Dual Function Materials (DFMs) have been proposed for the integration of CO2 capture and subsequent conversion when exposed to green H2. DFMs typically combine a CO2 storage metal (e.g., Na, K, Ca, Ba) with a catalyst metal (e.g., Ru and Ni for methanation) dispersed over the same support. Interactions between the active phases are the determining factors for parameters such as CH4 yield and formation rate and CO2 conversion. Although the intimacy between Ru and sorbent is generally beneficial towards CH4 yield and CO2 conversion [1], CH4 formation rate suffers from that intimacy due to hydrogenation inhibition effects, typically observed for alkali metals [2].
Methods. Catalysts have been prepared by dry impregnation of γ-Al2O3 (Sasol) or TiO2 (Norpro) followed by calcination at 500 °C for 5h to obtain CO2 sorbents (4.6 wt.% Na/Al2O3 and 7.6% K/Al2O3) or CO2 methanation catalysts (1 wt.% Ru/Al2O3 and 1 wt.% Ru/TiO2). Traditional DFMs were obtained through sequential impregnations of Ru and Na or K on alumina (Ru/Na/Al2O3 and Ru/K/Al2O3). All samples have been characterized and then tested (microreactors and spatially-resolved operando FT-IR) in isothermal cyclic conditions (CO2 capture, purge, and reduction phases) in the 250-350 °C temperature range. Results and discussion. Under isothermal and cyclic conditions Ru+K physical mixtures outperform the DFM in terms of both CH4 formation rate and CH4 yields. The superior performance of the physical mixture is attributed to the efficient H2 activation on Ru and inter-particle spillover to the stored CO2 to trigger its hydrogenation to CH4. On contrary, in DFMs the similar intra-particle pathway is slower due to the K inhibition on Ru hydrogen activation, reducing CH4 formation rate and selectivity. Indeed, when alumina is replaced with a support granting a higher H spillover (i.e., Ru/TiO2 + K/Al2O3), methane yield and formation rate increases. This was further confirmed by a systematic study on different metals, supports and storage elements

Oral Presentation

Environmentally-friendly and sustainable Chemicals

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

SCB0030

Tuning the acid-base properties of lignin-derived carbon modulated ZnZr/SiO2 catalysts for selective and efficient production of butadiene from ethanol

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Abstract Category: *Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Biomass*

Keywords: Ethanol, Butadiene, Lignin

Abstract Body.

The direct selective conversion of ethanol to butadiene (ETB) is a competitive and environment-friendly process compared to the traditional crude cracking route. The acidbase properties of catalysts are crucial for the direct ETB process. Herein, we report a rationally designed multifunctional lignin-derived carbon modulated ZnZr/SiO2 (L-ZnZr/SiO2) catalyst with suitable acid-base properties for the direct ETB reaction. A variety of characterization techniques are employed to investigate the relationship between the acidbase properties and catalytic performance of the multifunctional lignin-modulated ZnZr/SiO2 catalysts. The results revealed that the rationally additional lignin-modulated carbon enhances both acidic and basic of the ZnZr/SiO2 catalysts and provides a suitable acid-base ratio that boost the direct ETB reactivity. Meanwhile, the 1%L-ZnZr/SiO2 possessed ethanol conversion and butadiene selectivity as high as 98.4 % and 55.5 % respectively and exhibited excellent catalytic stability.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

SCM0153

Synthesis of Beta-Type Titanoaluminosilicates via an Interzeolite Transformation and Their Catalytic Activity in Glucose Conversion

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Materials (Zeolite, MOF etc)

Keywords: Bi-functional catalyst, glucose conversion, interzeolite transformation, titanoaluminosilicate

Abstract Body.

Purpose

Bottom-up control of active site composition in bifunctional zeolites is essential for optimizing cascade reactions but remains challenging. Conventional top-down approaches, such as impregnating Lewis acid metal species into H-form zeolites, often suffer from poor metal dispersion and limited control over active site distribution. Interzeolite transformation enables incorporation of active phases from a parent zeolite into a daughter zeolite phase, allowing the synthesis of bifunctional zeolite catalysts with high dispersion and tunable loadings. This study aims to derive optimal acidic properties for the glucose conversion reaction by tuning the Ti and Al compositions of Beta-type titanoaluminosilicates through interzeolite transformation.

Method

The precursor Ti- and Al-MWW materials were synthesized via traditional hydrothermal synthesis. Titanoaluminosilicates with Beta structure (TixAl1-x-BEA) were synthesized by interzeolite transformation of the calcined Ti- and Al-MWWs, which were mixed in various molar ratio, Ti : Al = x : (1-x), x = 0.0, 0.2, 0.4, 0.6, 0.8, and 1.0. Structural characterization was performed using PXRD analysis. The compositions of the synthesized materials were investigated by ICP-OES analysis. The acidic properties of samples were investigated by using py-IR. The glucose conversion reaction was carried out at 160 °C for 1–24 h.

Results

PXRD patterns confirmed that the synthesized TixAl1-x-BEAs exhibit only diffraction patterns of the Beta structure, without any residual peaks attributable to the MWW. ICP analysis was performed to verify the distinct Ti and Al contents in TixAl1-x-BEAs. when the Ti/Al molar ratios of parent mixtures were plotted against those of TixAl1-x-BEAs, a linear relationship was observed with an R2 value of 0.9998 and a slope of 0.82 (Fig. 1). Py-IR was performed to characterize the acidic properties of TixAl1-x-BEAs. It is clearly observed that both the Brønsted acid concentration and the B/L ratio increased as the Al content increased. The

glucose conversion to 5-HMF (5-hydroxymethylfurfural) reaction was performed. As the reaction proceeded, distinct glucose conversion and 5-HMF yield behaviors emerged, with higher Al contents leading to enhanced the catalytic performance.

Conclusions

TixAl1-x-BEAs were synthesized via interzeolite transformation of Ti- and Al-MWW precursors. By controlling the mixture ratios of the two parent precursors, the compositions of the daughter phase could be finely tuned. The controlled framework composition significantly influenced the acidic properties. As the Al content increased, both the concentration of Brønsted acid sites and the B/L ratio increased. These results demonstrate that interzeolite transformation is a promising strategy for optimizing acid properties tailored to reactions through compositional tuning of bifunctional zeolites.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

KN0117

Synthetic methods to position acid sites in zeolites for selective arene methylation catalysis

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Abstract Category: Invited Lecture - Keynote Lecture

Keywords: Zeolite, active site, catalysis

Abstract Body.
Arene methylation occurs via complex reaction networks on Brønsted acid zeolites, wherein the confinement of transition states strongly influences rate constants, selectivities of forming similarly-sized regioisomers, and deactivation kinetics. As a result, marked differences in catalytic behavior are observed among zeolites of different topology, and even for a given zeolite framework at acid sites located within distinct void environments. Here, we investigate arene methylation reactions across substrates of varying size (benzene, toluene, xylene), microporous and mesoporous aluminosilicates of varying pore size and topology (TON, MFI, BEA, FAU, MCM-41), and MFI zeolites that differ both in framework heteratom identity (Al3+, Ga3+, Fe3+, B3+) and in acid site distribution between smaller channel and larger intersection voids. We present evidence that MFI samples can be synthesized with fixed framework heteroatom content, but varied distributions of acid sites between channel and intersection voids, using different organic and inorganic structure-directing agents (SDAs). We show that kinetically-controlled arene methylation rates and product selectivity vary markedly at acid sites confined in channels or intersections, irrespective of framework heteroatom identity. These conclusions are supported by density functional theory (DFT) calculations that assess how different SDAs influence trivalent heteroatom siting in MFI frameworks and how arene methylation transition state free energies depend on acid site location in MFI and other zeolite frameworks. Overall, these findings highlight the importance of combining experimental and theoretical approaches to elucidate how active site distributions influence reaction rates, product selectivity, and deactivation in complex reaction networks in microporous zeolite catalysts.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

SCM0225

Replacing HCl with Hierarchical Zeolite Catalysts in the Production of Polyurethane Intermediates

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Materials (Zeolite, MOF etc)

Keywords: polyurethane, methylenedianiline, LTL zeolite, 3-stage reaction

Abstract Body.

The production of methylenedianiline (MDA) and oligomeric MDAs, key intermediates for polyurethane synthesis, has traditionally relied on homogeneous HCl catalysis, which suffers from severe drawbacks including corrosion, large salt waste generation, and limited process sustainability. Although numerous solid acid catalysts have been investigated as environmentally benign alternatives, their industrial implementation has been hindered by insufficient selectivity toward the desired 4,4′-MDA isomer, poor controllability over oligomer formation, and rapid catalyst deactivation caused by pore fouling. Herein, we present a comprehensive catalytic and process-level strategy that enables the selective, stable, and tunable production of polyurethane precursors using solid acid catalysts. Through detailed kinetic, mechanistic, and structural analyses, we identify hierarchical LTL zeolite as an exceptionally effective catalyst for the conversion of aminobenzylaniline intermediates into 4,4′-MDA. The unique one-dimensional, cage-like micropores of LTL selectively stabilize bimolecular assemblies of para-aminobenzylaniline, thereby promoting the formation of 4,4′-MDA while suppressing undesired isomers and bulky oligomeric byproducts. The introduction of intracrystalline mesoporosity alleviates mass-transfer limitations, resulting in high catalytic activity and unprecedented resistance to deactivation under continuous-flow conditions. Building on this mechanistic understanding, we further develop a versatile three-stage fixed-bed reactor system employing distinct solid acids optimized for each reaction step. In the first stage, aminal is selectively converted to para-aminobenzylaniline over amorphous silica–alumina (ASA) at low temperature under thermodynamic control, maximizing the precursor selectivity for downstream reactions. In the second stage, hierarchical LTL zeolite enables highly selective transformation of aminobenzylanilines into 4,4′-MDA with minimal oligomer formation and excellent long-term stability. In the final stage, controlled oligomerization is achieved over purely mesoporous ASA at elevated temperatures, allowing the coproduction of monomeric and oligomeric MDAs in tunable ratios without catalyst fouling. This staged catalytic approach synergistically combines shape selectivity, mass-transfer enhancement, and fouling resistance, delivering 4,4′-MDA/(2,4′-MDA + 2,2′-MDA) isomer ratios far exceeding those of conventional HCl-based processes while maintaining stable operation over extended time-on-stream. Overall, this work establishes a scalable and eco-friendly solid acid–based platform for polyurethane precursor production, bridging fundamental catalyst design with industrially viable continuous processes.

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2026 / SEOUL, KOREA

SCM0542

Encapsulation of Metal Nanoparticles in Zeolites Enabled by Organic Molecules

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Materials (Zeolite, MOF etc)

Keywords: Zeolite, Metal nanoparticles, Encapsulation

Abstract Body.
Encapsulating metal nanoparticles (NPs) within microporous zeolites provides a robust route to sintering-resistant catalysts, as long as metal precursors can be stabilized within the zeolite micropore network. Here we present an organic-molecule-assisted approach to encapsulate metal NPs inside zeolite crystals via both post-synthetic and in-situ routes. In this approach, organic molecules serve as practical tools to keep metal precursors inside zeolite crystals and suppress deposition on external surfaces. Simple functional groups (e.g., -SH and -NH2) anchor metal precursors in the micropores and promote intracrystalline nucleation, either after zeolite synthesis or during zeolite crystallization. Overall, organic molecules are not the final active component, but a practical handle to guide metal precursors into zeolite micropores and induce intracrystalline nucleation, providing a general pathway toward stable, high-loading zeolite-encapsulated metal nanocatalysts.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

SCM0623

Ti-MWW Zeolite for Sustainable Lactide Production from Methyl Lactate: Origin of Its Catalytic Superiority

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Keywords: Ethyl lactate dehydration; Ethyl acrylate; ZSM-5; Zeolite-catalysed mechanism

Introduction. The growing reliance on fossil resources and environmental concerns associated with petrochemical plastics have intensified the need for sustainable alternatives. Polylactic acid (PLA), a biodegradable polymer derived from renewable resources, is regarded as a promising substitute because of its favorable properties and closed-carbonloop potential. However, its commercialization is limited by the high cost of conventional lactide (LD) production, which requires energy-intensive lactic acid polycondensation and high-temperature transesterification, often leading to racemization and byproduct formation. One-step gas-phase transesterification of methyl lactate has emerged as a more efficient alternative because it lowers energy demand and suppresses side reactions. Here, titaniumcontaining MWW-type zeolites and their delaminated form were investigated to clarify their structure-activity relationship in LD production.

Methods. TiO_2-supported MCM-22 and ITQ-2 were prepared by incipient wetness impregnation, while Ti-MWW and delaminated Ti-MWW were obtained by framework Ti insertion after acid treatment [2]. Methyl lactate transesterification was conducted in a continuous-flow fixed-bed reactor, and products were analyzed by online GC-FID.

Results and discussion. Consistent with previous reports, LD production over TiO_2supported silicates was governed primarily by Ti-O-Si bond formation rather than structural sensitivity. In contrast, Figure 1 indicates that structural sensitivity is significant in Tiincorporated zeolites. Although Ti-MWW and Ti-MWW-del share two-dimensional sinusoidal channels and half 12-membered-ring MWW cages, Ti-MWW-del contains more externally exposed pockets. This structural difference likely modifies the distribution and electronic environment of Ti active sites, leading to measurable changes in LD production performance.

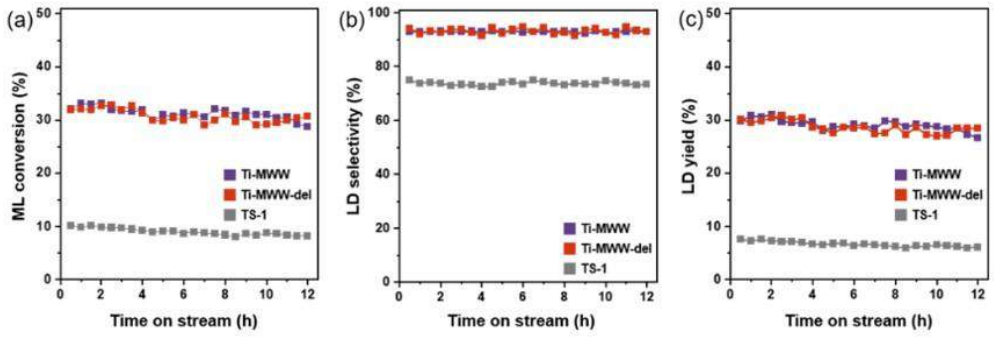

Figure 1. Methyl lactate oligomerization performance over Ti-incorporated catalysts.

Acknowledgments

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ISCRE29 & APCRE11
2026 / SEOUL, KOREA

SCB0149

Thermodynamic Prediction of Advanced Distillation Curves for Bio-Oil and Complex Sustainable Fuel Mixtures

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Biomass

Keywords: Advanced distillation curve, Bio-oil, Thermodynamic modeling, UNIFAC-DMD, Sustainable fuels

Abstract Body.
Bio-oil produced from biomass and waste pyrolysis represents a promising renewable feedstock for sustainable fuels and chemicals; however, its complex composition, wide boiling-point distribution, and thermal sensitivity pose significant challenges for separation and process design. Vacuum distillation is commonly applied to mitigate thermal degradation, yet experimental determination of distillation curves remains expensive, time-consuming, and subject to uncertainty. In this work, a computational framework is developed to predict vacuum batch distillation curves using thermodynamic modeling. An algorithm integrated with the UNIFAC-DMD activity coefficient model is proposed to generate distillation curves based on bubble-point, dew-point, and flash calculations. A Flash Pθ formulation is employed to simultaneously solve the $2C+1$ equations required to determine the still-pot temperature, liquid-phase composition, and vapor-phase composition under reduced pressures.
The proposed methodology is validated against experimental data for a broad range of systems, including binary mixtures (n-decane + n-tetradecane, benzene + ethanol, benzene + isopropanol, acetone + chloroform), a ternary system through residue curve map analysis (2-ethoxyethanol + ethylbenzene + DMSO), surrogate mixtures for Jet-A/JP-8 fuels, fatty acid–levulinate biodiesel blends, fast pyrolysis bio-oil, and tail-gas reactive pyrolysis mixtures. The predicted distillation curves show good agreement with experimental results across different pressure levels, demonstrating the robustness and accuracy of the approach. Finally, the distillation behavior of fast pyrolysis bio-oil and plastic waste pyrolysis oil is analyzed, and the separation characteristics of their constituent components are discussed. This computational methodology provides a cost-effective and reliable tool for vacuum distillation analysis, supporting process design and optimization for complex and sustainable chemical systems.

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SCB0257

High-rate biohydrogen production and granule formation in an upflow bioreactor packed with ceramic hollow balls and granular activated carbon

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Biomass

Keywords: High-rate biohydrogen production, Biocarrier, Upflow velocity, Granular biomass

Abstract Body.
Dark fermentative hydrogen production was investigated in a packed-bed bioreactor using glucose (20 g/L) as substrate and sludge (3 g/L) as inoculum at an upflow velocity of 0.5 m/h under various hydraulic retention times (HRTs) of 4, 2, and 1 h. The ceramic hollow balls (CHB) and granular activated carbon (GAC) were employed as biocarriers in a 50:1 weight ratio, with CHB serving as the primary structural biocarrier and GAC as the auxiliary functional biocarrier. The performance of the bioreactor with and without GAC was evaluated in terms of hydrogen production rate (HPR), hydrogen yield (HY), volatile fatty acids production, total solids, volatile solids, substrate degradation efficiency, granule particle size distribution, granule porosity, sludge volume index, extracellular polymeric substance, microbial population, and morphology of granules and biocarriers. Compared with the system without GAC, the presence of GAC increased HY and HPR, and promoted granulation at shorter HRT, resulting in more stable hydrogen production without washout, and improved bioreactor performance. The highest HY was achieved at HRT of 2 h, reaching 1.97 mol H2/mol glucose, followed by an HRT of 1 h with 1.85 mol H2/mol glucose. In contrast, the highest HPR was obtained at HRT of 1 h (48.3 L H2/L/d), followed by 2 h (39.54 L H2/L/d glucose).

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SCB0470

Efficient production of xylitol via xylose hydrogenation under relatively low hydrogen pressure

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Biomass

Keywords: catalytic hydrogenation, carbon-supported copper catalysts, xylitol, alcohol solvents

Abstract Body.
Catalytic hydrogenation process is one of the key reaction processes for chemical use of biomass. This process generally consists of a solid metal catalyst, a liquid reaction solution, and high-pressure gaseous hydrogen. But high-pressure hydrogen raises the equipment costs of the processes and heightens the risks associated with its handling. Therefore, we have investigated the development of the efficient catalytic hydrogenation process at relatively low hydrogen pressure. We selected the hydrogenation of xylose into xylitol as the model reaction. In previous work, we revealed that the carbon supported copper catalysts (Cu@C) prepared from a weakly-acidic cation exchange resin selectively produced xylitol via hydrogenation of xylose under the hydrogen pressure below 1.1 MPa. However, the xylitol production rate was small because the low hydrogen pressure decreased the concentration of hydrogen on the catalyst surface. Thus, in this study, we examined the enhancement of the xylitol production rate at low hydrogen pressure by varying the reactant solvent; namely water, ethanol, 2-propanol, and 2-butanol. The Cu@C catalysts were synthesized by loading copper ions onto weakly acidic cation-exchange resin via ion-exchange at room temperature, followed by carbonizing the copper ion-loaded resin at 500 °C in an inert atmosphere. The xylose hydrogenation was performed at 130 °C for 3 h using a 97 cm3 of Teflon-lined autoclave. The 0.26 g of Cu@C catalyst pretreated at 350 °C for 1 h in 50 % H2/N2 stream and 30 g of xylose solution at the concentration ranged from 10 to 480 mol/dm3 were put into the reactor. Subsequently, the atmosphere in the reactor was replaced with hydrogen gas at 0.15 to 1.1 MPa. The xylitol yield was 79 and 65 % for ethanol and 2-propanol solvents at initial xylose concentration of approximately 160 mol/dm3 and hydrogen pressure of 0.6 MPa; meanwhile, it was 14 and 10 % for water and 2-butanol solvents. The reaction rate of the xylose hydrogenation in each solvent was explained by the Langmuir-Hinshelwood mechanism. The differences in the reaction rates were reflected in the adsorption-desorption equilibrium constant of reactants. Therefore, high xylitol production rates obtained in ethanol and 2-propanol are attributed to relatively high solubility of both hydrogen and xylose. This finding indicates that the selection of solvents with high solubility of reactants are important keys to enhance the hydrogenation reaction rate without increasing hydrogen pressure.

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SCB0490

Role of inorganics during the hydrothermal liquefaction of OFMSW

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Biomass

Keywords: Hydrothermal liquefaction, inorganics, biocrude, waste valorization, PCA, biofuel

Abstract Body.
Introduction. Hydrothermal liquefaction (HTL) is gaining increasing interest for the energy valorization of the organic fraction of municipal solid waste (OFMSW). HTL performance depends strongly on biochemical composition, with biocrude yields typically following: lipids > proteins > carbohydrates. However, the role of inorganics in HTL remains poorly understood. This study examines their effects by adding selected inorganics to a fixed biochemical mixture (63% cellulose, 19% albumin, and 18% sunflower oil), representative of average OFMSW.
Methods. Experiments were conducted in 20 mL batch reactors submerged in a preheated sand bath under constant conditions: 350 °C, 30 minutes, 1.78 g daf biomass, 1.8 mmol inorganic cations, and 9.0 g total slurry. The selected inorganics (Figure 1), chosen for their prevalence in biomass, were tested individually while maintaining a fixed molar cation content representative of typical biomass (20-40 g cation/kg dry feedstock).
Results and discussion. Even at low levels, the tested inorganics significantly influenced HTL performance, from both quantitative and qualitative perspective. Figure 1 shows the results of the principal component analysis (PCA) of the complete dataset. Figure 1A reports the distribution in the PC1-PC2 space, distinguishing between quantitative (blue) and properties-related data (red). The quantitative variables were explained mainly by PC1, whereas the properties-related variables loaded primarily on PC2. It can be observed that higher inorganic basicity favored carbon distribution toward biocrude at the expense of the solid fraction. Focusing on the distribution of the performed tests (Figure 1B), a consistent pattern emerged within each anion group. Specifically, the four metal cations were arranged in a rectangular configuration: Na and K exhibited higher PC1 values (with Ca and Mg at lower PC1 values), while Na and Mg showed higher PC2 values (with K and Ca at lower PC2 values). This recurring trend suggests that the metal cations exerted a coherent and direct effect on HTL performance. Na and K promoted biocrude production and solid conversion more effectively than Mg and Ca, whereas K and Ca generally yielded biocrudes with lower oxygen content and higher energy density.

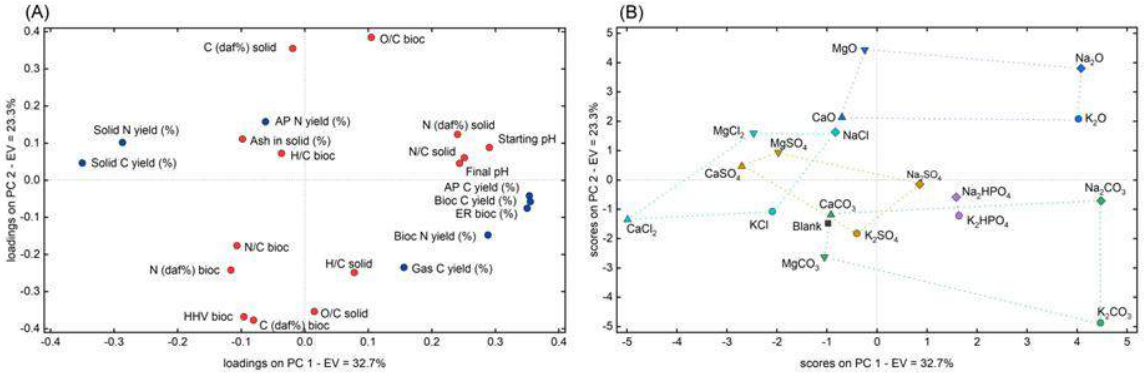

Figure 1: Loadings (A) and scores (B) obtained from the principal component analysis (PCA) of the complete experimental dataset.

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SCB0526

CATALYTIC HYDROLYSIS OF HEMICELLULOSE TO SUGAR MONOMERS

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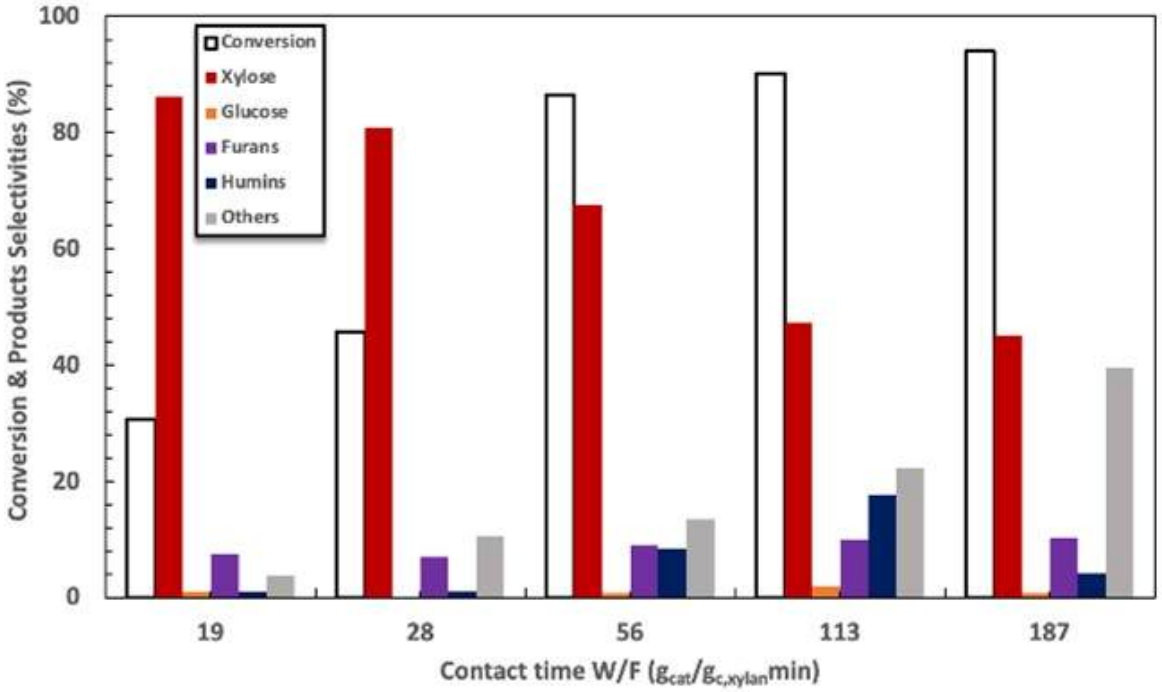
Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Biomass

Keywords: Hemicellulose, biomass waste, tungsten catalyst, sugars

Abstract Body.

Keywords: Hemicellulose; biomass waste; tungsten catalyst; sugars
Introduction.
Hemicellulose, a major component of lignocellulosic biomass, is an abundant carbon resource, consisting of C5 (xylose) and C6 (glucose) sugars linked together with glycosidic bonds1. Its catalytic depolymerization to sugar monomer(s), which can be further valorized to chemicals and fossils, via hydrolysis is a new unexplored topic in the open literature2,3. This work studies the continuous flow hydrolysis of hemicellulose over a homemade WOx/TiO2 catalyst.
Methods.
The WOx/TiO2 catalyst was prepared as previously described2. Hydrolysis experiments were performed in a fixed bed reactor using aqueous commercially available xylan hemicellulose from corncob, whereas catalyst performance was evaluated over a wide range of conditions (T:100-200 oC, C:10-50 g/L, W/F:15-915 gcat/gc,feedmin). The unreacted xylan was determined by post-hydrolysis2, while the hydrolysates were analyzed by HPLC (RID and PDA).
Results and discussion.
Non-catalytic hydrolysis was initially explored to evaluate homogeneous feed conversion, indicating only partial depolymerization at high temperatures (180 oC) and low conversion levels (below 20%) across all operating conditions studied. In contrast, the WOx/TiO2 catalyst remarkably enhanced both catalytic activity and sugars selectivity. Increasing temperature from 100 to 200 oC significantly boosted conversion, which remained low until 130 oC and reached nearly 100% at 180 oC. whereas sugars formation was greatly promoted. Higher temperatures enhanced the formation of secondary degradation reactions leading to furans and humin, thus restricting sugars formation. Additionally, feed concentration was also found to play a key role affecting both catalytic activity and sugars selectivity, with higher concentrations promoting sugars production at lower W/F values, hence improving reaction efficiency and minimizing energy consumption. According to figure 1, maximum sugars selectivity of 86% (mostly xylose) was achieved at 180 oC, 50 g/L feed concentration and 19 gcat/gc,feedmin W/F for 31% conversion, whereas further increase in W/F enhanced degradation reactions. The reaction pathway was further explored by using both sugars and furans as reactants at the same conditions providing insights into reaction kinetics.



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SCB0649

Effect of Different Environmental Gases on the Catalytic Pyrolysis of Organic Waste

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Biomass

Keywords: Pyrolysis, organic waste, Methane, Biogas

Abstract Body.
Introduction. The growing volume of organic waste has created an urgent need for efficient thermochemical valorization strategies. Catalytic pyrolysis has emerged as a promising route for converting such waste into valuable fuels and chemicals, with the aid of tailored catalysts and optimized reaction environments. While many studies have focused on catalyst design and pyrolysis temperature, the composition of the reaction atmosphere, or environmental gas, is also known to play a crucial role in determining product distribution, coke formation, and reaction efficiency. Methane (CH44), a representative C1 gas, can act as a co-reactant that enhances aromatization through hydrogen transfer and methylation reactions, potentially improving the yield of valuable hydrocarbons. Carbon dioxide (CO22), although chemically inert under standard conditions, may suppress coke formation via mild oxidation and promote gas-phase reforming. Biogas, typically a mixture of CH4 and CO22, offers a synergistic environment that can balance these effects, providing both reactivity and coke control. In this study, we investigated the effect of different environmental gases, specifically N22, CH4, CO22, and biogas, on the product distribution during the catalytic pyrolysis of organic waste using zeolite-based catalysts.
Methods. Catalytic pyrolysis of organic waste was performed using zeolite-based catalysts under different gas atmospheres (N22, CH44, CO22, and biogas). Reactions were conducted in a fixed-bed reactor at desired temperatures. Liquid products were analyzed by GC-MS and GC-FID, and gas products by GC-TCD and GC-FID.
Results and discussion. The product distribution from catalytic pyrolysis of organic waste was significantly influenced by the pyrolysis atmosphere gas. Compared to the inert N2 atmosphereatmosphere, CH4 notably enhanced the formation of aromatic hydrocarbons, especially BTEX (benzene, toluene, ethylbenzene, xylene), likely due to enhanced hydrogen transfer and methylation reactions with reactive intermediates. However, coke formation also increased under CH44, indicating accelerated secondary reactions. In contrast, CO2 suppressed coke deposition and facilitated mild reforming reactions, which helped reduce the accumulation of heavy residues. Although the aromatic yield under CO2 was lower than in CH44, it contributed to greater catalyst stability. The biogas atmosphere exhibited a synergistic effect, enhancing aromatic hydrocarbon formation while limiting coke generation. The results

highlight the crucial role of pyrolysis atmosphere in optimizing both yield and stability in catalytic pyrolysis systems.

Acknowledgments
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SCB0653

Hydrogen production from waste cigarette filters via steam gasification over waste-derived Ni/MFe_2O_4 spinel catalysts synthesized from acid mine sludge effluent

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Biomass

Keywords: Steam gasification, Acid mine sludge, Spinel catalysts, Cigarette Butts

Abstract Body.

Introduction. The increased smoking of cigarettes worldwide has resulted in the generation of trillion cigarette butts (CBs) [1], with limited biodegradability, acting as long-term environmental contaminants [2]. CBs contains a complex mixture of hazardous compounds, including nicotine, heavy metals, polycyclic aromatic hydrocarbons [3], posing serious risks to ecosystems and public health. In this context, valorization of CBs into hydrogen-rich synthesis gas through catalytic steam gasification using Nickel-supported spinel ferrite catalysts (Ni/MFe2O4) can be proposed as a promising technology. Spinel ferrites with the general formula MFe_2O_4 are attractive catalyst supports due to their high thermal stability, redox flexibility, and strong metal–support interactions, which enhance resistance to sintering under harsh gasification condition. However, the costly precursors for the synthesize of MFe2O4 has limited its widespread application. In this study, Ni/MFe2O4 (M=Mg, Mn, Zn, and Co) catalysts in which the iron was extracted from hazardous acid mine sludge, has been synthesized for the first time and used during the catalytic steam gasification of CBs, providing both environmental and economic benefits.

Material and Methods

Iron was extracted by pre-leaching acid mine sludge with dilute HCl to remove soluble metal oxides as chlorides, followed by filtration and drying. Stoichiometric amounts of metal precursors were added to synthesize MFe2O4, with polyethylene glycol used as a porosity agent, followed by drying at 110 °C and calcined at 800 °C for 4 h. Subsequently, a known amount of nickel was loaded onto the support, followed by drying at 110 °C and calcination at 550 °C. The resulting powder was reduced under a constant flow of N2 and H2 at 600 °C for 3 h and labeled as the Ni/MFe2O4 catalyst.

Results and discussion.

The catalytic performance of Ni/MFe2O4 was assessed through the catalytic steam gasification of CBs in a dual-zone reactor at 800 °C. The Ni/MnFe2O4 catalyst outperformed all others, exhibiting the highest H_2 selectivity (53.0 vol%). This superior performance is likely because of highly dispersed Ni nanoparticles, and high reducibility which provides abundant accessible Ni^0 sites, as confirmed by H2-TPR analysis. Nickel, as the active phase, promotes tar cracking, C–C and C–H bond cleavage, steam reforming, and water–gas shift reactions, thereby enhancing hydrogen production. Overall, this work demonstrates a novel circular approach that couples CB steam gasification with the utilization of acid mine sludge effluent

for catalyst synthesis, offering a sustainable solution for hazardous waste management and renewable hydrogen production.

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SCB0272

Electronic-structure control of source-dependent hydrogen utilization in selective C–O bond cleavage in furfural conversion

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Keywords: electronic-structure effect; hydrogen utilization; C-O bond cleavage; furfural hydrogenation, 1,5-pentanediol

Selective conversion of furfural (FFA) to 1,5-pentanediol (1,5-PDO) requires precise control over hydrogen activation [1], and charge redistribution in the catalyst surface [2]. Here, we demonstrate that modified electronic structures of Co-Zr mixed oxides regulate hydrogen partitioning and reaction selectivity in the on FFA to 1,5-PDO productions.

Two distinct methods were used to modify the surface electronically of Co-Zr mixed oxide: the first approach is a chemical reduction method with 1 M $NaBH_4$, named the catalyst as $Co_{2.5}Zr_1$-CR, and the second approach with *in-situ* reduction process named $Co_{2.5}Zr_1$-IR. By systematic comparison of *in-situ* reduced and chemically reduced Co–Zr mixed oxides, we show that as $Co_{2.5}Zr_1$-CR achieves a markedly higher 1,5-pentanediol yield (70.5%) than its named $Co_{2.5}Zr_1$-IR catalyst (55.4%).

Based on spectroscopy analysis, ZrO_x nanoclusters act as interfacial electron reservoirs that capable of stabilizing Co^{2+} centers rich in unpaired electrons within O_v-Co_3O_4, which generating electronically asymmetric and spin-polarized catalytic environments capable of heterolytic hydrogen activation and C−O cleavage of furan ring. Isotope labelling and kinetic isotope effect uncover unique hydrogen chemical potential on the catalyst surface, where ethanol-derived hydrogen preferentially participates in the rate-determining C2−O bond cleavage, while H_2-derived hydride do selective hydrogenation of FFA carbon backbone. Density functional theory calculations further confirm that C2−O bond scission is the ratelimiting step and show that rich O_v-Co_3O_4 in the Co-Zr mixed oxide system lowers the activation barrier by inducing charge depletion at the reaction carbon and charge accumulation in the furan ring. These findings signify that electronic asymmetry, spin polarization (unpaired electron of Co^{2+} in Co_3O_4), and hydrogen partitioning are the key descriptors for selective biomass-derived FFA hydrogenation and C−O bond activation in mixed oxide catalysts.

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SCW0157

Catalytic upgrading of waste tire pyrolysis vapors in a circulating fluidized bed reactor

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Waste Valorization

Keywords: Tires, recycling, catalytic pyrolysis, aromatics, circulating fluidized bed

Abstract Body.
Purpose: Global tire sales are projected to reach 1.5 billion units annually by 2030, with 1.2 billion units annually entering the end-of-life tire (ELT) pool. Current ELT recycling routes are not circular, while limited recycled product demand means that ELTs present a largely untapped resource for energy and materials recovery. Previously, we reported the production of highly aromatic oils from the ex situ catalytic pyrolysis of waste tires in batch fixed bed and continuous bench-scale fluidized bed systems (Ind. Eng. Chem. Res. 2025, 64, 19342). Follow up work in a pilot continuous system with a fixed catalytic bed produced consistent results, but catalyst coking was a limiting factor. Here, we report the ex situ catalytic pyrolysis of ELTs in a pilot continuous system with a circulating fluidized bed (CFB).

Methods: ELTs were pyrolyzed in a continuous fluidized bed reactor at 500 °C in contact with an inert heat carrier. The vapors were transferred to a CFB reactor for upgrading with ecat FCC (USY) or steamed ZSM-5 catalysts at 500-600 °C. Catalyst circulation between a regeneration and a reaction vessel ensured the continuous supply of coke-free catalyst for the reaction. Reference tests were conducted with the CFB offline. The pyrolysis oils were analyzed to determine composition and aromatics content.

Results: Non-catalytic pyrolysis of the ELT feedstock yielded ~50 wt% oil. Catalytic upgrading of the pyrolysis vapors in the CFB resulted in a drastic oil yield decrease to 32-38 wt% in favor of gas products. However, of the C/H ratio of the oil product increased, indicating increased aromaticity. Increasing catalyst circulation and/or temperature further increased the C/H ratio with limited impact on oil yield. The increased aromaticity was confirmed quantitatively by HPLC, which revealed up to 82 wt% aromatics content.
Simulated distillation analysis indicated that the ELT pyrolysis vapors were composed of ~25 wt% heavy compounds, which were catalytically cracked in the CFB towards gasoline- and diesel-range compounds.

Conclusions: Ex situ catalytic pyrolysis of ELTs in a pilot CFB unit yielded oil with significantly increased aromaticity compared to non-catalytic pyrolysis. On the downside, a reduction of

the oil yield from 50 wt% to 32-38 wt% was observed. Temperature and vapor residence time optimizations in the pyrolysis and catalytic upgrading reactors are crucial to minimize secondary thermal cracking reactions and obtain aromatic oil yields at the level reported previously from smaller scale systems.

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SCW0159

Solvent-free hydrogenolysis of waste PET to p-xylene over a PtSn bimetallic catalyst

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Waste Valorization

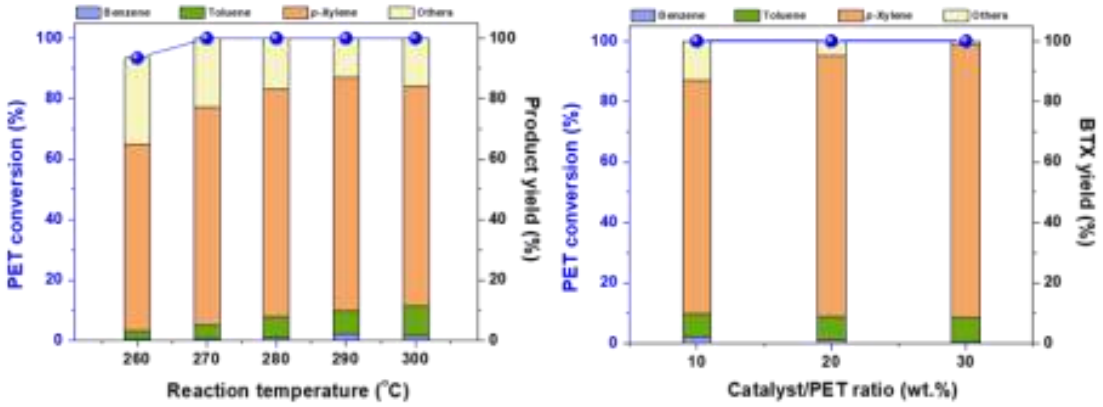
Keywords: PET, Hydrogenolysis, p-Xylene, Solvent-free, Bimetallic catalyst

Abstract Body.
Introduction. The accumulation of waste PET has increased interest in chemical recycling routes that convert PET into value added chemicals. Hydrogenolysis is an attractive approach because it enables selective cleavage of carbon-oxygen and carbon-carbon bonds, allowing direct conversion of PET into aromatic hydrocarbons such as benzene, toluene, and xylene (BTX). Of particular interest is the selective formation of p-xylene, a key precursor for purified terephthalic acid, which avoids energy intensive separation from mixed xylene streams. Achieving high BTX yield and p-xylene selectivity requires precise control of hydrogenation activity and ester carbon-oxygen bond cleavage through catalyst design, motivating the development of Pt-Sn bimetallic catalysts for solvent free PET hydrogenolysis.

Methods. PtSn bimetallic catalysts supported on Al2O3 were prepared by incipient wetness impregnation followed by calcination and hydrogen reduction, and characterized by XRD, XPS, H2 TPR, TEM, XANES, and EXAFS. PET hydrogenolysis was conducted in a mechanically stirred stainless steel batch reactor under hydrogen pressures up to 85 MPa and temperatures up to 290 °C. Reaction products were identified and quantified by gas chromatography.

Results and discussion. A systematic evaluation of mono and multimetallic catalysts including Cu, Ni, Pt, Ru, and Sn identified the Pt Sn bimetallic system as the most effective catalyst for solvent-free hydrogenolysis of PET. At an optimal Pt to Sn molar ratio of 0.5, complete PET conversion and a BTX yield of 77.3% were achieved at 270°C with a catalyst to PET weight ratio of 10 wt.%. Increasing the Pt to Sn ratio beyond this optimum led to pronounced decreases in both PET conversion and BTX yield, demonstrating the critical role of precise bimetallic stoichiometry in controlling catalytic activity and selectivity. XRD and EXAFS analyses revealed the coexistence of metallic Pt and PtSn alloy phases, with their relative abundance strongly influencing p-xylene formation. Cooperative interactions between Pt and PtSn phases promote selective C=O hydrogenation and facilitate efficient ester C-O bond cleavage, which are key steps in BTX formation and p-xylene enrichment. The effects of reaction conditions were systematically examined (Fig. 1). Optimal performance was obtained at 290°C, delivering a BTX yield of 86.8% with 77.1% p-xylene selectivity. Higher temperatures

favored excessive hydrogenation. Under solvent-free conditions, increasing the catalyst to PET ratio to 30 wt.% further enhanced performance, yielding 99.1% BTX with 90.5% p-xylene selectivity. These results establish PtSn as a benchmark system for efficient PET hydrogenolysis and provide insight into alloy driven selectivity control for plastic waste valorization.



ISCRE29 & APCRE11
2026 / SEOUL, KOREA

SCW0234

Waste Polyoxymethylene Valorization Using Reusable Polymeric Acid Catalyst

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Waste Valorization

Keywords: Waste valorization; Polyoxymethylene; Heterogeneous catalysis; Microwave chemistry

Abstract Body.
Introduction. Polyoxymethylenes (POM) are engineered thermoplastics used in products such as kitchen utensils, joints, buckles, and gears, known for their strength and water repellency. However, disposing of POM plastics poses environmental issues, as incineration increases greenhouse gas emissions. Waste POM valorization methods using Bi(OTf)3 show promise but require high catalyst loadings and the use of solvents.1 Moreover, the catalyst is not reusable.
Methods. A mixture of plastics (1 mol equiv), PAFR II (260 mol ppm), and alcohol/amines (1.2 mol equiv) was introduced into a microwave reaction tube. The tube was sealed and subjected to microwave irradiation at 130 °C (max 80 W) using a microwave reactor, with temperature monitored by an infrared sensor and pressure maintained below 10 bar. Results and discussion. We have developed a method for waste polyoxymethylene valorization using m-phenolsulfonic acid-formaldehyde resin (PAFR II) as a reusable heterogeneous catalyst in solvent-free conditions.2 The method achieves up to 99% yield of upcycled products with just 260 mol ppm sulfur loading, demonstrating remarkable efficiency. Microwave irradiation proved more efficient, yielding 99% compared to 73% with conventional heating. This approach enables the synthesis of valuable chemicals, including solvents, herbicides, insecticides, and pillar[5]arenes, from biomass-derived reactants such as alcohols, amines and water. Notably, the catalyst maintains stability over six cycles without any loss of activity. This strategy effectively depolymerizes POM from various sources, including carbon-fiber-reinforced polymers (CFRP) and microplastics. The reaction was successfully scaled up to 40 g. A detailed investigation of the substrate scope and plausible catalytic pathway will be discussed.

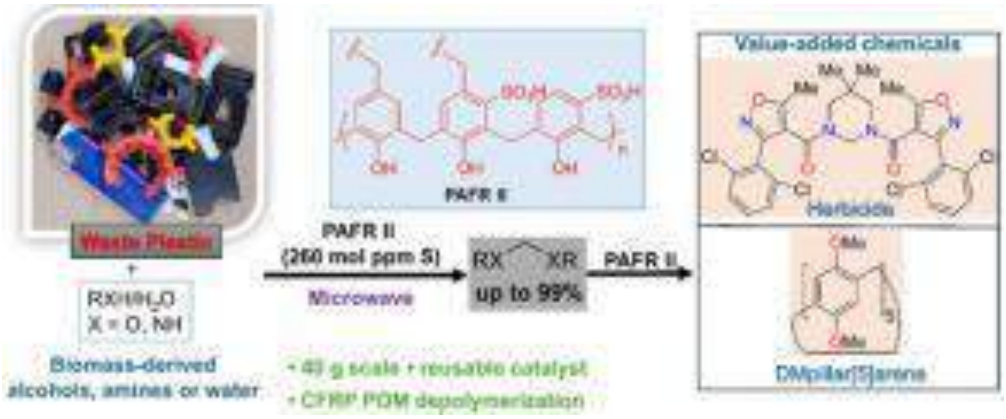

Figure 1. Upcycling waste polyoxymethylene to value-added chemicals.

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KN0024

Design Synthesis of Novel Metallosilicates for Selective Oxidation Catalyses

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Abstract Category: Invited Lecture - Keynote Lecture

Keywords: titanosilicate; ketone ammoximation; hydrogen peroxide; ketoxime

Abstract Body.
Cyclohexanone oxime (CHO) and methyl ethyl ketoxime (MEKO) are important bulk or fine chemicals. Traditional production of ketoxime relies on the hydroxylamine method. The firstgeneration TS-1 titanosilicate developed a transformative technology for the one-step ammoximation of ketone, ammonia, and hydrogen peroxide in a t-BuOH solvent system to produce ketoximes. The new-generation titanosilicates of large-pore Ti-MWW and Ti-MOR not only provide new ammoximation technology in t-BuOH, but also enable the development of aqueous-phase technology, which has been applied and promoted on a large scale in the production of MEKO and CHO. In the future, it is expected to develop greener ammoximation technologies using bifunctional catalysts, as well as coupling electrocatalytic oxygen reduction reaction and thermocatalysis by titanosilicates.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

SCW0235

Environmentally Friendly Production of Sustainable Olefins from Plastic Waste via Catalytic Cracking of Crude Pyrolysis Oil in a Circulating Fluidized Bed Reactor

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Waste Valorization

Keywords: plastic recycling, plastic waste, pyrolysis oil, catalytic cracking, light olefin, circulating fluidized bed reactor

Abstract Body.

Introduction. Plastic waste represents one of the most pressing environmental challenges and, at the same time, a largely untapped resource for sustainable chemical production. Conventional recycling routes for waste plastic pyrolysis oil (WPPO) rely on hydroprocessing followed by thermal steam cracking, which are energy-intensive, hydrogen-demanding, and constrained by strict feedstock specifications for olefin content and impurities. These limitations hinder large-scale deployment of plastic waste valorization as a circular-economy solution. This study presents an environmentally friendly and scalable catalytic strategy that directly converts crude WPPO into high-value light olefins, eliminating hydrogen-intensive post-treatment steps and enabling complete utilization of heterogeneous plastic-derived feedstocks.

Methods. A hydrothermally stable microspherical phosphorus-modified steam-treated ZSM-5 catalyst (ms-P-HZSM5-S) was rationally designed for successive reaction-regeneration cycles and integrated into both lab-scale and pilot-scale systems. Catalytic cracking was first investigated in a micro-activity test unit to establish structure-activity relationships and identify optimal operating windows. The process was then scaled up to a pilot-scale circulating fluidized bed reactor (CFBR, 1000 g·h^{-1} throughput), where the catalyst circulation rate, feed rate, and catalyst-to-oil ratio were systematically varied. Product distributions were quantified using online and offline gas chromatography, and catalyst stability was evaluated under continuous operation with in situ regeneration.

Results and discussion. Compared with thermal cracking and naphtha-based benchmark processes, the catalytic route delivered substantially higher C_2 -C_4 olefin yields and superior energy efficiency. In the pilot CFBR, total C_2 -C_4 olefin yields reached up to 46.2 wt% at temperature of 680 °C, outperforming conventional naphtha cracking despite operating at significantly lower reaction severity. The tailored ms-P-HZSM5-S catalyst exhibited excellent hydrothermal stability and maintained high activity and selectivity during 24 h continuous operation, enabled by continuous coke removal and regeneration. The circulating fluidized

bed configuration ensured steady-state operation, uniform heat management, and long-term robustness, demonstrating the feasibility of industrial deployment. Compared with state-of-the-art commercial schemes, the proposed process achieves higher olefin productivity, reduced energy demand, elimination of hydrogen consumption, and complete utilization of crude WPPO without hydroprocessing, offering a compelling pathway for sustainable plastic waste valorization.

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ISCRE29 & APCRE11
2026 / SEOUL, KOREA

SCM0651

Investigating external surface accessibility effects of hierarchical and nanosponge zeolite Beta in polyolefin chemical recycling

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Materials (Zeolite, MOF etc)

Keywords: Waste Plastic, Chemical Recycling, Hierarchical Zeolite, Zeolite Beta

Abstract Body.
Polyethylene (PE) waste, which accounts for a significant portion of plastic waste, is accumulating rapidly due to its chemical inertness and high production volume. Chemical recycling has therefore gained attention as a route to convert polyolefin waste into valuable products, thereby contributing to mitigation of plastic waste and carbon neutrality. Thermal pyrolysis, which is already commercially available, has limitations such as high operating temperatures, high energy demand, and the production of olefin-rich products. Utilizing zeolite catalysts offers an effective approach by enabling milder reaction conditions with improved product selectivity. However, the conversion of long-chain polymers is often governed by catalyst accessibility and mass-transfer constraints.
In our previous studies on polyolefin decomposition over zeolite Beta (*BEA), varying the Si/Al ratio and crystal size in an open-batch reactor system, we identified the external surface area of zeolite Beta as a key factor affecting the catalytic performance in both PE catalytic cracking and PE hydrocracking.
To investigate the effects of external surface area and accessibility on PE conversion, we applied a series of pore-structure-engineered zeolite Beta catalysts, which vary in external surface area and pore structure, to PE catalytic cracking and PE hydrocracking in an open-batch reactor setup. Hierarchical and nanosponge zeolite Beta catalysts were synthesized to provide varied pore structures and external surface areas relative to conventional zeolite Beta. These catalysts were tested in an open-batch reactor system for PE catalytic cracking and PE hydrocracking. Introducing mesoporosity led to increased conversion and enhanced selectivity compared to conventional zeolite Beta. Reaction results were correlated with catalyst properties to assess the contributions of external surface area, mesoporosity, and morphology. This work contributes to a deeper understanding of how pore structure, external surface area, and morphology influence PE conversion and selectivity. The resulting structure–performance relationships will offer guidance for designing zeolite Beta architectures for efficient polyolefin chemical recycling.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

SCW0134

Technical and environmental assessment of wheat straw biochar for soil application

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Waste Valorization

Keywords: Wheat straw; Biochar; Soil conditioner; Life Cycle Assessment

Abstract Body.

Introduction.

The management of agricultural residues is a key component of the transition toward efficient, resilient, and climate-neutral agri-food systems. Wheat straw (WS), one of the most abundant by-products of cereal cultivation, represents a strategic resource due to its composition and wide availability. Globally, cereal production produces nearly 60% of total crop residues, of which a substantial fraction of WS is available for off-farm uses. This study evaluated the technical feasibility and environmental performance of WS-derived biochar production and application as a bio-based soil conditioner, supporting circular economy strategies and the decarbonization of agro-systems. The WS-derived biochar was applied in a greenhouse on tomatoes and compared with conventional mineral fertiliser through an integrated experimental and environmental assessment.

Methods.

WS was converted into biochar using slow pyrolysis in a horizontal fixed-bed reactor at three temperatures (400, 500, and 600 °C; heating rate 10 °C min^{-1}, residence time 30 min). The produced biochars were chemically and physically characterised. Greenhouse experiments were conducted on tomato plants (Solanum lycopersicum L.) using three rates of biochar (1% v/v, 100 kg N ha^{-1}, and 10 t ha^{-1}) and compared with mineral fertiliser (NPK 16-4-8) and an untreated control. Plant height and fresh and dry biomass were monitored during growth.

A cradle-to-gate Life Cycle Assessment (LCA, ISO 14040–44:2006) was performed with SimaPro 9.5 software, Ecoinvent 3.8 database, and the ReCiPe Midpoint (H) 2016 method. The functional unit was defined as 100 kg N ha^{-1} applied, and a consequential approach was adopted, accounting for avoided impacts from fossil fuel substitution by pyrogas.

Results and discussion.

The biochar obtained at 500 °C (BC500) was selected for agronomic trials due to its balanced nutrient content and energetic self-sustainability. Agronomic results showed that high application rates (10 t ha^{-1}) negatively affected plant height, suggesting potential phytotoxicity, while no significant differences in fresh or dry biomass were observed among treatments. At lower dosages (1% v/v and 100 kg N ha^{-1}), BC500 performance was comparable to mineral fertilizer.

LCA results highlighted a substantial reduction in environmental impacts compared to mineral fertiliser, with climate change impacts of 1.84E−03 kg CO2 eq/FU versus 1.65E−02 kg CO2 eq/FU and a negative fossil resource scarcity impact due to fossil fuel substitution.

The study demonstrates that WS-derived biochar can be a technically feasible and

environmentally advantageous bio-based soil conditioner when applied at appropriate rates, contributing to greenhouse gas mitigation, resource efficiency, and circular agricultural systems.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

SCW0237

Catalytic Hydrothermal Valorization of Hydrocarbon Residue and Plastic Waste to Chemicals: Experimental and Machine Learning Insigts

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Waste Valorization

Keywords: Waste Valorization; Machine learning; Sustainable chemical

Abstract Body.
Owing to the rising demand for plastics, the generation of massive volumes of waste remains a hurdle in waste management. The heavy hydrocarbon residues from refining processes also remain underutilised despite their high carbon content. Hence, the catalytic hydrothermal co-valorisation (HTCV) of heavy hydrocarbon residues and plastic waste offers a promising route for sustainable resource recovery, aligning with the Sustainable Development Goals. This study addresses these challenges by transforming plastic waste and heavy hydrocarbon residues into chemicals, delivering a dual benefit: diverting waste from landfills and producing high-value platform chemicals. Accordingly, both feedstocks were co-processed in a batch autoclave reactor using a supported iron-based catalyst under hydrothermal conditions. Real-time data were recorded alongside gas chromatography analysis of the products for machine learning (ML) modelling. Experimental results revealed that feed composition and catalyst loading significantly influenced selectivity. Furthermore, ML models were developed to capture the complex relationships between operating parameters. Tree-based algorithms demonstrated superior predictive performance ($R2 > 0.97$), and feature importance analysis corroborated experimental observations, highlighting HHR content, reaction time, temperature, and catalyst loading as key drivers. These findings underscore the synergy between feed composition and ML modeling to maximize value chemical production from challenging waste streams, advancing circular-economy strategies and carbon-neutral chemical processes.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

SCW0292

Efficient polyolefin upcycling to liquid fuels via Ru–zeolite physical mixtures and pathway control

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Waste Valorization

Keywords: polyolefin upcycling; physical mixing; spatial separation; pathway switching; hydrocracking; gasoline-range products

Abstract Body.
Introduction. Chemical recycling of polyolefin waste into liquid fuels is a promising route to reduce the environmental burden of plastics while recovering high-value hydrocarbons. Ru-based catalysts are highly active for polyolefin hydrogenolysis under relatively mild conditions, but they often favor terminal C–C scission, which drives deep cracking and substantial methane formation [1], limiting liquid-fuel selectivity and practical utility. Even when Ru is directly supported on zeolites (e.g., Ru/BEA), the strong intrinsic hydrogenolysis tendency of Ru can remain dominant [1]. Here, a simple catalyst design principle is introduced: physically mixing Ru/TiO2 with BEA zeolite to spatially separate metal and acid functions, aiming to suppress Ru-mediated deep hydrogenolysis while selectively activating bifunctional hydrocracking toward gasoline-range liquids.
Methods. Catalysts included 5 wt% Ru/TiO2, BEA zeolite (Si/Al2 = 25), and 5 wt% Ru/BEA prepared by wet impregnation. LDPE (Mw ~4 kDa) was reacted in a 25 mL Parr stainless-steel batch reactor at 270 °C for 3 h under 50 bar H2. Gas and liquid products were quantified and identified using GC-FID, TCD, and MS.
Results and discussion. Ru/TiO2 alone converted 87% PE but produced 7% methane, confirming monofunctional hydrogenolysis pathway. Physical mixing of Ru/TiO2 and BEA dramatically suppressed methane to <0.5% while achieving 100% PE conversion and 83% gasoline yield with 77% isomers—a clear pathway switching to bifunctional hydrocracking. In contrast, Ru/BEA retained significant methane production (13%), suggesting that confining Ru within zeolite micropores sustains direct hydrogenolysis due to restricted intermediary diffusion [1]. The superior performance of the physical mixture compared to Ru/BEA demonstrates that spatial decoupling, rather than mere metal-acid proximity, is critical for suppressing hydrogenolysis and achieving selective gasoline production from polyolefin depolymerization.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

SCW0343

Unlocking BTX from Epoxy–Polyethylene Waste: Catalytic Vapor Upgrading over Ga/Zn HZSM 5

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Waste Valorization

Keywords: Chemical Recycling, Pyrolysis, Zeolites, Plastic, Waste, Catalysts

Abstract Body.
Purpose. Plastics are indispensable in modern applications such as construction, transportation, electronics, and packaging; however, the increasing generation of mixed plastic waste streams poses significant recycling challenges. While pyrolysis has been extensively explored for polyolefinic plastics, thermoset polymers such as epoxy resins remain difficult to valorize due to their crosslinked structure and oxygen-rich degradation products. Although epoxy resins are not typically co-processed with polyethylene (PE), they can enter the same waste streams through electronic components and multilayer packaging materials, where mechanical recycling is not feasible. Our previous study on the catalytic upgrading of PET pyrolysis vapors demonstrated that gallium- and zinc-promoted HZSM-5 catalysts are highly effective in converting oxygenated compounds into BTX aromatics [1]. Given the chemical similarity of PET- and epoxy-derived oxygenates, this catalytic strategy is expected to be applicable to epoxy-containing waste streams.
Methods. Thermal pyrolysis experiments of epoxy resin and epoxy–polyethylene mixtures were conducted using a micro-pyrolyzer system to establish baseline product distributions and quantify oxygenated compounds. The resulting pyrolysis vapors were analyzed using comprehensive GC×GC coupled with flame ionization detection and time-of-flight mass spectrometry, enabling detailed characterization of gaseous and liquid products.
Based on insights obtained from prior catalytic PET pyrolysis studies, Ga- and Zn-modified HZSM-5 catalysts were selected for forthcoming catalytic upgrading experiments. These experiments will be performed in a two-stage reactor configuration, in which thermal pyrolysis is followed by vapor-phase catalytic upgrading (Figure 1), allowing direct comparison between non-catalytic and catalytic pathways.
Results and discussion. Thermal pyrolysis experiments revealed that epoxy resin generates a substantial fraction of oxygenated compounds, accounting for approximately 40 wt.% of the products. These oxygenates, dominated by phenolic and aromatic species, significantly deteriorate pyrolysis oil quality and highlight the limitations of non-catalytic epoxy pyrolysis. In our previous work on catalytic PET pyrolysis, Ga- and Zn-promoted HZSM-5 catalysts enabled efficient deoxygenation via decarbonylation, decarboxylation, and aromatization pathways, resulting in BTX selectivities of up to 90% in the pyrolysis oil during co-pyrolysis with polyethylene. However, PET pyrolysis and catalytic upgrading are accompanied by substantial CO and CO2 formation (>35 wt.%), leading to significant carbon loss from the liquid product pool [1]. In contrast, preliminary epoxy resin pyrolysis results show significantly lower CO and

CO2 generation (~5 wt.%), indicating a higher potential for carbon recovery of liquid hydrocarbons, preferably BTX aromatics. These observations form the foundation for the ongoing catalytic epoxy–polyethylene co-pyrolysis study.

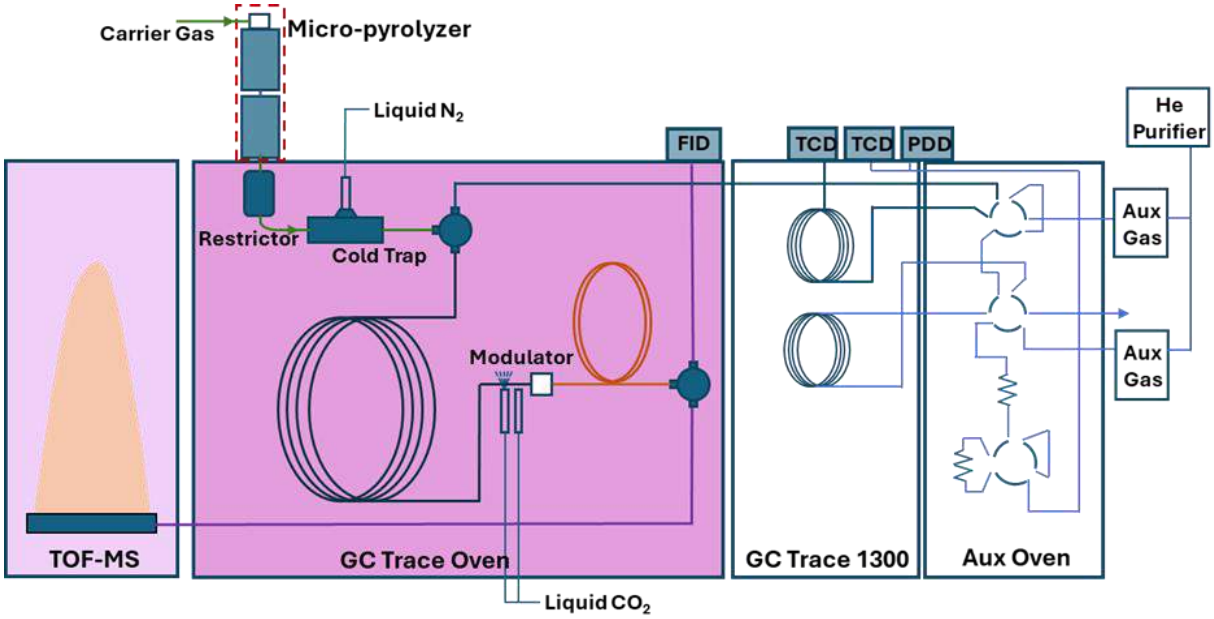

Figure 1. Micropyrolyzer facility.

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ISCRE29 & APCRE11
2026 / SEOUL, KOREA

SCW0440

High-conversion Fischer-Tropsch Technology for Waste to Fuels applications

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Waste Valorization

Keywords: Waste to fuels, Fischer-Tropsch synthesis, novel catalytic reactor

Abstract Body.
Introduction The conversion of waste-derived synthesis gas into liquid fuels and chemicals via Fischer–Tropsch (FT) synthesis is a promising route toward sustainable carbon utilization. Although FT is commercially established route to liquid fuels, waste valorization applications bring new challenges such as diluted synthesis gas, fluctuating feed quality, and inefficient single-pass conversion in conventional FT reactors. This work addresses these challenges through a reaction-engineering assessment of a novel high-conversion FT reactor concept, based on patented technology [1,2]. The objective is to apply an experimentally validated model of the novel high-conversion FT reactor to demonstrate the advantages in waste valorization applications and compare it to established FT reactor technologies.
Methods Pilot-scale experiments were conducted using synthetic and waste-representative syngas feeds with varying CO/H_2 ratios, dilution levels, and flow rates. Experimental data were used to validate a mechanistic reactor gPROMS model [3,4] incorporating gas–liquid mass transfer, dissolved-gas transport in a circulating wax phase, intrinsic FT kinetics, and heat removal via external liquid circulation. The validated model was then employed to perform a systematic, sustainability-oriented comparison of the high-conversion reactor with slurry bubble column reactors, multitubular fixed-bed reactors, and microchannel reactors. Performance metrics included single-pass carbon monoxide conversion, syngas recycle requirements, thermal control, and sensitivity to feed variability typical of waste valorization processes.
Results Model predictions are in good agreement with pilot-scale measurements for conversion, temperature profiles, and product selectivity. The high-conversion reactor achieves single-pass CO conversions exceeding 80% for dilute syngas feeds while maintaining small temperature gradients (1°C temperature change across the catalyst bed) and stable operation. Reaction-engineering trade-offs between gas solubility, liquid circulation rate, and catalyst effectiveness will be quantified and contrasted with mass- and heat-transfer limitations characteristic of conventional FT reactor designs.
Conclusions The experimentally validated model demonstrates that the high-conversion FT reactor offers distinct advantages for sustainable waste valorization, enabling efficient processing of dilute and variable syngas streams with reduced energy intensity. The high-conversion reactor concept enables use of FT reactors in waste valorization applications by allowing complete elimination of syngas recycle for diluted syngas feeds. Same technology is suitable for processing concentrated CO2 feeds as the syngas recycle can be significantly

reduced. Relatively low conversion of conventional FT reactor technologies makes the traditional FBCR or SBCR designs discredited for use in waste valorization applications.
The results highlight the importance of reactor concepts that decouple gas conditioning from catalytic reaction in advancing waste-to-chemicals and waste-to-fuels technologies.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

SCW0552

Pyrolysis of Contaminated Mixed poly-olefins: Feedstock Characterization and Impurity Partitioning into Oil Fractions

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Waste Valorization

Keywords: mixed waste plastic, pyrolysis, additives, halogens, TGA-FTIR, ICP-OES, 2D-GC

Abstract Body.

Introduction: Pyrolysis of mixed polyolefin-rich plastic waste (MPO) is complicated by the coexistence of multiple polymers and diverse contaminants in the feedstock. MPO typically contains polyethylene (PE), polypropylene (PP), and polystyrene (PS), together with impurities such as biomass, PVC, PET, and polyamides [11,12]. Post-consumer packaging waste often includes multilayer materials (cardboard, aluminum foils), adhesives (polyurethanes, epoxies), organic residues, and absorbed salts. At the same time, industrial and construction plastics introduce mineral fillers ($CaCO_3$, SiO_2, clays) and additives such as plasticizers, antioxidants, and flame retardants. These impurities complicates mechanical recycling, therefore chemical recycling processes such as pyrolysis becomes the viable pathway for recycling. The composition of the produced pyrolysis oil is severely impacted by the contaminants present in the feed and consecutive petrochemical processes, as the presence of halogens, sulfides, and heavy metals can lead to corrosion in the steam cracker, coke formation, and potential poisoning of downstream catalysts. In this study, pyrolysis of three surrogate mixed polyolefin (MPO) feedstocks and two contaminated real MPW feedstocks were investigated to assess how feedstock composition and impurity levels affect pyrolysis oil characteristics.

Methods: Polyolefin content, non-polyolefin polymers, and additives in the feedstocks were identified using Thermogravimetric analysis-Fourier Transform Infrared Spectrometry TGA–FTIR. Elemental and halogen concentrations in MP) and pyrolysis oil samples were determined by Induced Coupled Plasma-Optical Emission Spectrometry (ICP-OES) and combustion ion chromatography (CIC). Detailed hydrocarbon group composition of the pyrolysis oils was obtained using comprehensive two-dimensional gas chromatography with flame ionization detection (GC×GC-FID).

Results and discussion: TGA–FTIR analysis revealed three primary degradation regions: 170–370 °C (biomass, PVC, PS), 370–550 °C (polyolefins), and 500–900 °C (fillers and mineral residues). The MPW feeds exhibited elevated concentrations of Ca (>2000 ppm), Si (>1000 ppm), Mg (>700 ppm), Fe (>500 ppm), Zn (>100 ppm), and Cl (>300 ppm), highlighting the significant inorganic and halogen burden. Impurities were preferentially enriched in the heavy pyrolysis oil fraction compared to the naphtha fraction. The heavy fraction showed higher

levels of Cl (>50 ppm), Fe (>2 ppm), Cu (>2 ppm), and Zn (>5 ppm), whereas the naphtha phase contained only trace concentrations of Si, Ni, Co, Cu, and Zn. Notably, high-temperature extrusion feeding during pyrolysis reduced Cl-, O-, and N-containing species in the produced oil fractions, indicating its potential as a process-based impurity mitigation strategy.

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2026 / SEOUL, KOREA

CET0150

Facile and efficient microwave strategy for upcycling of plastic wastes into high-yield hydrogen and carbon nanotubes

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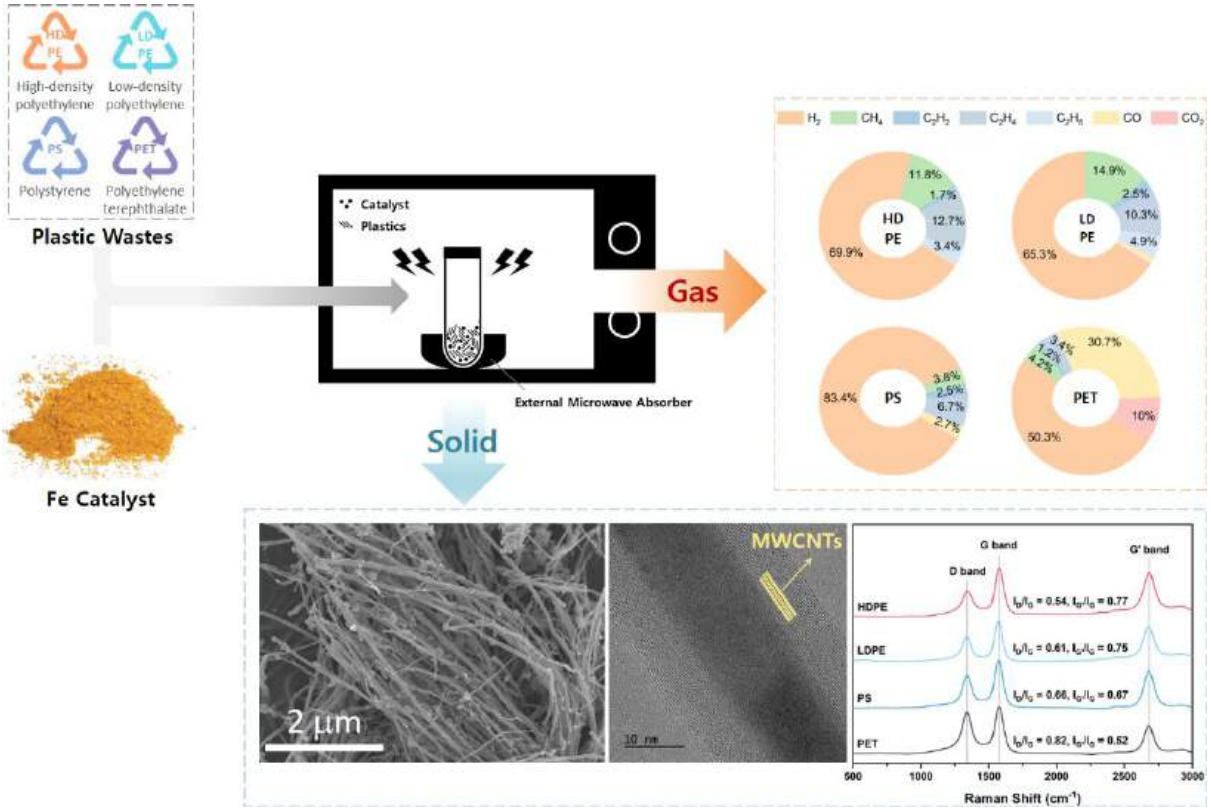
Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: plastic waste upcycling, microwave-irradiated pyrolysis, microwave absorber, hydrogen, carbon nanotube

Abstract Body.
Plastics are indispensable in modern society, yet their persistence and low degradability impose a growing environmental burden. Accordingly, the establishment of sustainable and practical plastic waste management strategies has been considered one of the most urgent and non-negotiable agendas. To address this issue, various thermochemical valorization routes have been widely explored to convert plastic waste into value-added products. Among them, microwave-assisted pyrolysis has been particularly attractive because it has enabled rapid volumetric heating and short reaction times. However, practical implementation of microwave-driven upcycling has often been limited by the need for purpose-built microwave cavities, specially designed reactors, and sophisticated control systems to stabilize temperature profiles and product selectivity. In this work, we present a facile and efficient microwave-assisted plastic-waste upcycling strategy that operates in a common household microwave oven, providing a low-infrastructure alternative for rapid conversion. In the presence of an Fe catalyst and an external silicon carbide (SiC) microwave absorber, plastic wastes (HDPE, LDPE, PS, PET, and their mixtures) were rapidly decomposed into high-yield H2 and carbon nanotubes (CNTs) within 1–2 min of microwave irradiation. SiC played a decisive role by triggering an abrupt thermal surge, raising the reaction temperature to as high as 1123 K, which preferentially accelerated C–H bond cleavage and enabled simultaneous CNT growth. Microwave-irradiated pyrolysis of HDPE and LDPE exhibited high H2 selectivity (up to ~70%) and produced high-quality CNTs (Raman ID/IG = 0.54) with an ~95% filamentous carbon yield after purification, indicating efficient carbon utilization in the solid phase with negligible formation of undesired liquids. Indeed, liquid products were undetectable, and CO2 formation was minimal except for PET. Even for oxygen-rich PET, CO production was approximately three times higher than CO2 production. It is noted that microwave-irradiated pyrolysis of mixed plastic wastes generated syngas with tunable H2/CO ratios (0.75–2.5). Since other gaseous products such as CH4 and C2Hx do not participate in the reaction, the resulting syngas can be directly used for the Fischer–Tropsch reaction for e-fuel production. These results established a practically deployable, SiC-boosted household-microwave pathway that coupled ultrafast H2 liberation with in-situ CNT synthesis from real-world plastic wastes.


HDPE
LDPE
High-density polyethylene
Low-density polyethylene
PS
PET
Polystyrene
Polyethylene terephthalate
Plastic Wastes
Fe Catalyst
Catalyst
Plastics
External Microwave Absorber
Gas
Solid
H2 CH4 C2H2 C2H4 C2H6 CO CO2
HD PE
LD PE
PS
PET
2 μm
MWCNTs
G band
D band
G' band
HDPE
LDPE
PS
PET
Raman Shift (cm-1)

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

CET0256

Accelerated Design of Wide-Temperature-Range Molten Salts via Transfer Learning with Small Sample Sizes of data

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: Energy Storage Molten Salts; Wide Temperature Range; Machine Learning

Abstract Body.

Introduction. Concentrated Solar Power (CSP) and thermal power retrofits extensively utilize molten salts.[1] The current commercial salt, Solar Salt, operates within a limited temperature range (220–565°C). However, the development of advanced multi-component salts faces distinct challenges.[2] Traditional approaches are inefficient for exploring the vast compositional space. While machine learning strategies offer acceleration, they are severely constrained by the small sample size of data.[3] Direct training on such limited datasets is prone to noise, which obscures the true chemical trends. This study proposes a transfer learning framework to design wide-temperature-range molten salts, specifically to overcome small sample size limitations.

Methods. To address the challenge of small sample sizes in energy storage materials, a hierarchical dataset was constructed. This comprised a foundational dataset of low-fidelity historical data to capture general trends and a high-quality dataset generated via strictly controlled experiments. A non-linear regression model was utilized as the base learner to capture interactions between salt components (KNO3, NaNO3, NaNO2, LiNO3, Ca(NO3)2). A transfer learning strategy was employed, where the model was pre-trained on lower-fidelity data and subsequently fine-tuned using the small set of high-fidelity experiment data. This approach avoids the noise and bias introduced by simply aggregating datasets of varying fidelity. Screening was then applied to predict candidates with optimal thermal properties.

Results and discussion. The transfer learning strategy successfully mitigated the limitations imposed by the small sample size of data, allowing the model to accurately predict thermal stability limits even when the data is noisy and sparse. The model-guided screening identified novel multi-component molten salt formulations with temperature range exceeding 500°C. Remarkably, this represents a 50% increase over commercial salts. This study provides a framework for accelerating the discovery of next-generation thermal energy storage materials despite limited data.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

CET0288

Revealing the active Cu species in Cu/ZSM-5 catalysts for the selective catalytic oxidation of ammonia

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: NH3-SCO, Cu/ZSM-5, ammonia, oxidation, active sites

Abstract Body.

Introduction.

Ammonia slip, a by-product of NH_3 processes such as selective catalytic reduction (SCR) of NO_x and emerging NH_3-fueled energy systems, poses significant environmental and health risks, necessitating its removal via the selective catalytic oxidation of ammonia (NH3-SCO; 4NH3 + 3O2 → 2N2 + 6H2O). Recent studies have demonstrated the potential of Cu/zeolite catalysts for NH_3-SCO reactions, owing to their intrinsic oxidation activity and high N2 selectivity. However, the precise nature of the active Cu sites governing NH3-SCO has not been fully established and remains controversial.

Methods.

In this study, a series of Cu/ZSM-5 catalysts with varying Cu loadings was synthesized via an aqueous ion-exchange method. The structural properties were characterized by XRD and BET, while the nature and distribution of Cu species were examined using H2-TPR, EPR, and UV-Vis DRS. In addition, NH3 adsorption behavior and reaction pathways were investigated through NH3-TPD and in situ DRIFTS. The reaction rate and apparent activation energy (E_a) were determined under conditions with NH_3 conversion maintained below 20% to avoid mass diffusion limitations.

Results and discussion.

Among the catalysts with various Cu loadings, the 2.1Cu/ZSM-5 catalyst, corresponding to the maximum Cu content achievable via ion exchange, exhibited up to 99.5% NH_3 conversion and 99.4% N_2 selectivity at 400 °C. To investigate the active Cu sites in the NH3-SCO reaction, the distribution of the Cu species quantified by H2-TPR and EPR was correlated with the reaction rate, revealing that isolated Cu2+ ions exhibited the strongest linear correlation. A controlled experiment involving the selective reduction of Cu2+ to Cu+ resulted in a significant decrease in the NH3 conversion, confirming that Cu2+ ions are more active than Cu+ ions in the NH3-SCO reaction. Furthermore, the turnover frequency (TOF), calculated based on the number of Cu2+ ions, remained nearly constant with a slight increase at higher Cu loadings, confirming the primary role of Cu2+ ions in the catalytic oxidation process and the minor contribution of other Cu species. Further NH3-TPD and in situ DRIFTS analyses demonstrated that Cu ion-exchange enhances NH3 adsorption capability, thereby contributing to the improved catalytic activity in the NH3-SCO reaction.

These results collectively indicate that both the population and intrinsic reactivity of isolated Cu^{2+} ions are key factors governing NH3-SCO performance. This study identifies the most active Cu sites and their role in NH_3 oxidation within ion-exchanged Cu/ZSM-5 catalysts,

providing insights for developing future strategies to achieve enhanced NH3-SCO performance.

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CET0410

Performance Evaluation of Cation-Exchanged Zeolites for CO_2/CH_4 Separation

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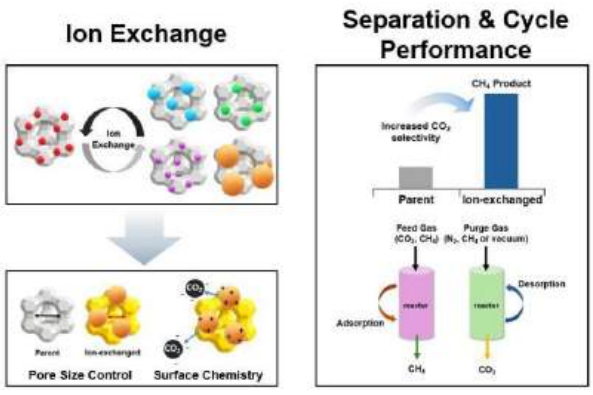
Keywords: Ion-exchanged zeolite; CO_2/CH_4 Separation; Vacuum pressure swing adsorption (VPSA)

The technology for efficiently separating CO_2 and CH_4 from natural gas and biogas is crucial for achieving energy sustainability and climate goals. Zeolite-based adsorption processes are well-recognized as promising technologies due to their high stability and structural tunability. However, to enhance separation efficiency, it is necessary to simultaneously optimize physical pore size and chemical surface properties. This study aimed to confirm the enhancement of CO_2/CH_4 separation performance by controlling the pore structure and surface charge density (acid sites) through cation exchange in zeolites, utilizing both electrostatic interactions and kinetic mechanisms between the zeolite framework and CO_2 molecules.

Cation-exchanged zeolites were synthesized using a conventional ion-exchange method. Typically, 10g of the base zeolite was dispersed in a 1.0 M metal-nitrate aqueous solution and stirred at 80°C for 6h. To ensure maximum exchange capacity, the process was repeated four times by replacing it with a fresh solution. The ion-exchanged zeolites were washed with deionized water, dried in an oven for 12h, and calcined at 500°C for 5h. The physicochemical properties of synthesized samples were characterized using X-ray diffraction (XRD), X-ray fluorescence (XRF), X-ray photoelectron spectroscopy (XPS), temperature-programmed desorption (TPD), and N_2 and CO_2 specific surface area analysis (BET). Dynamic separation properties were investigated using vacuum pressure swing adsorption (VPSA), where CO_2 adsorption capacity, CO_2/CH_4 separation performance and cyclic stability were evaluated under various purge gas conditions.



As a result of study, it was identified that the effective pore size of the zeolite was precisely controlled according to the ionic radius of the introduced cations.

Furthermore, characterization results revealed that changes in surface acid sites and electrostatic interactions following cation introduction were key factors determining CO_2 adsorption affinity. These changes in physicochemical properties effectively restricted CH_4 diffusion while maintaining CO_2 accessibility, resulting in differences in kinetic selectivity. In particular vacuum pressure swing was performed to confirm CO_2 adsorption capacity and CO_2/CH_4 separation performance. Cyclic experiments using various purge gases suggest that desorption efficiency and adsorbent regeneration are influenced by the type of purge gas.

Acknowledgments

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ISCRE29 & APCRE11
2026 / SEOUL, KOREA

SCB0274

Pyrolysis and in-line catalytic cracking of olive stone-derived volatiles

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Biomass

Keywords: fast pyrolysis, olive stone, catalytic cracking, spouted-bed reactor

Abstract Body.
Introduction. The transition toward a less fossil-dependent circular economy requires efficient technologies for producing fuels and chemicals from renewable resources. Olive stone is an abundant Mediterranean residue, generated at roughly 0.2 ton per ton of raw olives [1]. Ex-situ catalytic fast pyrolysis offers a promising valorization pathway for such lignocellulosic waste.
Methods. In this work, olive-stone pyrolysis vapours were upgraded using a dual spouted-bed/fixed-bed bench-scale unit. Spouted-bed reactors are well established for biomass and plastic conversion, offering intense solid–gas circulation, rapid particle heating, and effective mitigation of agglomeration issues common in bubbling beds [2]. The study examines the influence of pyrolysis temperature, cracking temperature, and catalyst space-time on product yields, quality, and catalyst deactivation. Preliminary insights into the effect of catalyst type on product distribution are also reported.
Results and discussion. Increasing catalyst space-time and cracking temperature enhanced water and gas formation at the expense of organics. Char yield remained insensitive to catalytic conditions but decreased with higher pyrolysis temperatures. Micro-GC analysis showed that HZSM-5 (zeolite used as catalyst) favoured decarbonylation and dehydration as primary deoxygenation routes. The catalyst significantly reduced light oxygenates in bio-oil and promoted the production of aromatic hydrocarbons, but its strong Brønsted acidity also drove secondary condensation to PAHs. Spent-catalyst analysis indicated rapid deactivation, with ~10 wt% coke deposition and substantial losses in surface area and porosity within 45 min. Type I coke—poorly ordered deposits in meso- and macropores—was more abundant than type II, and acidic sites (measured by NH3-TPD) were progressively masked by coke and condensed hydrocarbons. A screening of different catalysts demonstrated that the functionality must be tailored to the targeted upgrading outcome. HZSM-5 remained the most effective for aromatization and for suppressing light oxygenates, whereas calcined dolomite showed exceptional deacidification performance. In contrast, γ-Al2O3-based catalysts and Fe/dolomite exhibited limited improvements, indicating the need for further research.

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2026 / SEOUL, KOREA

SCB0642

Acrylamide-Tuned Tobacco Biochar–Hydrogel Controlled Release Fertilizer for Alkaline Red Mud: Swelling, Water-Holding Capacity, and Medium-Dependent N–P Release

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Biomass

Keywords: Red mud, Biochar–hydrogel composite, Controlled-release fertilizer, Water-holding capacity

Abstract Body.
Red mud (bauxite residue) is a highly alkaline industrial waste whose low organic matter, limited water retention, and constrained nutrient bioavailability hinder revegetation. This study engineers a red-mud-compatible controlled-release fertilizer (CRF) by integrating NPK-impregnated tobacco-stem biochar with an acrylamide-tuned hydrogel network to jointly enhance moisture storage and regulate macronutrient delivery under alkaline conditions. Tobacco-stem biochar was produced via pyrolysis at 600 °C, loaded with NPK, and subsequently immobilized within a polymer network formed using acrylamide (2.5–15% w/w) to systematically tune composite architecture. Increasing acrylamide content improved product formation and nutrient immobilization, reaching the highest composite yield (96.03%) and nutrient retention at 15% acrylamide (N: 28.61%, P: 13.37%, K: 7.05%). In contrast, hydration performance in alkaline media exhibited a clear structure–property trade-off: the 10% acrylamide formulation delivered the most favorable physicochemical response, achieving a swelling index of 1606.91% at pH > 7 and a water-holding capacity up to 92.25%. The enhanced alkaline swelling is attributed to increased ionization of acidic functionalities within the composite matrix, promoting osmotic-driven water uptake and electrostatic expansion of the network. Nutrient release depended strongly on the testing medium, highlighting the importance of evaluating CRF behavior beyond aqueous systems. Nitrogen release was substantially higher in water (95.56%) than in red mud (40.53%), indicating stronger retention and/or reduced mobility in the highly alkaline, ion-rich red mud matrix. Conversely, phosphorus release was enhanced in red mud (89.66%) relative to water (58.35%), demonstrating substrate-selective release behavior. Overall, acrylamide network tuning provides a practical route to biochar–hydrogel CRFs that combine high water retention with medium-dependent nutrient partitioning, offering a promising amendment to support early-stage plant establishment and accelerate revegetation of red mud disposal sites.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

SCW0481

Sustainable Upcycling of Polyolefin Plastic Waste Using Spent FCC Catalysts

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Waste Valorization

Keywords: Polyolefin, Upcycling, Plastic waste, FCC Catalyst, Chemical recycling

Abstract Body.
Introduction. Despite advances in catalytic upcycling technologies, the global recycling rate of plastic waste remains 11% [1]. Compared to mechanical recycling, chemical recycling has contributed only marginally to plastic waste management, and most existing chemical recycling approaches rely on pyrolysis-based routes [2, 3]. A major impediment to broader implementation is that numerous high-performing catalytic systems depend on noble metals or require large-scale catalyst production, which raises concerns regarding economic feasibility, material availability, and process scalability. In this study, we propose a potentially economically and environmentally viable upcycling strategy that employs a spent fluid catalytic cracking (FCC) catalyst, a widely available industrial byproduct generated through decades of the petrochemical industry [4]. By utilizing an industrially mature and readily accessible waste catalyst, this study aims to advance the practical deployment of chemical recycling technologies and emphasizes the importance of integrating catalytic performance metrics with considerations of process maturity and material supply.
Methods. Reactions were performed in a 50 mL batch reactor using PP (1.0 g) and a catalyst (0.2-0.5 g). After purging with Ar, the reactor was pressurized to 2 bar and heated to 350 °C. Products were analyzed by gas chromatography equipped with FID and TCD detectors.
Results and discussion. The catalytic upcycling of waste PP (Fig. 1a) was investigated over HY(60) and a spent FCC catalyst. HY(60) achieved 60.4% conversion with a 52.6% naphtha yield (Fig. 1b). In contrast, the spent FCC catalyst exhibited lower activity, showing a conversion of 20.4% and a naphtha yield of 14.2%. NH3-TPD analysis indicated a lower total acid density for the spent FCC catalyst (0.337 mmol/g) compared with HY(60) (1.053 mmol/g) (Fig. 1c), suggesting that insufficient acid sites limit its performance. To address this limitation, the catalyst loading was increased, resulting in an increase in conversion to 63.3% and naphtha yield to 55.8% (Fig. 1d). These results demonstrate that, given a sufficient number of acid sites, the spent FCC catalyst can achieve catalytic performance comparable to that of a zeolite, supporting the feasibility of incorporating spent catalysts into plastic upcycling processes.

Acknowledgments
This work was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education (RS-2025–25414560).

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Oral Presentation

Clean Environmental Technologies

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

CET0193

Unlocking catalyst potential: Forced dynamic operation for modern emission control

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: Forced dynamic operation; Emission control; Heterogeneous catalysis; Methane conversion; Ammonia conversion

Abstract Body.
Meeting increasingly stringent emission regulations requires innovative strategies to maximize catalyst performance. Forced dynamic operation (FDO) has emerged as a versatile approach to overcome kinetic and thermodynamic limitations in emission control systems. This work explores FDO across three representative applications: three-way catalysis under stoichiometric conditions, methane oxidation in lean environments, and selective ammonia oxidation in oxygen-rich gas streams.
For this, Pd-based catalysts were prepared and subjected to comprehensive kinetic evaluation (Fig. 1) combined with ex situ and in situ characterization, both as powders and washcoated substrates. In three-way catalysis, high-frequency lean-rich cycling mitigates surface poisoning by CO and O2, enabling temperature-dependent frequency control for improved activity and selectivity. For CH4 oxidation, introducing short rich pulses during lean operation significantly enhances light-off behavior and stabilizes long-term performance. Spatiotemporal studies revealed axial gradients in palladium oxidation state and removal of hydroxyl species as key factors for robust CH4 activation. Similarly, FDO applied to NH3 oxidation promotes coexistence of metallic Pd and PdO phases, outperforming state-of-the-art catalysts in both activity and selectivity. These dynamic strategies not only enable efficient low-temperature pollutant abatement but also open pathways to reduce catalyst volume and material costs.
By leveraging fundamental insights into structure-activity relationships and reaction mechanisms, this work demonstrates how rationally designed dynamic operation unlocks previously untapped catalyst potential. FDO thus represents a promising route toward cleaner air and more sustainable catalytic processes, reducing reliance on scarce resources while meeting future emission standards.

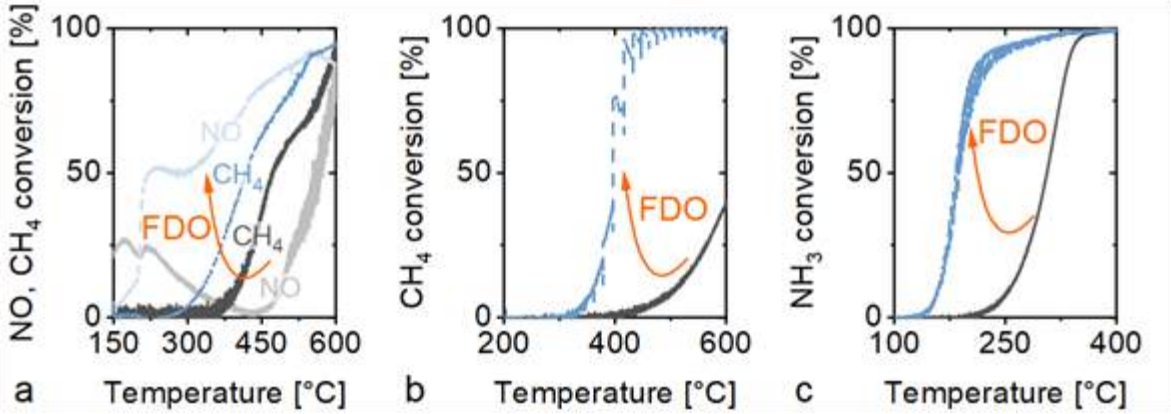

Figure 1: Pollutant conversion in time-invariant constant gas streams (solid lines) and in forced dynamic operation (dashed lines) for a) three-way catalysis, b) lean methane oxidation, and c) selective ammonia oxidation in excess O2. Data from [1-3].

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ISCRE29 & APCRE11
2026 / SEOUL, KOREA

CET0271

Co-modulated Ag/Al2O3 IPA-SCR catalyst for NOx emission control in semiconductor FAB exhaust

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: IPA-SCR, AgCo/Al2O3, deNOx, semiconductor FAB exhaust

Abstract Body.

Co-modulated Ag/Al2O3 IPA-SCR catalyst for NOx emission control in semiconductor FAB exhaust

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Keywords: IPA-SCR; AgCo/Al2O3; deNOx; semiconductor FAB exhaust

Introduction. Semiconductor fabrication facilities (FAB) emit nitrogen oxides (NOx) together with large amounts of isopropyl alcohol (IPA) from wafer cleaning processes [1]. Although IPA can serve as an on-site reductant for selective catalytic reduction (IPA-SCR), conventional Ag/Al2O3 catalysts are severely deactivated under the water-deficient conditions of indoor FAB exhaust due to preferential IPA dehydration to SCR-inactive propene [2]. Here, a cobalt-modulated AgCo/Al2O3 catalyst is proposed to regulate IPA activation under low-humidity conditions, enabling stable NOx reduction using IPA as an intrinsic reductant.

Methods. AgxCoy/Al2O3 was synthesized by co-impregnation using aqueous precursor solutions over g-Al2O3. x:y denotes molar ratio of x:y and x represents the Ag loading (wt.%).

Results and discussion. Under water-deficient conditions (1.6% H2O), conventional Ag1/Al2O3 predominantly promoted IPA dehydration to propene, an SCR-inactive pathway, resulting in poor NOx conversion. In contrast, Co-modified Ag1Co5/Al2O3 exhibited significantly enhanced and stable deNOx performance over a wide humidity range (Fig. 1). Structural and spectroscopic analyses revealed that cobalt incorporation suppressed strong acid sites associated with Ag–Al interactions and induced the formation of Ag-O-Co interfacial sites anchored on alumina defect centers. These interfaces redirected IPA activation toward acetone formation and enabled rapid utilization of dehydration-derived propene via thermodynamically favorable migration to interfacial sites. In-situ DRIFTs confirmed enhanced formation of surface isocyanate and cyanide intermediates, identifying the Ag-O-Co interface as the dominant SCR-active center.

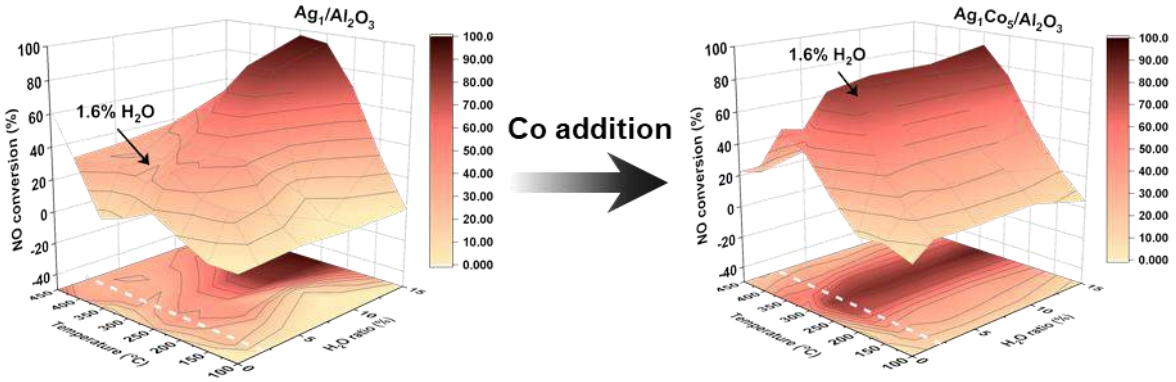

Fig. 1. 3D-plots for NO conversion as a function of the reaction temperature and H2O concentration during the IPA-SCR reaction over Ag/Al2O3 (left) and Ag1Co5/Al2O3 (bottom).

Acknowledgments
This work was supported by the National Research Foundation of Korea (RS-2021-NR060081 and RS-2023-00282392) and Samsung Advanced Institute of Technology (SAIT), Samsung Electronics Co., Ltd.

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ISCRE29 & APCRE11
2026 / SEOUL, KOREA

CET0350

Pd-ceria catalysts for complete CH4 oxidation: influence of Pr-doping on water and sulfur resistance

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: methane oxidation, Pd-ceria, Pr-doping, sulfur tolerance, catalyst deactivation

Abstract Body.

Introduction. Natural gas is regarded as an important energy vector for the energy transition, but CH4 emissions must be minimized due to its high global warming potential. Catalytic total oxidation is a state-of-the-art method to abate methane in exhaust gases, and Pd-based catalysts are usually employed for activating the CH4 dissociation. In the last years, Pr-doping was proven to be beneficial for Pd-ceria materials, promoting the stability of Pd2+ sites which are crucial species for high-temperature activity [1]. An intermediate Pr content also resulted in higher activity and stability in wet conditions [2]. Besides water, sulfur traces in natural gas also deactivate Pd-based catalysts [3]. Hence, this work thoroughly investigates the resistance of Pd/Ce-Pr materials to sulfur poisoning and the role of Pr-doping in this phenomenon.

Methods. Well-defined ceria nanostructures with different Pr contents (0-10-50-100 at%) were prepared through hydrothermal synthesis. Pd was deposited via incipient wetness impregnation (2 wt%) using a palladium nitrate solution. Catalytic tests of methane oxidation (0.3% CH4 + 1.2% O2 in N2, GHSV = 50000 h-1), consisting of repeated heating and cooling cycles up to 900 °C (see Fig. 1A), were carried out before and after exposure to SO2 during isothermal reaction (20 ppm, 500 °C, 6 h). Fresh and spent catalysts were comprehensively studied with several techniques, including XRD, Raman, TPO, FESEM, TEM, EDX, XPS.

Results and discussion. Upon exposure to SO2 during methane oxidation, different behaviors were observed depending on the Pr loading. In particular, Pd/CeO2 exhibited a rapid drop in activity as soon as SO2 was sent to the reactor (Fig. 1B), while Pr doping increased the resistance of the catalysts and led to improved activity in the second reaction cycle after sulfation (4th cycle, Fig. 1C). XRD, Raman, and XPS investigations coupled with TEM-EDX mapping evidenced that sulfates form on the catalyst surface, but sulfur can also penetrate the bulk of Pr-rich supports, causing structural distortion and defect formation, but without damaging the palladium activity. This results in a weakened metal-support interaction, which positively affects activity at low temperature, despite reducing the beneficial effect of Pr on Pd2+ stabilization at high temperature. The best overall performance was obtained with 10 at% Pr-doping, thanks to optimized PdO/Pd ratio.

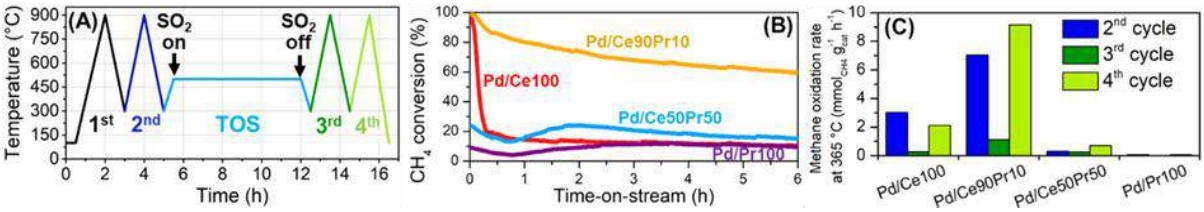

Figure 1. (A) Scheme of the catalytic tests. (B) Evolution of CH4 conversion over time-on-stream in the presence of SO2. (C) Specific reaction rate of methane oxidation through the three heating cycles.

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CET0329

N2O Abatement on Fe-CHA Catalysts: Transient Experiments and Kinetic Modelling

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: N2O decomposition, Fe-CHA, redox mechanism, auto-reduction, kinetic model

Abstract Body.
Introduction. Nitrous oxide, N2O, is a powerful greenhouse gas and ozone-depleting species, whose mitigation requires efficient abatement technologies. The catalytic decomposition of N2O (N2O→N2+½O2) over Fe-CHA is emerging as a promising solution thanks to the combination of high activity, hydrothermal stability, and cost-effectiveness. However, the decomposition mechanism remains debated due to the coexistence of multiple iron species. In this work, we combine transient response methods and kinetic analysis to elucidate the kinetically relevant steps of the N2O decomposition redox cycle.
Methods. The experimental activity was carried out on a model Fe-CHA catalyst (Fe loading = 1.7 % w/w, SAR = 13), to study N2O decomposition by means of Transient Response Methods. The catalyst is exposed to a step feed of N2O, while monitoring the outlet gas dynamics: this protocol was repeated varying T, N2O inlet concentration, initial catalyst oxidation state, with and w/o O2/H2O co-feed. The kinetic analysis was based on an integral plug-flow dynamic reactor model, with mass balances for gas species and Fe site fractions. Several mechanistic schemes from the literature were compared, with particular focus on the Cano-Blanco et al. model, which introduces both active and inhibited Fe sites.
Results and discussion. The experiments showed a strong effect of temperature on N2O conversion, which increased from 10.2 to 74.5 % between 330 and 480 °C, confirming the key role of Fe-sites auto-reduction in controlling catalytic activity. Varying the N2O concentration preserved similar transient shapes with a moderate decrease in steady-state conversion, suggesting an overall reaction order close to one with respect to N2O. The reductive vs. oxidative pretreatment markedly affected the initial transients but led to comparable steady-state performance. Cofeed of O2 and, even more strongly, H2O exerted a significant inhibiting effect, attributed to the formation of Fe-OH species, a poorly reactive oxidized state. The model based on the Cano-Blanco et al. mechanism successfully reproduced transient profiles and conversions under pre-reduced conditions and, with some limitations, under pre-oxidized and O2 co-fed conditions, providing a coherent picture of the redox cycle on Fe-CHA for N2O decomposition.

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KN0348

Unravelling the Standard/NH3-SCR Redox Chemistry: A Decoupled Kinetic Approach for Cu-CHA Catalysts

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Abstract Category: Invited Lecture - Keynote Lecture

Keywords: SCR, DeNOx, Cu-CHA catalyst, redox mechanism

Abstract Body.

Introduction. Decoupling the reduction and oxidation half-cycles of the low-temperature Standard-SCR mechanism over Cu-CHA catalysts is crucial to elucidate the elementary steps governing DeNOx activity and to develop predictive kinetic models. In this work, Transient Response Methods were adopted to independently study the Reduction Half-Cycle (RHC), where Cu2+ is reduced to Cu+ by NO and NH_3, and the Oxidation Half-Cycle (OHC), where Cu+ is re-oxidized to Cu2+ by O2. This approach builds upon previous advances in transient kinetic analysis of Cu-CHA systems [1-3] and employs an integral plug-flow reactor model to derive intrinsic kinetic constants and bed-averaged oxidized Cu fractions.

Methods. Cu-CHA catalysts differing in Cu loading (0.5-2.7 wt%), SAR (10-25), and hydrothermal aging level were tested under varying NO (300-500 ppm), O2 (1-8 %), H2O (0-2 %), and T (150-500 °C) conditions. For each sample, RHC and OHC rate constants independently estimated from transient runs were combined to predict steady-state NO conversion and oxidized Cu fraction under Standard-SCR conditions, showing excellent agreement with experimental data [3].

Results and discussion. H2O exerts a mild inhibiting effect on the RHC at high SAR, but significantly promotes the OHC at all SARs, consistent with mechanistic insights on water-assisted Cu redox chemistry from DFT and operando UV-Vis spectroscopy studies [4,5]. Hydrothermal aging has a negligible impact on RHC, but markedly depresses OHC.

At temperatures above 250 °C, our results reveal that the characteristic “seagull” in SCR activity originates exclusively from a sharp decline in the OHC rates between 250 and 350 °C, while the RHC rates retain the Arrhenius-type monotonic trend with T. This confirms the central role of Cu oxidation kinetics in limiting medium-temperature SCR performance.

Overall, the redox-decoupling framework provides mechanistic clarity on the interplay between Cu2+/Cu+ species during both low- and high-temperature Standard-SCR and offers a powerful tool for guiding the rational design of more active and durable Cu-CHA catalysts for automotive emission control.

Acknowledgments

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HTT0546

Modeling of propylene oxidation rate and selectivity on Cu/SSZ-13 catalysts for NH3-SCR

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: SCR, mathematical modeling, kinetics, pore diffusion, exhaust gas aftertreatment

Abstract Body.

Introduction

Cu/SSZ-13 catalysts are used for selective catalytic reduction of NOx (SCR). A close-coupled SCR not preceded by an oxidation catalyst is being considered to meet stringent emission regulations during cold start. However, the influence of hydrocarbon oxidation on the SCR catalyst remains unclear. Our work extends current understanding by incorporating new oxidation reactions in a mathematical model of an SCR catalyst, including C3H6 oxidation to CO, CO2, CH3CHO, HCHO and HCN (via ammoxidation).

Methods

2 wt.% Cu/SSZ-13 catalysts were synthesized via incipient wetness impregnation of copper acetate solution into HSSZ-13 with Si/Al ratios of 5.5 and 15 (ACS Materials). Powder samples were examined in a lab microreactor in the fresh state and after mild hydrothermal aging, resulting in a varying distribution of ZCuOH and Z2Cu sites [1]. Oxidation of 1000 ppm C3H6 was tested at 150–550 °C with or without 200 ppm NH3.

Results and discussion

Based on the experimental data, a kinetic model for propylene and ammonia oxidation on Cu/SSZ-13 was developed. The ZCuOH sites, the occurrence of which closely related to the Si/Al ratio of the zeolite, promote total oxidation of the undesired by-products, Figure 1. During mild hydrothermal aging, however, ZCuOH is gradually transferred to Z2Cu, decreasing the oxidation activity [1]. Hydrothermal aging further induces formation of extra-framework Al, which decreases the effective diffusivity of propylene into zeolite micropores and thus effectively reduces propylene conversion as well as byproduct formation.

Conclusions and significance

The developed kinetic model can predict propylene conversion and selectivity depending on Cu sites speciation and catalyst aging state. The new insights help optimize the SCR catalyst performance under realistic operating conditions.

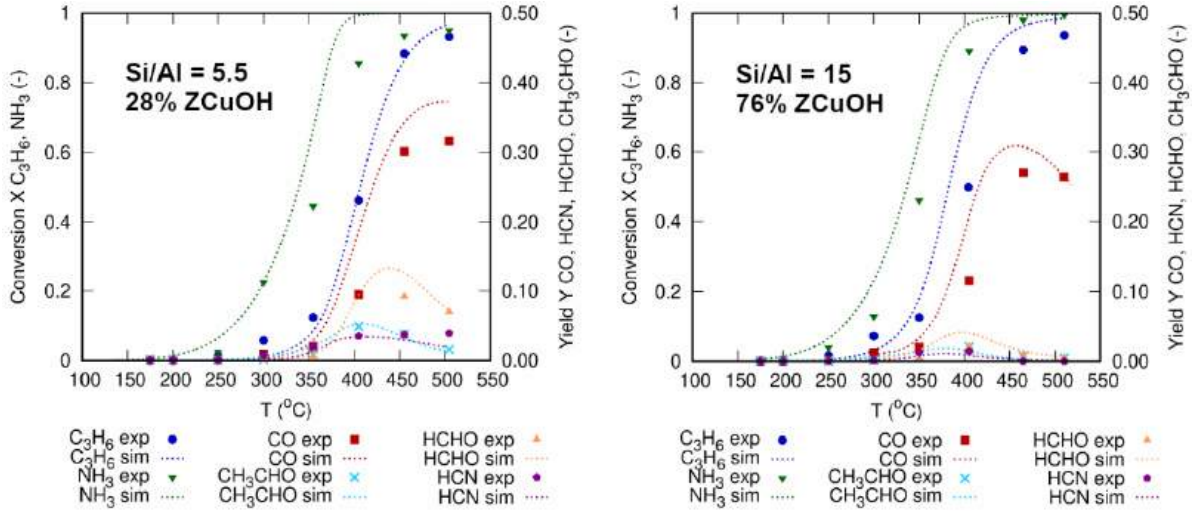

Figure 1. Impact of Si/Al and ZCuOH fraction of Cu sites on C3H6+O2+NH3 conversion and selectivity. The same kinetic parameters were used for both catalysts, effect of ZCuOH concentration considered.

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CET0083

On the thermal degradation of a functionalized ionic liquid for reactive removal of acid gases and its synthesis mixtures

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: Ionic liquids, Stability assessment, Calorimetric analysis, Reactive acid-gas treatment, Reactor safety

Abstract Body.
Purpose:
The transition toward safer and more sustainable chemical processes requires thermally robust and tunable reaction media to replace conventional volatile solvents. Ionic liquids (ILs) have emerged as promising candidates due to their negligible vapor pressure, chemical versatility, and suitability for reactive separation processes. Their use as reactive solvents for acid gases such as CO_2, H_2S, and SO_2 is particularly attractive. However, industrial deployment is limited by gaps in understanding their thermal stability under operating conditions and safety concerns associated with their synthesis and scale-up. This work investigates the thermal stability of tetramethylguanidinium imidazolate ([TMG][Im]), focusing on both operational performance and its synthesis route.
Methods:
Accelerated Rate Calorimetry (ARC) was employed to determine decomposition onset temperatures, heat release characteristics, and degradation kinetics of [TMG][Im]. The study also examined the upstream synthesis via neutralization of tetramethylguanidine (TMG) with imidazole (Im) in ethanol. ARC experiments were conducted on pure TMG, pure Im, their binary mixtures with ethanol, and the complete ternary system (TMG + Im + EtOH) to assess the influence of reactant interactions and solvent presence on thermal stability and process safety.
Results:
Pure TMG exhibited slow decomposition starting at approximately 250 °C, without a pronounced exothermic peak. In contrast, the presence of ethanol significantly increased decomposition intensity, lowering the onset temperature to about 130 °C, just above ethanol's boiling point. Pure imidazole, both neat and in ethanol solution, showed no detectable decomposition under the tested conditions. The thermal behavior of the ternary mixture and the synthesized [TMG][Im] followed these trends, indicating that ethanol primarily reduces stability during synthesis. Additionally, within the mixture, the presence of imidazole appears to have a dominant effect over TMG, as no distinct exothermic decomposition peak was

observed within the analyzed temperature range. Figure 1 shows thermograms of TMG and Im in mixtures with ethanol at different mass ratios, measured at a heating rate of 2.5 °C/min.

Conclusions:

The findings provide a comprehensive understanding of [TMG][Im] thermal stability from synthesis to application in reactive acid-gas treatment. Ethanol significantly lowers decomposition thresholds during synthesis, highlighting the need for careful process design. Combined with literature data, these results support preliminary design of emergency relief systems for industrial-scale operations, enabling safer and scalable implementation of ionic liquids in next-generation clean technologies.

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CET0156

Kinetics analysis of pure and industrial hematite powder reduction using hydrogen and carbon monoxide mixture.

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Keywords: Gas solid reaction; iron oxide reduction; kinetic.

Introduction.

The steel industry plays an important role in the world's industry and economy, arriving at a yearly production of 1950 mega tons in 2020 that corresponds to a large emission of carbon dioxide due to the Blast Furnace (BF) process. In the BF, carbon monoxide produced from coke acts as reducing agent. Steel production is responsible for approximately 8% of industrially based global CO2 emission, that corresponds to around 4 Giga tons yearly. The principal alternative to classic fossil fuel routes are direct reduction (DR) processes in which natural gas reduces iron ore in a shaft furnace by solid state reaction. It offers several advantages such as the reduction of CO2 emissions by about 48% and less process and energy cost because of the lower temperature. They represent the first important step towards the decarbonization of the ironmaking process. On other hand, these technologies don't offer an adequate upgrade to convert the old BF route and fossil feedstock is used and CO2 is still emitted. Moreover, the introduction of hydrogen complicates the reaction pattern promoting side reactions in which influence on the intrinsic kinetic of iron oxide reduction using mixture of hydrogen and carbon monoxide is not clarified yet.

Main reactions

$$3Fe_2O_3 + H_2|CO \rightleftharpoons Fe_3O_4 + H_2O|CO_2$$
$$Fe_3O_4 + 4H_2|CO \rightleftharpoons 3Fe + 4H_2O|CO_2$$
$$FeO + H_2|CO \rightleftharpoons Fe + H_2O|CO_2$$

Side reaction

$$2CO \rightleftharpoons C + CO_2$$
$$CO + H_2O \rightleftharpoons CO_2 + H_2$$

In this work, the intrinsic kinetic of iron oxide reduction for pure material and for commercial pellet powder derived from both BF and DR plants, has been studied. The seemingly simple overall reaction displays interestingly complex behavior, which depends on gas phase, surface and solid phase phenomena. The progressive complexity of the reaction pattern and the influence of the catalytic role of iron and iron oxide phases coupled to the thermodynamic convolution make this system an open challenge to investigate and understand in detail. The fundamental issues are crucial in designing and operating the steel making process in the future.

Methods.

The kinetics of pure hematite (Fe_2O_3) and industrially sourced iron oxide (mainly hematite) reduction was studied using a novel approach. In fact, respect the traditional thermogravimetric method, the off gases composition is used to follow the reaction. The experimental set up consists of three flowmeters, a glass reactor, a water trap and a microGC. Experiments were performed with a thin layer of hematite powder to study the intrinsic kinetics of reduction. Solid-state properties were also analyzed to assure a correct interpretation of the obtained data and for a correct understanding of the influence of morphology and crystal structure of the material.

Results and discussion.

As can be seen on Fig.1, the reduction kinetics differs between pure and commercial samples. The results are in agreement with the profile observed using hydrogen and carbon monoxide as single reducing agents. Moreover, the physical- chemical characterization of the material (before, during and after reaction) at various experimental conditions supports the interpretation of the kinetic data, indicating that the local thermodynamics influences the overall kinetics. In addition, the morphological changes occurring during the reduction is a key point to consider. The observations are supported by data obtained on the gas composition and solid-state properties of the pure oxide and commercial samples obtained with SEM, CHNS, XRD. Finally, the rate of Boudourd reaction is also considered and investigated.

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CET0177

Optimization of process parameters for the esterase production from Trichoderma harzianum using both Taguchi orthogonal design and machine learning technique and hydromechanical stress study in a fermenter

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Abstract Category: Process Intensification - 선택 없음

Keywords: Esterase, Optimization, Machine Learning, Data Augmentation

Abstract Body.
Esterase is a hydrolytic enzyme plays the important role in sustainable bioeconomy. Hence, the optimization of significant upstream bioprocess parameter in the fermentation industries improves the esterase productivity with the economic process. The current study intends to optimize the most significant process parameter such as temperature, pH, agitation, and aeration using Taguchi method in 3-L bioreactor. Further, machine learning technique of data augmentation with variational autoencoder (VAE) and optimization with Bayesian optimization (BO) technique was used to improve the optimal condition for maximum esterase production. Also, the hydromechanical stress during the fermentation was studied in fermenter. The samples were taken at regular interval up to ten days of fermentation to analyse the optimal values of each day. In Taguchi optimization study, the optimal pH value of first day was found to be pH 5 and changed to pH 7 for the rest of the fermentation. Similarly, the temperature also found be 25 °C at the first day and found optimum at 30 °C for the rest of the fermentation period. The agitation rate was found to be in the range of 150 to 250 rpm and aeration was found to be 1 to 1.5 lpm. The maximum esterase activity of 4485.77 U/L was obtained on the seventh day of fermentation. Interestingly, machine learning technique of VAE+BO obtained the maximum esterase activity of 4668.16 U/L which was higher than the Taguchi optimization due to its optimization with a greater number of synthetic data. The hydromechanical stress study in the 3-L bioreactor reveals that the more stress induces at the mid of the log phase due to increasing cell diameter, viscosity and density. However, stress got decreased due to the reduction of cell diameter.

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2026 / SEOUL, KOREA

CET0280

CF4 Destruction via Oxidative Heat Assistance in a Sn-Mg Molten Metal Bubble Column Reactor

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: CF4 Destruction, Molten metal, Sn-Mg alloy, Bubble column reactor

Abstract Body.
Perfluorocarbons (PFCs) emitted from semiconductor manufacturing are potent greenhouse gases, and CF_4 is especially difficult to abate because of its exceptional thermodynamic stability. Molten metal–based thermochemical processes are promising for F-gas destruction, yet many systems still rely on very high operating temperatures. This study proposes an oxidative heat–assisted approach to enable efficient CF_4 destruction in a Sn–Mg molten metal bubble column reactor at reduced temperatures.
CF_4 destruction experiments were performed in a laboratory-scale bubble column reactor using a Sn–Mg alloy as the reaction medium. A Sn–Mg molar ratio of 40% was selected based on prior optimization showing high destruction performance. To reduce external heating demand, oxygen was co-injected with CF_4 at concentrations below 10% of the total gas flow to provide in situ oxidative heat release. In addition, SUJ2 beads were introduced as packing media to refine bubble size and increase the gas–liquid interfacial area, thereby enhancing mass transfer. CF_4 conversion was quantified by comparing inlet and outlet gas compositions over an operating temperature range of 600–800 °C.
Oxidative heat assistance combined with bubble refinement improved CF_4 destruction and enabled stable conversion at lower temperatures compared with non-assisted conditions. The results indicate that reactor hydrodynamics and kinetic enhancement, together with controlled oxidative heat input, can substantially improve performance beyond purely thermodynamic considerations.
In conclusion, integrating low-level oxygen co-injection with bubble refinement offers a practical route to lower-temperature, energy-efficient CF_4 destruction in Sn–Mg molten metal bubble column reactors, supporting industrially viable greenhouse-gas abatement.

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CET0613

Optimization of the Catalyst Layer Using Fluorine-Free Ionomers in GDE Half-Cell Configuration

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: fluorine-free ionomers; catalyst layer optimization; gas diffusion electrode; half-cell screening; proton exchange membrane fuel cells

Abstract Body.
Introduction. Catalyst layer (CL) optimization remains a central challenge in proton exchange membrane fuel cells (PEMFCs), where performance arises from a delicate balance between proton transport, oxygen accessibility, and catalyst utilization. Although perfluorosulfonic acid (PFSA) ionomers such as Nafion® are widely used as benchmarks, their cost and environmental impact motivate the development of fluorine-free alternatives. High–ion exchange capacity (IEC) sulfonated aromatic polymers (SAPs) are promising candidates, yet their application is often limited by excessive swelling and insufficient hydrolytic stability. In this work, crosslinked fluorine-free ionomers based on sulfonated poly(phenyl sulfone) (SPPSU) are investigated as CL binders. A gas diffusion electrode (GDE) half-cell configuration is employed to systematically explore the influence of ionomer chemistry and formulation on CL structure and electrochemical behavior.
Methods. Fluorine-free ionomers with high IEC (1.5–2 meq g^{-1}) were synthesized via PPSU sulfonation, followed by controlled thermal crosslinking promoted by dimethyl sulfoxide (DMSO) to improve mechanical and hydrolytic stability. Catalyst inks were prepared using a commercial Pt/VC catalyst (TEC10V50E), with systematic variation of ionomer-to-carbon (I/C) ratio and DMSO–water solvent composition. Electrodes were fabricated as GDEs and evaluated in a half-cell setup to enable rapid and reproducible screening of CL formulations. Ex situ characterization included field-emission scanning electron microscopy (FESEM) and nitrogen physisorption (BET) to assess CL morphology, thickness, and porosity. X-ray photoelectron spectroscopy (XPS) was used to probe catalyst–ionomer interfacial mechanism interactions and ionomer surface distribution. All results were benchmarked against Nafion®-based electrodes prepared under identical conditions.
Results and discussion. The GDE half-cell configuration provides a robust platform for isolating and comparing the effects of fluorine-free ionomers on CL structure and electrochemical response. The combined electrochemical and ex situ analyses highlight the importance of optimizing ionomer content and crosslinking degree to balance protonic connectivity and porous network accessibility. Morphological and surface-sensitive characterizations indicate that ionomer chemistry strongly influences CL homogeneity, porosity distribution, and catalyst–ionomer interactions, underpinning a clear structure–property relationship. Overall, this integrated methodology demonstrates the potential of

crosslinked fluorine-free ionomers as viable CL binders, offering performance-relevant features comparable to PFSA benchmarks while enabling enhanced control over interfacial and microstructural properties, establishing further performance KPIs for these materials.

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CET0660

Delayed Coking for Co-conversion of Biomass: Bench-scale Experiments and Multi-Objective Optimization

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: Delayed coking, Biomass co-processing, bioenergy, Multi-objective optimization

Abstract Body.

1. Introduction

The delayed coker unit (DCU) offers a unique opportunity for integrating renewable biomass into petroleum refineries due to its non-catalytic operation, high impurity tolerance, and operating temperatures compatible with biomass pyrolysis. When biomass is co-processed with vacuum residue (VR), the simultaneous decomposition of oxygen containing biopolymers and heavy petroleum hydrocarbons creates complex reaction interactions that can alter cracking severity, hydrogen transfer, and coke formation. Quantitative understanding of these trade-offs and their impact on product yields and quality is essential for scale-up of this technology.

2. Methods

Bench-scale delayed coking experiments were conducted at 460–490 °C and 1–3 kg cm²(g) with biomass dosing up to 20 wt%. Regression-based surrogate models were developed to predict product yields (fuel gas, LPG, naphtha, gasoil, coke) and key quality indicators (TAN, sulfur content, calorific value). These models were embedded within a multi-objective optimization framework employing NSGA-II and simulated annealing to obtain optimum conditions for six real-life refining operation scenarios such as simultaneous maximization of selected product yields and calorific value of liquid product in combination with minimization of undesirable product yields, liquid product TAN, and sulfur in coke and liquid product.

3. Results and discussion

Increasing biomass content led to higher coke yields (from ~32.5 wt% for VR alone to ~35–38 wt% at 10–20 wt% biomass) and reduced liquid yields, while promoting hydrogen transfer reactions that suppressed polycyclic aromatics and enhanced the saturates in the liquid products. Synergy in terms of lower than estimated metal impurity content, and TAN (Fig. 1 (a)) due to deoxygenation of acidic compounds were observed in liquid products. Though the biomass coprocessing increased the contents of Fe and alkali/alkali earth metals as well as ash in liquid products, majority were concentrated in the coke.

Optimal operating conditions for six cases were obtained through multi-objective optimization. Pareto-optimal solutions revealed strong trade-offs between coke yield, liquid yield, TAN, sulfur content, and fuel gas production. Low biomass dosing (≤5 wt%), higher temperatures, and moderate pressures were found to be optimal for maximizing naphtha + gasoil yield while minimizing TAN and sulfur content in liquid product (Fig. 1(b)). In contrast, coke-oriented

operation benefited from higher biomass dosing and lower temperatures. The optimal operating conditions and the reasons for the formation of Pareto fronts will be discussed in the full paper.

ISCRE29 & APCRE11
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CET05684

Sub/supercritical water gasification of hydrothermal carbonization-derived wastewater: influence of feedstock on the energy recovery

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Keywords: Supercritical water gasification; Hydrogen production; Wastewater treatment

Introduction. Sub- and super-critical water gasification converts biomass with high moisture content into value-added gaseous products, such as H_2 and CH_4. While this process is mostly investigated starting from solid biomass, it can also be particularly promising when recalcitrant components are present in a wastewater (AP). This is the case of the aqueous phase derived from hydrothermal processes, where organics like cyclic and N-containing molecules are refractory to conventional abatement. In this work, sub- and super-critical water gasification was investigated with the aim of improving the energy recovery with respect to stand-alone hydrothermal carbonization (HTC), evaluating feedstock influence on reaction performance.

Methods. The HTC-AP was kindly provided by CEA Cadarache. The feedstocks were different in nature, and included non-digested urban sewage sludge, lignocellulosic green waste, soda industry sludge, and microalgae (Feed 1, 2, 3, and 4, respectively). They were characterized by complementary techniques to identify and quantify organic and inorganic compounds (e.g., GC-MS, HPLC, TOC, ion chromatography). The gasification tests were carried out in an unstirred batch reactor, investigating several reaction conditions. The influence of the catalyst was evaluated using a commercial 5% Ru/Al_2O_3 and an assessment of the energy recovery from the reactions was performed.

Results and discussion. The figures below show two representative outcomes. On the left, it is shown that, at 400 °C, catalyst addition significantly improved H_2 productivity for each feedstock but urban sewage sludge. Green waste and microalgae led to the highest hydrogen productivity, above 80 mmol H_2/g_C, with the latter reaching more than 80% of carbon conversion into gaseous molecules. On the right, the beneficial integration of HTC with microalgae gasification is reported: the supercritical water gasification step increased the recovered energy by about 27% with respect to HTC alone, raising total recovery from 69% to 96%, corresponding to 20.6 MJ/kg_{feed}. Furthermore, the carbon conversion to gas allows the aqueous phase to be recycled to the microalgae growth stage, reducing the freshwater need.

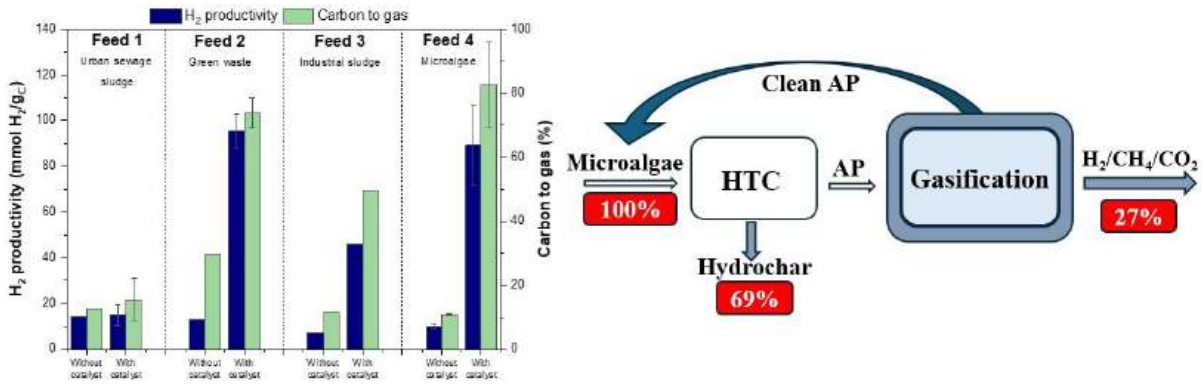

Figure 1: Influence of feed and catalyst on H_2 productivity and on carbon to gas (left) and energy recovery of the coupled process (right).

Acknowledgments The project leading to this research has received funding from the Horizon Europe research and innovation program under Grant Agreement No 101146861 (NIAGARA Project).

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

CET0330

Investigating Effect of Angle of Attack on Methane-Oxidation Reaction in Exhaust After-Treatment Process

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: Exhaust aftertreatment, methane oxidation, catalytic structures, structure-resolved CFD simulations

Abstract Body.

Introduction: Maritime transport is increasingly utilizing natural gas-fueled engines to meet stringent emission regulations, owing to their lower CO2, SOX and particulate emissions. However, a major concern is the release of unburned methane (methane slip). Methane is a highly potent greenhouse gas which significantly contributes to global warming. Consequently, without dedicated exhaust gas treatment, methane slip not only affects the global climate but also has direct impact on marine and coastal ecosystems. Therefore, exhaust after-treatment systems based on catalytic methane oxidation represent an effective way to mitigate methane slip before its release into the atmosphere. In view of this, the present work aims to investigate the effect of flow angles and effect of various catalytic structures on methane conversion in exhaust after-treatment process under different operating conditions using CFD simulations.

Methods: In present study, a cylindrical computational domain (diameter = 18 mm) consisting of hexagonal monolithic structure (bed diameter and height = 18 and 16 mm, respectively) is considered to investigate the effect of flow angles (i.e., 90°, 120° and 150°) on methane oxidation reaction [see Figure 1(a)]. The Reynolds-averaged continuity, momentum, energy and species transport equations are solved using Ansys CFX v2025R2.

Results and discussion: The effect of flow angle on methane oxidation conditions is investigated by introducing an artificial source of 1 Watt. The simulations are performed at a pressure of 6 bar and temperature of 673 K. A typical velocity distribution for various flow angles is shown in Figure 1(b). The 90° case exhibited higher stagnation and recirculation zones due to normal flow impingement on the catalytic bed, leading to increased viscous dissipation resulting in higher pressure drop (ΔP). Whereas, with increase in flow angle, recirculation zone decreases as the flow angle becomes more axially aligned with the bed, resulting in lower ΔP for the 150° case. While intermediate ΔP are observed for the 120° case [see Figure 1(b)-(d)]. The influence of flow angle is found to be more pronounced at high velocity, as suggested by large ΔP difference between flow angle cases. The marginal variation in temperature is found for all cases due to introduction of small heat source values [see Figure 1(e)]. A detailed discussion of reaction simulations of flow angles and different catalytic configurations will be presented at the conference.

Conclusions: These findings highlight the importance of flow angle on flow characteristics, therefore important to investigate their influence on methane oxidation performance under actual reaction conditions.

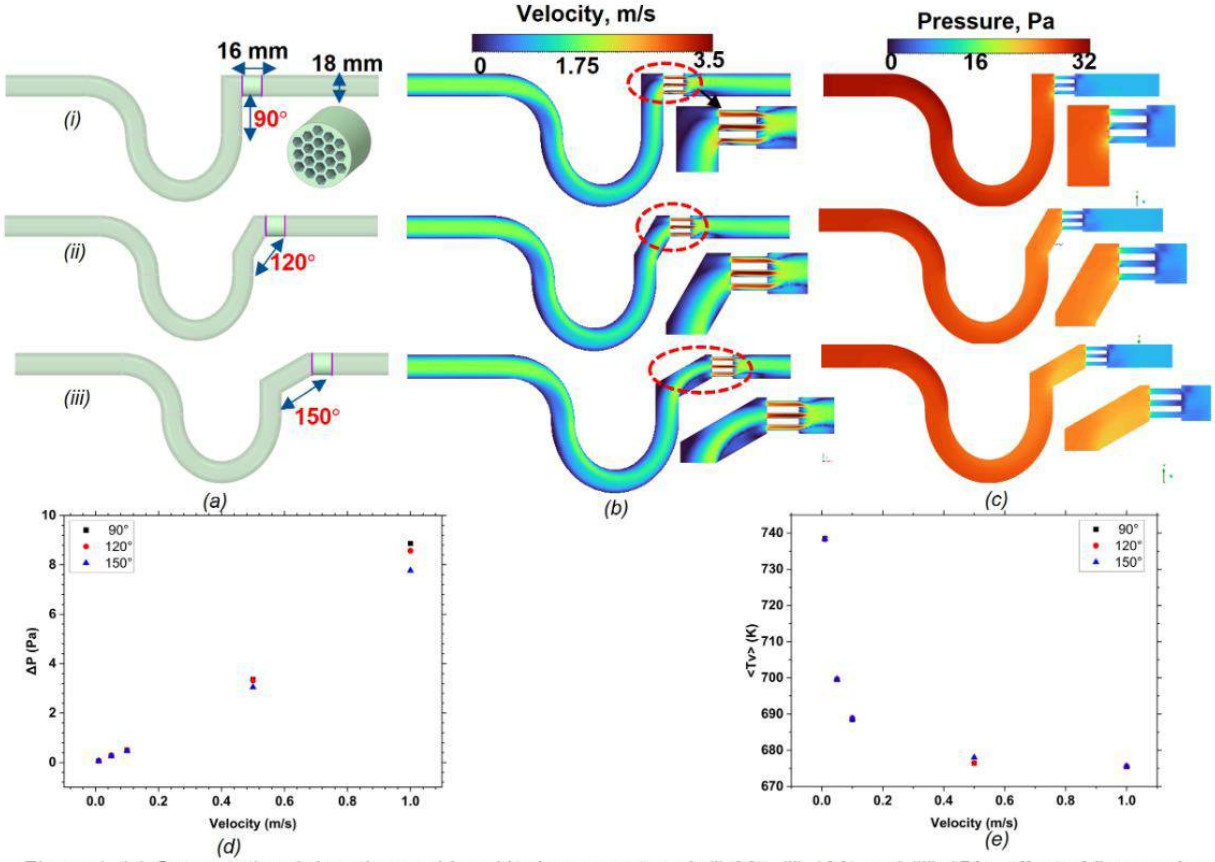

Figure 1. (a) Computational domain considered in the present work (i) 90°, (ii) 120° and (iii) 150°, effect of flow angle on (b) velocity distribution, (c) pressure distribution, (d) pressure drop and (e) solid temperature distribution.

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CET0163

From Mixed Plastic Waste to Olefins: Techno-Economic and Life-Cycle Impacts of Pyrolysis-Oil Co-Feeding and Electrified Steam Cracking under Korean electricity grid

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: Petrochemical Decarbonization, Electrified Steam Cracking, Waste-to-Olefins

Abstract Body.
Purpose: South Korea's petrochemical industry must reduce greenhouse-gas emissions to meet the 2050 carbon-neutrality goal while maintaining cost competitiveness in global olefin markets. Steam cracking, essential for olefin production, is energy- and carbon-intensive, with its Scope 1-2 emissions increasingly restricted by policy and market pressures. This study explores a dual decarbonization pathway combining (i) electrified pyrolysis of mixed plastic waste (MPW) to produce pyrolysis oil (Py-oil) and (ii) electrified steam cracking to convert this Py-oil (pure or blended with conventional feedstocks) into High Value Chemicals (HVC). The goal is to assess trade-offs among economic performance, operating costs, and cradle-to-gate climate impacts under Korean conditions.
Methods: Five electrified steam-cracking configurations were evaluated and compared against a conventional naphtha steam cracker (CSC). For each, eleven Py-oil substitution levels from 0 to 100 wt% were modeled. Mass and energy balances were generated using first-principles process modeling with COILSIM integrated into Petro-SIM flowsheets, explicitly accounting for utilities and heat-recovery systems in downstream separation. These inventories fed into an integrated cradle-to-gate life-cycle assessment (LCA) and techno-economic analysis (TEA). TEA metrics included discounted payback period (DPP), operating expenses, and sensitivity to electricity price and carbon intensity, while LCA quantified net greenhouse-gas emissions relative to the naphtha-based CSC benchmark.
Results: The benchmark CSC has a DPP of 14.3 years, indicating limited incentives and high uncertainty for new fossil-based cracking assets. In the steam-cracking unit, increasing Py-oil substitution improves capital recovery, reducing DPP to approximately 1.5-2.5 years once substitution exceeds 70 wt%. When considering the full waste-to-olefins chain, DPP values drop to around 5 years at 100 wt% Py-oil substitution, compared with approximately 8 years for pyrolysis alone, showing that integration with steam cracking enhances overall economics. Partial electrification – using high-temperature electric heating combined with steam-turbine

integration and heat recovery – delivers the lowest operating costs under current energy prices. From an emissions standpoint, full electrification can nearly eliminate Scope 1 emissions; however, net climate benefits depend heavily on the carbon intensity of electricity. Net GHG savings over conventional naphtha cracking occur only if grid emissions are below roughly 0.2–0.3 kg CO2/kWh, a threshold Korea's current electricity mix does not yet meet.

Conclusion: The results support a phased transition strategy: immediate deployment of moderate Py-oil blending in existing crackers alongside expanding MPW pyrolysis capacity; medium-term partial electrification with advanced heat integration; and long-term full electrification driven by decarbonization of the power sector and decreasing costs of low-carbon electricity.

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CET0195

Does H2 Temperature-Programmed Reduction Always Probe Solid-State Redox Chemistry?

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: H2-TPR, Pt, CeO2, Kinetics

Abstract Body.
Redox reactions on the surface of transition metal oxides are of broad interest in thermo, photo, and electrocatalysis. H2 temperature-programmed reduction (H2-TPR) is commonly used to probe oxide reducibility by measuring the rate of H2 consumption during temperature ramps, assuming that this rate is controlled by oxide reduction. However, oxide reduction involves several elementary steps, such as H2 dissociation and H-spillover, before surface reduction and H2O formation occur. In this study, we evaluated the kinetics of H2 consumption over CeO2 and Pt/CeO2 with varying Pt loadings and structures to identify the elementary steps probed by H2-TPR. Literature often attributes changes in H2-TPR characteristics with Pt addition to increased CeO2 reducibility. However, our analysis revealed that the H2 consumption rate is measurement of the rate of H-spillover at Pt-CeO2 interfaces and is determined by the concentration of Pt species on Pt nanoclusters that dissociate H2. Therefore, lower temperature H2 consumption observed with Pt addition does not indicate higher CeO2 reducibility. Measurements on samples with mixtures of Pt single-atoms and nanoclusters demonstrated that H2-TPR can effectively quantify dilute Pt nanocluster concentrations, suggesting caution in directly linking H2-TPR characteristics to oxide reducibility while highlighting alternative material insights that can be gleaned.

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CET0313

Tailored catalytic selectivity in small-pore environments: A case study of Mn/TiO_2 in the NOx reduction

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: Selective Catalytic Reduction, MnTiO2, Pore confinement

Abstract Body.
Controlling selectivity in heterogeneous catalysis is essential for designing processes that minimize the production of undesired byproducts. For example, TiO2-supported manganese oxide, a promising material for catalyzing the selective reduction of NO with NH3 at very low temperatures, is currently restricted by poor selectivity because of the production of unwanted N2O, which has a greenhouse gas potential 300 times higher than that of CO2. In this study, we located manganese oxides in microporous TiO2 with small pores of molecular dimensions and found that this catalyst exhibited superior N2 selectivity (more than 98% at 100–200 °C) as compared to that of conventional Mn/TiO2 nanoparticles. The enhancement in N2 selectivity was consistently observed regardless of the amount of Mn active sites, demonstrating that the confining void environment is able to affect the site-specific selectivity of manganese oxides. When the reaction was performed at a low temperature (175 °C), it was found that the same reactive intermediate, possibly ammonium nitrate, was formed and deposited on both catalysts. However, the N2 selectivity in the reaction of this intermediate and NO was greatly improved in small-pore environments. In addition, it was demonstrated that such reactive intermediates are effectively stabilized when confined in small pores, thereby blocking the reaction pathway in which the intermediates directly decompose into N2O. This approach to confining active sites within the pores of support materials provides a rational strategy for designing highly selective catalytic materials.

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KN0022

Cyclic unsteady-state reactions on catalyst surfaces for CO_2 utilization, exhaust purification, and mechanistic studies

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Abstract Category: Invited Lecture - Keynote Lecture

Keywords: unsteady-state reactions, heterogeneous catalysis, CO_2 utilization, exhaust purification, reaction mechanism

Abstract Body.

CO2 capture and reduction with H2 (CCR) has been studied for utilization of CO2 from combustion exhaust gas. In this study, the CCR system and a membrane direct air capture (DAC) were combined to demonstrate direct air capture and utilization (DAC-U) for continuous production of CH4 or CO from the air. Screening tests for model CCR system showed that Ni nanoparticle (NP) on Ca-loaded Al2O3 (Ni-Ca/Al2O3) was the best catalyst for methanation. Pt NPs on Na-loaded Al2O3 (Pt-Na/Al2O3) was the best catalyst for CO formation. In the DAC-U system, a membrane DAC module was connected to a vacuum pump, and the outlet of the pump was connected to the CCR system, to which H2 and CO2/air mixture (from the DAC) were periodically fed. The DAC-U system successfully was utilized for continuous CCR to produce CH4 or CO from the air for a few thousand cycles of CCR operation. Similar sorption/reduction systems was developed for CH4 production from combustion exhaust model gas (10% CO2/10% O2 mixture). By adjusting catalyst and adsorption systems, NH3 production from 0.1% NO/10% O2 mixture as well as 100% reduction of N2O under 10% O2 was also demonstrated.

In the latter half of the lecture, operando modulation excitation spectroscopic studies (under cyclic unsteady-state conditions) are shown to clarify catalytic mechanism for some catalytic systems. As an example, NH3−SCR mechanism over sulfate-loaded ceria (S/CeO2) was studied using operando IR, UV−vis, and XANES. Combination of operando spectroscopy with modulation excitation method is shown to be powerful methodology to identify active species.

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CET9697

Effect of Enhanced Support Surface Area of Red Mud-Derived Al2O3 on Catalytic CO2 Methanation over Ni Catalysts

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: CO2 methanation, Red-mud-derived alumina, Mesoporous alumina

Abstract Body.

Introduction. Bayer-process alumina refining produces vast amounts of highly alkaline red mud, mostly stored despite improved practices like dry stacking, leaving persistent environmental and safety risks. Meanwhile, CO2 emissions from fossil fuels spur interest in carbon-neutral energy routes such as CO2 methanation (Sabatier reaction), which converts CO2 and H2 to grid-compatible CH4 but requires efficient low-temperature catalysts. Ni-based catalysts are cost-effective and active, yet their performance strongly depends on the support, particularly Al2O3, which influences CO2 adsorption, Ni dispersion, and stability. This study valorizes red mud by extracting alumina to form high-surface-area γ-Al2O3 supports and benchmarks Ni/γ-Al2O3(r) against commercial Ni/γ-Al2O3(c), linking structure to methanation activity (250 – 450 °C).

Methods. Red mud from a Korean supplier (XRF: Fe-rich, ~20 wt% Al2O3) was processed to obtain high-purity alumina for CO2 methanation catalysts. Ca was first removed by leaching in 0.2 M HCl (75 °C, 2 h), followed by 3 M HCl leaching (75 °C, 2 h) to dissolve impurities and enrich Fe/Al. The filtrate was precipitated with NH4OH to pH 9, then treated with NaOH to pH 14 to dissolve Al as NaAlO2, enabling separation from Fe/Ti/Ca; Al(OH)3 was re-precipitated (pH 9), washed, dried, and calcined to yield ~98.6 wt% Al2O3. CO2 methanation was tested in a 1 atm fixed-bed reactor after H2 reduction.

Results and discussion. Catalyst characterization shows that red-mud–derived alumina (Al(r)) possesses a much higher surface area and mesoporosity than commercial alumina (Al(c)) (SBET 287.5 vs 120.7 m2g-1; pore volume 0.71 vs 0.20 cm3g-1), and both decrease after Ni impregnation. XRD indicates Al(c) is more crystalline, whereas Al(r) exhibits broader γ-Al2O3-like features; metallic Ni reflections appear for Ni/Al(r) but not Ni/Al(c) after 550 °C reduction, consistent with H2-TPR showing easier NiO reduction on Al(r) (~550 – 600 °C) than on Al(c) (~700 °C). NH3-TPD suggests similar total Lewis acidity for both supports, implying acidity is not the main performance driver. TEM and STEM-EDS reveal Al(r) is composed of loosely agglomerated nanoscale crystallites that promote uniform, fine Ni dispersion, while Al(c) favors more heterogeneous Ni distribution. In activity tests, 10 wt% Ni/Al(c) outperforms 10 wt% Ni/Al(r) across 250 – 450 °C and at high GHSV, likely due to transport advantages and larger Ni ensembles. However, at low Ni loading (2 wt%), Al(r) becomes superior, especially

at low temperature, highlighting dispersion-controlled kinetics.

Acknowledgments

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Poster Presentation

Reaction Mechanism and Kinetics

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

MKF0101

Sorption-Enhanced Methanol Synthesis: Reaction and Adsorption Modeling

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Fundamental

Keywords: Methanol synthesis, Adsorption modelling, Process kinetics

Abstract Body.

Introduction

Rising atmospheric CO_2 continues to drive climate change, making its conversion into valuable chemicals increasingly important. Methanol synthesis from CO_2 and H_2 over $Cu/ZnO/Al_2O_3$ catalysts offers a promising route for carbon utilization and supports the transition to sustainable chemical manufacturing. Methanol not only serves as a versatile C_1 building block but also represents a potential precursor for sustainable aviation fuels via methanol-to-jet pathways. The reaction, $CO2+3H2 \leftrightharpoons CH3OH+H2O, \Delta\square 298=-49.5$ kJ mol−1, is exothermic and equilibrium-limited at elevated temperatures, selective removal of water can shift the equilibrium toward higher methanol yields. Sorption-enhanced methanol synthesis (SEMS) exploits this effect by incorporating water-selective sorbents. Accurate modeling of sorption and reaction behavior is therefore crucial for designing and optimizing SEMS processes.1,2

Methodology and Approach

To generate reliable simulations, reaction kinetics are developed based on lab-scale experiments conducted in a tubular fixed-bed reactor. Baseline tests without sorbent evaluated the intrinsic performance of the $Cu/ZnO/Al_2O_3$ catalyst under standard methanol synthesis conditions (250 °C, 40 bar, H_2/CO_2 = 3, WHSV = 15,000 mL g^{-1} h^{-1}). SEMS experiments employed catalyst–sorbent mixtures prepared by dry blending CZA with molecular sieves 3A or 4A at a mass ratio of 1:8. Initial kinetic modeling applied established literature models for classical methanol synthesis to develop a one-dimensional reactor model for comparing conventional and sorption-enhanced performance. MATLAB was used to fit kinetic parameters to experimental data.

Outlook

Preliminary validation indicates that CO conversion cannot be neglected in methanol formation, suggesting a possible contribution from the reverse water–gas shift reaction. This finding requires further investigation to clarify the extent of an indirect CO pathway. The validated classical model provides a foundation for extending the SEMS model. Future work will expand the current one-dimensional framework to a two-dimensional reactor model capable of representing temporal effects such as sorbent saturation. This development will enable improved simulation of dynamic behavior and support designing efficient sorption-enhanced methanol systems.

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MKF0147

Temperature effect on oxidation and coking kinetics of aviation oils using thermal analyses

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[2] *Simulation and Experimental Analysis, IFPEN, France*
[3] *Kinetics, Thermodynamics and Energy, Universite de Lorraine - CNRS, LRGP, France*

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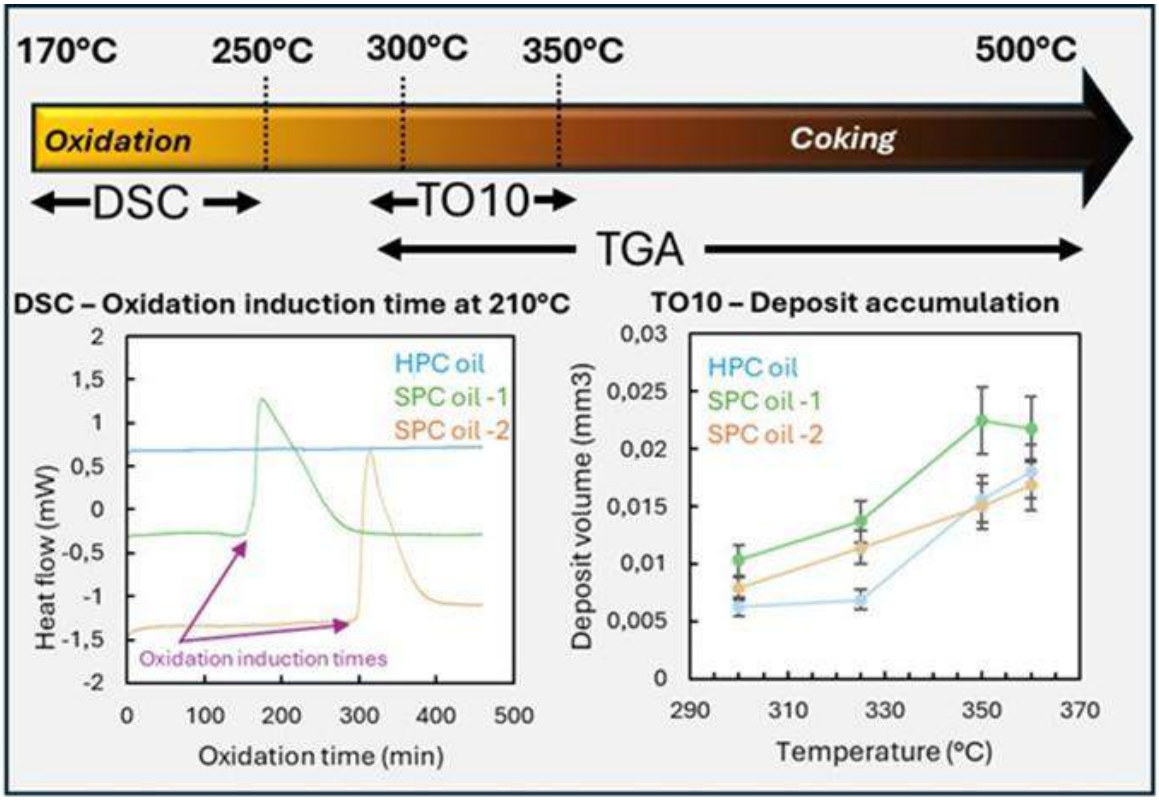
Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Fundamental

Keywords: coking, lubricants, deposits, kinetic, thermal analyses

Abstract Body.
Aviation lubricants are exposed to high temperatures and oxidative atmospheres within aircraft engines. This contributes to oil degradation through different mechanisms: oxidation and coking. Understanding these regimes is essential for predicting lubricant behavior across different formulations. This study investigates thermal analysis methods for evaluating degradation kinetics of three aviation oils: one High Performance Capability (HPC) oil and two Standard Performance Capability (SPC) oils. A protocol was developed to determine the oxidation induction time using Differential Scanning Calorimetry (DSC) between 190°C and 250°C. The TO10 device (AD Systems), generally used to assess the thermal stability of jet fuels according to ASTM D3241, was also used to evaluate the kinetic of deposit formation of the three aviation oils between 300°C to 350°C. Results from TO10 tests were compared with those obtained from thermogravimetric analysis (TGA) in the same temperature range. Further TGA measurements were performed at higher temperatures to evaluate the propensity of the oils to form deposits as a function of temperature. DSC measurements confirmed the superior thermal stability of the HPC oil, which oxidizes at higher temperatures than the SPC oils. The HPC oil did not undergo oxidation below 230°C for up to 900 minutes, whereas the SPC oils exhibited oxidation at lower temperatures (<210°C). Both TO10 and TGA measurements showed the same stability ranking between 300°C and 350°C: at 300°C, both SPC oils produced more deposits than the HPC oil and at 350°C, one SPC oil produced more deposits than the two other oils. The use of complementary techniques (DSC, TGA, TO10) enables the quantification of the temperature's impact on the kinetics of oxidation and coking. Additionally, the TO10 method provides valuable comparisons of deposit formation kinetics across different oil formulations. These experimental results and testing protocols contribute to identifying critical operating conditions of existing lubricants and could be used for testing future formulations.


170°C
250°C
300°C
350°C
500°C
Oxidation
Coking
DSC
TO10
TGA
DSC – Oxidation induction time at 210°C
Heat flow (mW)
Oxidation induction times
Oxidation time (min)
HPC oil
SPC oil -1
SPC oil -2
TO10 – Deposit accumulation
Deposit volume (mm3)
Temperature (°C)

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2026 / SEOUL, KOREA

MKF0222

Kinetic Analysis of Polyethylene Terephthalate (PET) Upcycling to Xylene via Catalytic Hydrogenation and Hydrogenolysis

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Fundamental

Keywords: Polyethylene terephthalate (PET) upcycling, Catalytic hydrogenation and hydrogenolysis, Kinetic analysis

Abstract Body.

Purpose

The exponential accumulation of polyethylene terephthalate (PET) waste poses a critical environmental challenge, necessitating efficient recycling strategies beyond conventional methods. Catalytic upcycling of PET into value-added aromatic hydrocarbons offers a sustainable pathway to preserve carbon value. Specifically, xylene serves as a pivotal petrochemical feedstock for polymer synthesis. This study aims to elucidate the intrinsic kinetic parameters governing the catalytic hydrogenation of PET to xylene. The primary objective is to establish a foundational kinetic model to facilitate the design and scale-up of a continuous stirred-tank reactor (CSTR) for industrial application.

Method

The conversion of PET to xylene was investigated under controlled batch conditions to deduce reaction kinetics. The process involves the depolymerization of PET into terephthalic acid (TPA), followed by hydrogenation and hydrodeoxygenation to produce xylene. Experiments were conducted at temperatures of 270, 280, and 290 °C and hydrogen pressures of 30, 50, and 70 bar. To evaluate the impact of catalyst loading, PET-to-catalyst mass ratios were varied at 2.5:1 and 5:1. A power-law rate model was applied to the temporal concentration profiles of reactants and products, utilizing a lumped kinetic approach to simplify the complex reaction network.

Results

Preliminary experiments demonstrate consistently high selectivity toward aromatic products, with xylene selectivity exceeding 90% across a wide range of reaction conditions. Time-resolved product analysis indicates a sequential reaction network in which PET-derived intermediates are converted to BTX aromatics, followed by secondary hydrogenation to saturated cyclic hydrocarbons, including dimethylcyclohexane (DCH), methylcyclohexane (MCH), and cyclohexane (CH). To quantitatively describe this behavior, systematic experiments are being performed by varying reaction time, temperature, and pressure. Batch reactor data are used to extract apparent kinetic parameters based on power-law rate expressions, allowing estimation of reaction orders, rate constants, and activation energies. These results provide a mechanistic basis for distinguishing primary aromatic formation from

subsequent hydrogenation pathways.

Conclusions

This study aims to establish a kinetic framework for the catalytic upcycling of PET to BTX, with an emphasis on xylene production. Kinetic parameters derived from batch experiments form the basis for developing a validated reaction rate expression. This model is being implemented in a continuously operated CSTR to evaluate its predictive capability under steady-state conditions. By linking batch-derived kinetics with continuous reactor operation, this work supports rational reactor design and scale-up for PET valorization and advances the industrial relevance of PET-to-BTX conversion processes.

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MKF0226

Separate storage of electrons and protons at Ru and BaO through low-work-function carbons for ammonia synthesis under mild conditions

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Fundamental

Keywords: Ammonia synthesis, Ru catalyst, BaO promoter, Low-work-function carbon

Abstract Body.
There is a strong demand for developing catalysts to enable ammonia synthesis under mild conditions. We demonstrate that Ru catalysts supported on low-work-function carbon, along with a BaO promoter, exhibit unprecedented catalytic activity. Rigorous analysis of 22 carbon-supported catalysts commonly revealed that H atoms generated by H2 activation on Ru dissociate into H+/e– pairs. Subsequently, H+ migrates over the carbon surfaces to titrate basic BaO, while e– accumulates in conductive Ru/carbon bodies. With the decreasing work function of the carbon support, Ru gradually becomes enriched with e–, facilitating N2 activation via π-backdonation and alleviating H2 poisoning. The best catalyst synthesized using low-work-function N-doped multiwalled carbon nanotubes exhibited 5.8 times higher activity than Ba-Ru/MgO at 573 K and 10 bar, a benchmark catalyst.

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2026 / SEOUL, KOREA

MKF0243

Hydrodynamics meets kinetics: Copper sorption kinetics onto zeolite NaX in straight blade turbine stirred tanks

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Fundamental

Keywords: kinetics, sorption, copper, zeolite NaX, SBT impeller, CFD

Abstract Body.
Introduction.
Copper ion sorption kinetics were investigated using NaX zeolite, focusing on the influence of straight-blade turbine (SBT) impeller geometry, off-bottom clearance, and baffle presence on the sorption rate. The study addresses a gap in understanding how impeller and tank design affect sorption kinetics in solid–liquid systems. Although SBT impellers are common in stirred tanks, their effect on kinetics in these systems remains insufficiently understood. This work aims to clarify how impeller and tank configuration influence mass transfer, particle suspension, and sorption performance, providing guidance for laboratory-scale multi-phase reactors.
Methods.
Experiments were performed in baffled and unbaffled stirred tanks equipped with SBT impellers, investigating a range of impeller-to-tank diameter ratios (D/dT = 0.32–0.68) and off-bottom clearances (C/H = 0.10–0.50). Tanks were operated at just-suspended conditions (NJS) to ensure complete particle suspension. Key measurements included NJS determination, copper sorption kinetics, and power consumption per unit mass of NaX zeolite (PJS). Sorption rates were analysed using the Ritchie model and the Mixed surface reaction and diffusion controlled adsorption model. Complementary computational fluid dynamics (CFD) simulations provided insights into flow patterns and mixing velocity distribution within the tank.
Results and discussion. Impeller geometry, off-bottom clearance, and baffle presence affected NJS and flow patterns, which consequently affected power demands and sorption rate constants (surface reaction was identified as the rate-limiting step). NJS decreased with increasing D/dT and generally increased with C/H across all impeller sizes. Baffled reactors consistently required higher NJS than unbaffled ones, with power consumption per unit zeolite mass being 2–30 times higher in baffled tanks. At C/H = 0.10 the rate constant was generally higher in unbaffled reactor, while at C/H = 0.33 it was higher in baffled reactor. In all cases the differences in PJS between baffled and unbaffled reactors increased with D/dT. However, this trend for C/H = 0.50 was reversed. The highest sorption rate constant and power consumption were observed in the baffled reactor with C/H = 0.50 and the smallest impeller (D/dT = 0.32). CFD simulations revealed how impeller geometry and tank configuration shape fluid flow, with implications for mixing efficiency.
Conclusions
By combining experimental and computational approaches, this study demonstrates how reactor design can be optimised to achieve energy-efficient sorption processes, providing practical guidance for laboratory-scale stirred-tank operation and supporting energy-

conscious, low-impact chemical processing.

Acknowledgments
This research was funded by the project ANTARES (IP-UNIST-28) granted by the European Union-“NextGenerationEU”.)

ISCRE29 & APCRE11
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MKF0252

Mechanisms of charge transport dynamics in barium cerate-zirconate proton-conducting electrolytes

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Fundamental

Keywords: perovskite electrolytes; proton-conducting solid oxide cells; Cerate-ziconate-based electrolyte; ionic conductivity; proton transport; impedance spectroscopy.

Abstract Body.

Recent advances in proton-conducting oxides have made them appealing as electrolytes for protonic ceramic fuel and electrolysis cells (PCFCs/PCECs), hydrogen sensors, membranes for hydrogen, steam and syngas purification, and for ammonia synthesis. The low mass and high mobility of protons allow the fabrication of intermediate-temperature PCFCs/PCECs operating at 700-400 °C, compared to SOFCs which usually operate at temperatures above 700°C [1]. Perovskite materials of Ba(Ce,Zr)O3-□ family are excellent candidates as electrolyte materials in PCFCs/PCECs since they show high proton conductivity, low Ea to proton transport and good chemical stability.

In-house Ba1.1Ce0.6Zr0.2Y0.2O3-δ (BCZY) electrolytes were optimized in terms of morphology, density and crystallinity and tested under different environments to study the conduction behavior. Impedance Spectroscopy measurements (EIS) were performed in the range of 400-800 °C in dry air and dry/wet reducing environments with 5% H2 (Fig. 1a). Proton-conducting oxides, as BCZY, are mainly protonic ionic conductors in wet atmospheres, they show partial conduction by electrons in reducing atmospheres and by holes in oxidizing atmospheres. In operating fuel cells conditions (700-400°C in wet 5% H2), BCZY reached a conductivity of 0.73·10-2 S/cm at 600 °C. [3]

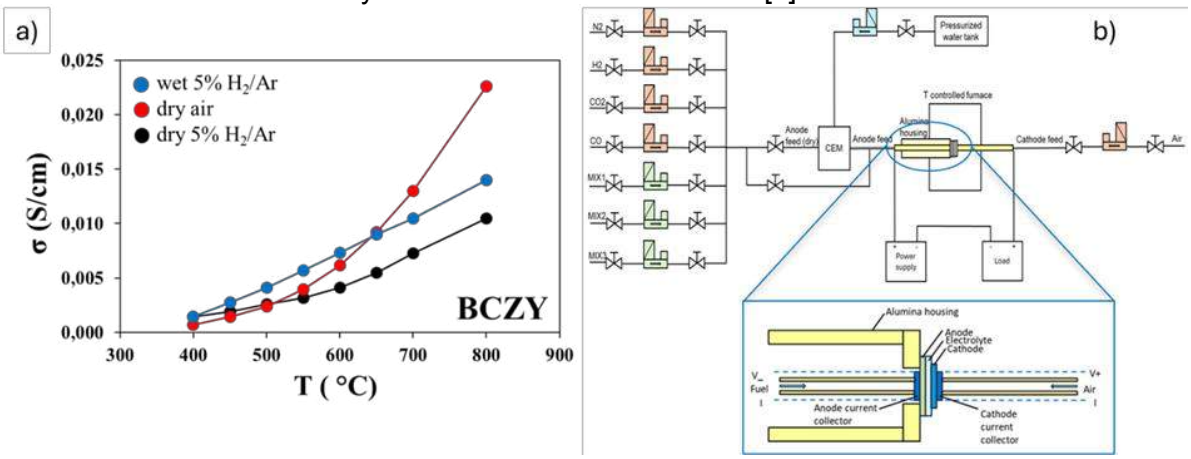

Fig.1: a) BCZY conductivities; b) Schematic of the button cell test-rig.

To gain better insight on charge transfer dynamics and proton conduction properties of Ba(Ce,Zr)O3-□ perovskites, in this work, a parametric investigation has been performed on ceramic electrolytes made of commercially available BaCe1-x-yZrxMyO3-□ either single doped or co-doped (i.e. Y3+, Yb3+). A button cell test rig (Fig. 1-b) was employed to evaluate the dependencies of the electrochemical processes with the variation of operating conditions, such as temperature, hydrogen and oxygen partial pressures and humidity content in the fuel mixture. The variations of both internal and polarization resistances in response to the variation of one single operating parameter at time were recorded by EIS. The Distribution of Relaxation Times (DRT) algorithm was then applied to shed light on each single process and its dependencies to the imposed variations.

Acknowledgments
This research was funded by the European Union - NextGenerationEU from the Italian Ministry of Environment and Energy Security, POR H2 AdP MEES/ENEA with involvement of CNR and RSE, PNRR - Mission 2, Component 2, Investment 3.5 "Ricerca e sviluppo sull'idrogeno", CUP: I83C22001170006

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MKF0285

Mechanism study of NH3 decomposition reaction with an electric field

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Fundamental

Keywords: NH3 decomposition reaction, Electric field, Mechanism

Abstract Body.

Introduction. Hydrogen is a promising carbon-free energy carrier with high gravimetric density, yet its large-scale adoption is hindered by low volumetric density and safety concerns [1]. NH3 has emerged as a viable chemical carrier due to its high hydrogen capacity (108 kgH2/m3NH3, 17.6 wt%) and established distribution infrastructure [2]. However, the efficient recovery of H2 is limited by the endothermic nature and sluggish kinetics of NH3 decomposition, necessitating high temperatures (>500 oC) [3]. While electric fields can enhance performance via joule heating and surface protonics [4], the precise underlying mechanisms remain poorly understood. This study investigates NH3 decomposition over Ni-exsolved ceria catalysts under an electric field, demonstrating that intentional oxygen vacancy formation critically facilitates surface protonic conduction and the N2 desorption step.

Methods. The catalysts were synthesized by the modified Pechini method. The amount of metal loading was fixed at 5 mol%. Precursors of metals used were nitrate for Ce and Ni. For the comparison, the other catalyst synthesized by the incipient wetness impregnation method, using same Ni precursors with an exsolved catalyst and a commercial CeO2 support.

Results and discussion. Fig. 1 illustrates the reaction mechanism modified by an electric field. A current donates electrons to the catalysts, induces surface protonics making H migrates. An ammonia molecule could be bonded with intermediates such as NxHy, then decomposed to the N2 and H2.

Acknowledgments

This work was supported by the Korea Institute of Energy Technology Evaluation and Planning (KETEP) and the Ministry of Trade, Industry & Energy (MOTIE) of the Republic of Korea (RS-2024-00469587). This work was also supported by the National Research Foundation of Korea (NRF) funded by the Ministry of Science and ICT (MSIT) (RS-2023-00261851).

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MKF0296

Trickle bed reactor studies of alkaline-aqueous phase glycerol oxidation over Pd-based catalyst

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Waste Valorization

Keywords: Pulse tracer experiments, Selectivity, Kinetic modeling, Hydrodynamics

Abstract Body.
Introduction: Glycerol oxidation, as a method for valorising glycerol, is important for the economy of the biodiesel industry. Recent kinetic studies by our group have shown that Pd-catalyzed alkaline-phase glycerol oxidation, when carried out in a mass transfer-controlled regime, yields better carbon conversion efficiency compared to a kinetically controlled regime. [1] In view of these results, we propose a trickle bed reactor for glycerol oxidation, and provide a proof-of-concept through extensive hydrodynamic and kinetic studies in such a reactor, in this study.

Methods: Factors such as dynamic/static liquid hold-ups, as well as mean residence times through pulse tracer experiments, were evaluated under the conditions of reaction to gain insights into the hydrodynamic behavior of TBR. A two-parameter PDE model has been proposed to explain the RTD profiles. Reaction studies on glycerol oxidation were performed over Pd/Activated carbon pellets, and the performance was compared with earlier results obtained under identical temperature and pressure conditions [2].

Results: The highlights of the results are summarized as follows.

1. C3 yields (Glyceric acid + Tartronic acid) increased to more than 60% compared to the batch reactor case, where C3 yields were less than 50%.
2. The selectivity to formic acid for TBR was very low compared to the batch reactor results obtained under the kinetic regime. Moreover, C1 selectivity decreased with increasing catalyst loading and bed length in TBR, confirming earlier conclusions [1].
3. The two-parameter PDE model was able to explain the RTD profiles reasonably well, as evident from comparisons of first, second, and third moments around the mean.

Conclusions: These results therefore show that reactors operated under industrially relevant, mass transport-limited conditions may be exploited to favor the selectivity to C3 compounds in the case of heterogeneously catalyzed glycerol oxidation while avoiding over-oxidation and C-C scission reactions.

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MKF0305

The Kinetics and Synergistic Mechanism of Co-Mn-Br Catalyzed Liquid-Phase Oxidation of 2,6-Dimethylnaphthalene to 2,6-Naphthalenedicarboxylic Acid

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Fundamental

Keywords: Kinetic model; catalytic oxidation; Effective collision theory; 2,6-Dimethylnaphthalene; 2,6-Naphthalene dicarboxylic acid

Abstract Body.

Introduction.

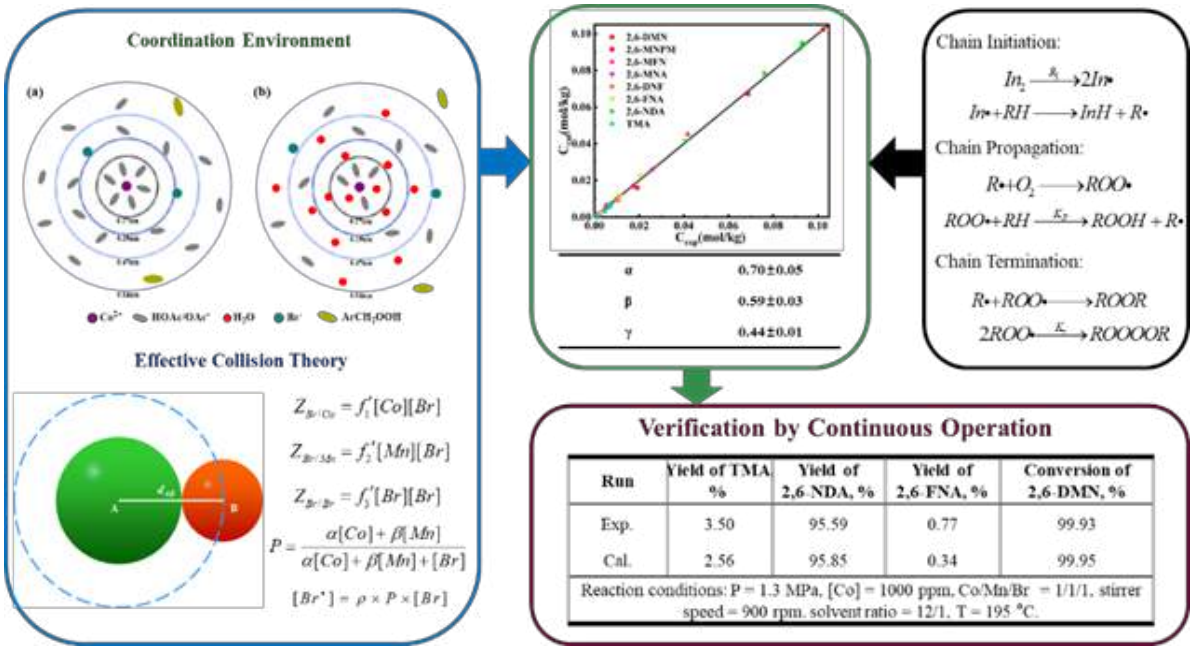
The extended π-conjugation of naphthalene imparts Polyethylene Naphthalate (PEN) with superior properties compared to Polyethylene Terephthalate (PET), enabling its application in advanced materials. Despite the industrial significance of 2,6-naphthalenedicarboxylic acid (2,6-NDA) synthesis via liquid-phase oxidation of 2,6-dimethylnaphthalene (2,6-DMN), the kinetic influence of Co/Mn/Br catalyst stoichiometry remains insufficiently quantified. This study employs effective collision theory to mechanistically elucidate the synergistic interactions governing catalytic performance, providing a fundamental framework for rational catalyst design in aromatics oxidation.

Methods.

2,6-NDA was synthesized through the liquid-phase catalytic oxidation of 2,6-DMN employing a ternary Co-Mn-Br catalyst. A comprehensive investigation into the coordination environment and dynamic evolution of the active catalytic species during oxidation enabled the formulation of an effective collision model. Based on the elucidated mechanism, a corresponding kinetic model was constructed and its parameters were optimized using lsqnonlin in MATLAB. The parameterized model was subsequently extrapolated, and its predictive validity was experimentally verified using a continuous- flow oxidation reactor.

Results and discussion.

Based on the catalyst coordination environment in acetic acid, parameters α and β were introduced to characterize the relative collision frequencies among Co/Br and Mn/Br and ρ to correct the effective concentration of Br·. The model quantitatively describes the effect of catalyst concentration on the reaction. Model parameters were obtained by fitting experimental data at different catalyst concentrations. Validation in a continuous oxidation reactor confirmed the model's predictive accuracy, guiding the industrial production of 2,6-NDA.



Verification by Continuous Operation

Run	Yield of TMA, %	Yield of 2,6-NDA, %	Yield of 2,6-FNA, %	Conversion of 2,6-DMN, %
Exp.	3.50	95.59	0.77	99.93
Cal.	2.56	95.85	0.34	99.95

Reaction conditions: P = 1.3 MPa, [Co] = 1000 ppm, Co/Mn/Br = 1/1/1, stirrer speed = 900 rpm, solvent ratio = 12/1, T = 195 °C.

Effective collision–based kinetic modeling of the Co-Mn-Br catalytic oxidation of 2,6-DMN

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MKF0353

Operando DRIFTS Insight into Methanol Activation and Hydrocarbon Pool Initiation on Zeolites

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Fundamental

Keywords: methanol-to-hydrocarbons, operando DRIFTS, carbenium ions, surface methoxy species, autocatalysis.

Abstract Body.

Introduction. The methanol-to-hydrocarbons (MTH) process over zeolites is still mechanistically debated, particularly regarding the first C–C bond formation and the nature of active hydrocarbon pool species1. Recent operando studies show that surface methoxy species (SMS) initiate C–C coupling, while alkenyl and aromatic intermediates sustain the autocatalytic cycle. Understanding these steps is essential for guiding catalyst design and improving product selectivity2.

Methods. Operando DRIFTS coupled with online mass spectrometry was used to monitor catalyst surface species and gas-phase products. Powdered zeolites were loaded into a Bruker Invenio S DRIFTS cell (ZnSe window, LN_2 -cooled MCT detector), pretreated at 380 °C under inert flow for 2 h, and cooled to the test temperature. Spectra were collected at 2 cm^{-1} resolution by averaging 32 scans, while changing temperature and gas composition, allowing real-time tracking of intermediates and products across different zeolite structures.

Results and discussion. Figure 1 shows that, upon methanol introduction into the DRIFTS cell, the Brønsted acid band at 3612 cm^{-1} and the silanol signal at ~3740 cm^{-1} disappeared immediately, accompanied by the formation of surface methoxy species (SMS), evidenced by the υ(C–O) band at 938 cm^{-1}. At 200 °C, changes in the υ(CH_3) stretching region (2840–3010 cm^{-1}) indicated the formation of dimethyl ether (DME), confirmed by MS as the main gas-phase product. Upon heating to 300 °C, new IR bands at 1610, 1515, and 1470 cm^{-1} appeared, marking the formation of hydrocarbon pool species. The 1610 cm^{-1} band is assigned to polymethylbenzenium ions, while the 1515 and 1470 cm^{-1} bands correspond to alkyl-substituted cyclopentenyl cations. MS detection of propane confirms hydrocarbon formation. Time-on-stream DRIFTs experiments show that SMS are transient species, formed at early reaction stages and progressively consumed as carbenium ions develop, which then take over their role and sustain the autocatalytic cycle3.

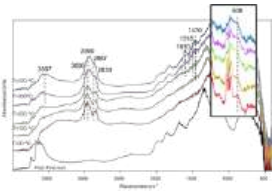

Figure 1: Operando DRIFTS spectra of methanol conversion on SSZ-13 from 30 °C to 370 °C. PCH3OH = 0,13 bar; flow = 50 ml/min; zeolite loading = 10−20 mg.

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MKF0495

Towards kinetic modelling of hydrodechlorination of model chlorinated compounds in diesel under hydroprocessing conditions

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Fundamental

Keywords: plastic pyrolysis oil, chemical recycling, hydrodechlorination, hydro processing, kinetic model

Abstract Body.
Plastic pyrolysis oil (PyOil) is a promising feedstock to produce high-value chemicals; however, its high chlorine content poses significant challenges for downstream upgrading, such as deactivation of catalysts and corrosion. Catalytic hydrodechlorination (HDC) has therefore emerged as a highly effective strategy for chlorine removal. In this context, this study aims (i) to elucidate the influence of operating conditions on the HDC process and (ii) to develop a comprehensive kinetic model, based on experimental data obtained during the HDC of a model PyOil.

The hydrodechlorination of 1-chlorohexane, selected as a representative chlorinated species, was investigated under hydrogen pressure using a commercial sulfided NiMo/γ-Al_2O_3 catalyst and hydrotreated diesel as solvent. Experiments were conducted in a fixed-bed reactor at an initial chlorine concentration of 250 ppm. Temperatures ranged from 120 to 210 °C, pressures from 1 to 3 MPa, and residence times from 15 to 60 min, at fixed H_2-to-liquid ratio of 80 NL.L-1.Total chlorine concentration was monitored by X-ray fluorescence spectroscopy, while reaction products and chlorine speciation were analyzed by gas chromatography (GC-FID and GC-ICP-MS/MS).

Negligible conversion was observed at 120 °C, whereas increasing the temperature from 150 to 210 °C enhanced HDC yields at all residence times. Hexane was the main reaction product, followed by 2-hexene and 3-hexene, consistent with thermodynamic predictions. Higher temperature and pressure favored selectivity toward hexane. Increasing pressure also promoted the recombination of HCl with olefins to form 2- and 3-chlorohexane. A preliminary kinetic model assuming pseudo-first-order behaviour with respect to 1-chlorohexane was thus developed, to describe experimental data. The estimated apparent activation energy and pre-exponential factor were 52 kJ.mol-1 and 600 s-1 and respectively, showing good agreement between model predictions and experimental data. Complementary batch experiments are currently being conducted to investigate intrinsic HDC kinetics while minimizing mass-transfer limitations (using catalyst with 300- 600 µm particles) and deactivation phenomena. Exploratory tests reveal a strong influence of chlorine concentration on the HDC of 1-chlorohexane. At initial concentrations of 500 and 1000 ppm, apparent inhibition effects were observed, as conversion remained nearly

constant with reaction time. Further experiments aim to investigate the simultaneous HDC of different chlorinated compounds (aliphatic, aromatic and oxygenated) to better approach real PyOil systems.

The final objective, in understanding the observed inhibition, is to develop a Langmuir-Hinshelwood kinetic model incorporating competitive adsorption between chlorides and HCl, parallel reactions, and inhibition phenomena. The resulting model is intended to predict outcomes under realistic PyOil upgrading conditions.

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MKF0512

Kinetics of Hydrochloric Acid Recovery from HCl-Saturated Potassium Chloride Solutions Using Tris(2 ethylhexyl)amine

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Fundamental

Keywords: Hydrochloric acid; TEHA; Extraction kinetics; Mass transfer; Diffusion control; Potassium chloride

Abstract Body.
Introduction. Potassium nitrate production generates HCl byproducts, requiring efficient recovery to prevent resource loss. This study investigates the extraction equilibrium and kinetics of HCl using tris(2-ethylhexyl)amine (TEHA) in a constant interfacial cell. The goal is to determine the rate-controlling step and develop a mathematical model for industrial design. Methods. A Lewis cell ensured a stable liquid-liquid interface. The aqueous phase contained 2.3 mol/L HCl and 1.8 mol/L KCl; the organic phase was TEHA in sulfonated kerosene. Experiments varied stirring speeds (250-450 rpm), temperature (288.15-328.15 K), and concentrations. HCl was analyzed by acid-base titration. Results and discussion. HCl extraction increased with TEHA concentration but was independent of temperature and KCl. IR spectroscopy confirmed an ion-pair complex mechanism. The extraction rate increased with stirring speed (>350 rpm) and was proportional to the interfacial area, suggesting a diffusion-controlled process. The apparent activation energy (Ea) of 18.76 kJ/mol confirms diffusion control, specifically within the organic phase boundary layer. Based on bilayer membrane theory, the derived rate equation is: r0 = k [HCl]0.3 [TEHA]1.8. The proposed model fits the experimental data well, providing mass transfer coefficients and apparent rate constants. This systematic analysis offers theoretical support for optimizing HCl recovery from high-salinity brines.

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MKF0520

CO2 Methanation over a Ni–Mg–Al2O3 Dual-Functional Material: Reaction Mechanism and Kinetics

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Fundamental

Keywords: CO2 methanation; dual-functional material; kinetic modeling

Abstract Body.
Introduction. Integrated carbon capture and utilization (ICCU) is a promising route to mitigate CO2 emissions from gas-fired power plants operating during periods of low renewable electricity availability. Captured CO2 can subsequently be converted to methane using green hydrogen once sufficient renewable electricity is available. Practical implementation benefits from dual-functional materials (DFMs) that integrate CO2 adsorption capacity and catalytic methanation activity within the CO2 desorption temperature window. Accordingly, a novel Ni–Mg–Al2O3 DFM is investigated, where MgO provides high CO2 uptake in the 250–400 °C range and Ni offers cost-effective, selective hydrogenation activity. This work focuses on the kinetic modeling of CO2 methanation under ICCU-relevant conditions.
Methods. Intrinsic kinetics were measured in a micro-packed bed reactor by systematically varying temperature, space time, and inlet partial pressures of reactants and products under kinetically controlled conditions, i.e., far from thermodynamic equilibrium. Candidate rate expressions were evaluated via parameter estimation and kinetic model discrimination using physicochemical and statistical assessments. The retained model was used to benchmark catalyst activity against a conventional methanation catalyst.
Results and discussion. CO2 conversion (XCO2) increased with temperature, space time, and inlet partial pressures of CO2 and H2. CH4 co-feeding had a negligible effect, whereas H2O co-feeding significantly decreased XCO2 (Figure 1a) due to competitive adsorption and a thermodynamic shift of the reverse water–gas shift (RWGS) reaction toward CO2, limiting CO formation. XCO2 increased with temperature and H2/CO2 ratio, while CH4 selectivity (SCH4) increased with H2/CO2 ratio but decreased with temperature (Figure 1b). These trends reflect enhanced hydrogenation at higher H2 availability and an increased contribution of the RWGS reaction at elevated temperatures due to its endothermic nature, as well as the exothermic nature of the overall CO2 methanation reaction. The CO detection confirms the formation of adsorbed CO or carbonyl intermediates during CO2 hydrogenation1. Ongoing work focuses on LHHW-type mechanistic modeling, parameter estimation, and kinetic model discrimination for CO2 methanation over Ni–Mg–Al2O3.

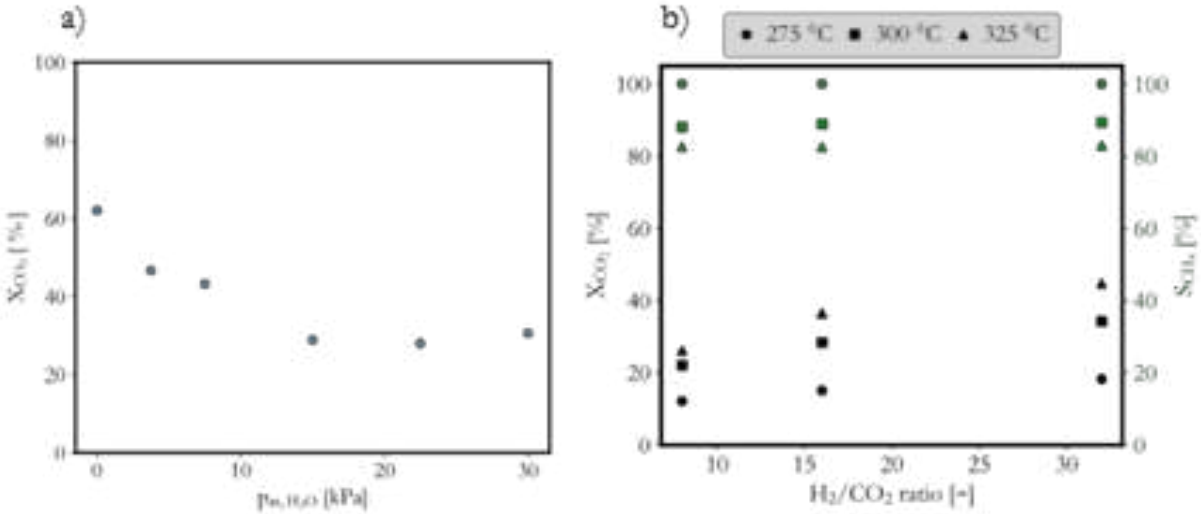

Figure 1: (a) XCO2 vs inlet H2O partial pressure; (b) SCH4 and XCO2 vs inlet H2/CO2-ratio and temperature.

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2026 / SEOUL, KOREA

MKF0544

On the contribution of bio-components to the global kinetics and speciation of lignocellulosic biomass pyrolysis: the case study of rice husk

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Fundamental

Keywords: biomass pyrolysis, reaction kinetics, lumped kinetic model, additive approach

Abstract Body.
Introduction. Understanding biomass pyrolysis kinetics is essential for the optimization of thermochemical conversion processes. In this context, lumped kinetic models are key engineering tools for reactor design and can be used to describe the pyrolysis of complex lignocellulosic feedstocks through an additive approach, where the overall behavior is reconstructed as the sum of the kinetics of the single biomass constituents: cellulose, hemicellulose and lignin [1]. However, the validity limits of this assumption remain uncertain.
Methods. In this work, the adequacy of the additivity hypothesis is investigated using rice husk as a representative real biomass. Rice husk pyrolysis was studied by thermogravimetric analysis coupled with mass spectrometry (TG-MS), providing detailed information on devolatilization behavior and product speciation. Chemical fractionation was performed to quantify the biomass main constituents, and a refined lumped kinetic model [2] was used to simulate their individual and combined pyrolysis behaviors.
Results and discussion. First, the TG-MS data of the individual biomass constituents were additively combined according to their measured proportions in the rice husk sample. As shown in Figure 1A, the resulting mixture surrogatereproduces the experimental devolatilization profile with good accuracy. In parallel, simulations of rice husk pyrolysis were carried out using the refined lumped kinetic models. Comparison with TG-MS data shown in Figure 1B confirms that the model satisfactorily captures both the global devolatilization profile and the main trends in product speciation. These results provide strong evidence to support the robustness of lumped kinetic models and the validity of the additivity assumption for describing the pyrolysis of real lignocellulosic biomasses. Ongoing work is focused on extending this assessment to additional feedstocks and larger-scale conditions, including packed-bed and fluidized-bed reactors, to evaluate whether the additive lumped model retains its predictive capability under more complex environments.

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MKF0549

Supercritical Catalytic Cracking of n-dodecane for Cooling in Scramjet Engines.

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Fundamental

Keywords: Cracking, Supercritical fluids, Catalysts, Heat sink.

Abstract Body.

Introduction:

Modern aircraft reach supersonic and hypersonic flight regimes, employing scramjet engines (Mach number > 5) face severe thermal management challenges, as the temperature of the incoming air becomes too high to cool the aircraft effectively.

One promising approach is coupling endothermic cracking reactions to the exothermic reactions of fuel combustion, enhancing heat removal and reducing wall temperatures. However, fuel cracking may produce significant amounts of coke, leading to catalyst deactivation. Operating under supercritical conditions can mitigate these challenges by improving the solubilization of coke precursors and enhancing catalyst stability.

n-dodecane is commonly used as a model compound for jet fuels. Previous studies under supercritical conditions show low conversion with negligible coke formation at low temperatures, while higher temperatures and pressures increase conversion but also promote coking. The present work aims to develop a simplified model that incorporates both reaction kinetics and catalyst deactivation as functions of temperatures and pressures. The model development will be based on empirical results and will enable robust system design.

Methods:

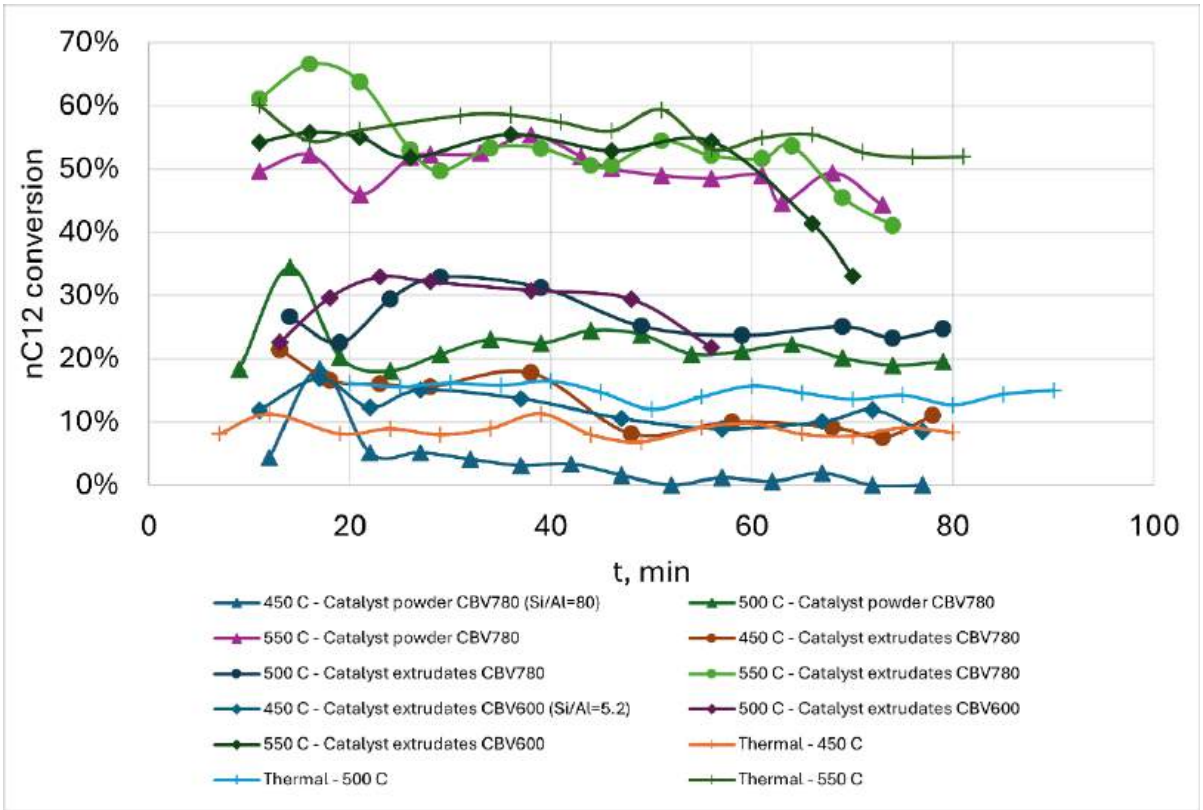
Catalytic cracking experiments were conducted using n-dodecane as a model compound in a lab-scale packed-bed reactor operating under supercritical conditions. The liquid reactant was pumped into the reactor, and the reaction products downstream were separated into gas and liquid products for quantitative analysis using GC-MS system. Thermal cracking experiments at 450, 500, and 550 0C and 25 bar were performed for comparison. Both powder and pellet forms of Y-zeolites were evaluated. A stabilization period was required due to the strong endothermicity of cracking reactions and the challenges of supercritical operation.

Results:

As shown in the figure, thermal cracking experiments exhibited relatively constant conversion over time, with average conversion increasing from approximately 10% at 450 0C to about 55% at 550 0C. All three Y-zeolite catalysts tested, differing in Si/Al ratio and morphology, displayed similar conversion trends, indicating a minimal influence of catalyst composition or form. At 450 0C and 500 0C, catalytic cracking significantly enhanced conversion relative to thermal cracking, reaching approximately 20% and 30%, respectively. In contrast, at 550 0C, catalytic and thermal cracking conversions became comparable (approximately 45-55%), which is attributed to significant coke formation leading to catalyst

deactivation.

Conclusions:
Supercritical cracking is a complex yet promising process with significant implications for thermal management. Catalytic cracking improves hydrocarbon conversion under supercritical conditions at moderate temperatures but is limited by catalyst deactivation at higher temperatures. Incorporating deactivation effects into simplified kinetic models is therefore essential for accurate prediction and system design.



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MKF662

Complex Network Approaches for Flow Regime Recognition in Gas-Solid Fluidized Beds

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Keywords: gas-solid fluidized bed; flow regime recognition; complex network; pressure fluctuation; machine learning; nonlinear dynamics

Introduction. Gas-solid fluidized beds are pivotal in chemical and energy processes, where flow regime transitions significantly influence operational efficiency. Traditional methods for analyzing pressure fluctuation signals—time-domain, frequency-domain, and state-space approaches—are often limited in capturing the nonlinear and nonstationary dynamics inherent in fluidization systems. Recent advances in complex network theory offer a novel paradigm for characterizing flow regimes and fluid dynamics by mapping time-series data into network structures, enabling the extraction of topological features that reflect underlying hydrodynamics.

Methods. This study presents three distinct complex network frameworks for flow regime analysis, including Flow Regime Complex Network (FRCN), Directed Weighted Complex Network (DWCN), and Horizontal Visibility Graph (HVG).

Results and discussion. FRCN achieved 98.2% accuracy in identifying single-bubble, exploding bubble, and transport regimes.[1,2] DWCN analysis revealed that key fluctuation modes dominate specific regimes. Network statistics (node strength, clustering, centrality) showed strong agreement with Kolmogorov entropy, confirming their utility as dynamics descriptors.[1,3] HVG metrics demonstrated high sensitivity to the bubbling-to-turbulent transition. When used as input features in machine learning models, HVG-based attributes enabled >95% accuracy in discriminating bubbling, transition, and turbulent regimes.[4] The integration of complex network theory provides a robust, multi-perspective framework for flow regime characterization in gas-solid fluidized beds. Each network construction method - FRCN, DWCN, and HVG - offers unique insights into flow dynamics, from regime identification to nonlinear feature extraction and machine learning compatibility. These approaches not only enhance the understanding of fluidization mechanisms but also pave the way for real-time monitoring and intelligent control of industrial fluidized bed systems.

Acknowledgments

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MKF0678

Reaction Mechanism and Kinetics of Ethane Oxychlorination on Cu-Ce/HZSM-5 Catalyst Through Inhibiting Gas-Phase Reactions and Promoting C2H5Cl Conversion

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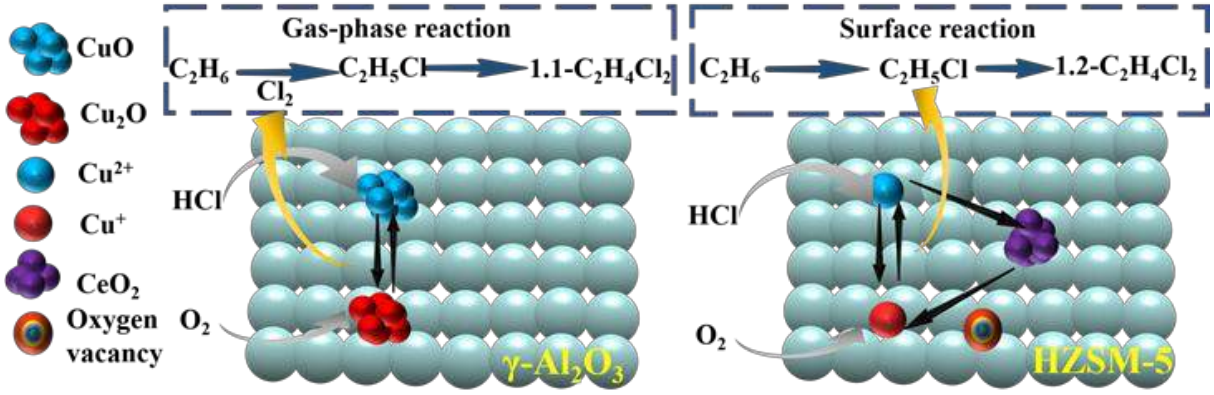
Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Fundamental

Keywords: Ethane oxychlorination; Cu-based catalyst; Reaction pathway; Selectivity control.

Abstract Body.
Introduction.
With the large-scale exploitation of shale gas resources, ethane oxychlorination to high-value-added chemicals has garnered growing significance. However, on conventional Cu-based catalysts, the accumulation of the intermediate C2H5Cl during ethane oxychlorination results in reduced selectivity toward the target products (C2H4 and C2H3Cl). Meanwhile, the predominant gas-phase chlorination of ethane generates 1,1-C2H4Cl2, which further inhibits the formation of C2H3Cl. Therefore, this study focuses on regulating the surface-dominated reaction pathway of C2H6 oxychlorination and promoting the conversion of the intermediate C2H3Cl, aiming to achieve dual-channel enhancement of the reaction process.
Methods.
In this study, a novel Cu-Ce/HZSM-5 catalyst was designed and prepared, using conventional Cu-Al2O3 serving as the reference. Initially, the catalytic performances of both catalysts were compared through steady-state activity tests. Subsequently, kinetic experiments were conducted to systematically investigate the potential reaction pathways of ethane oxychlorination over the catalysts. To elucidate the structure-activity relationship, a suite of steady-state characterizations (XRD, SEM, TEM, UV-Vis, EPR, Raman) and quasi-in-situ dynamic characterizations (H2-TPR, Py-FTIR, NH3-TPD, O2-TPD, XPS) was integrated.
Results and discussion.
Characterization results revealed that, unlike the conventional catalyst where agglomerated CuO phases predominated, the Cu species on Cu-Ce/HZSM-5 mainly existed as isolated Cu2+ ions. Further XPS and NH3-TPD analyses indicated that the abundant Cu2+ species not only provided more Lewis acid sites, lowering the energy barrier for HCl elimination from C2H5Cl, but also increased the surface chlorine coverage, thereby effectively suppressing the undesired gas-phase chlorination reactions. Integrated with steady-state kinetic data, it was found that the novel Cu-Ce/HZSM-5 catalyst, benefiting from the tailored interfacial Cu2+ species and the synergy with Ce, promoted surface-dominated reactions as the predominant pathway. Compared to the conventional catalyst, Cu-Ce/HZSM-5 achieved a 40% increase in C2H6 conversion and a 43% improvement in the overall selectivity toward the target products.



Schematic illustration of the reaction pathways for ethane oxychlorination.

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MKF0768

Deciphering Consecutive Protonation Steps in Photocatalytic CO2 Reduction with Plasmonic Au Nanorods Embedded in a Metal-Organic Framework

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Fundamental

Keywords: Keywords: CO2 Photoreduction; Protonation; Plasmon; In-situ Raman; Reaction mechanisms

Abstract Body.
Abstract: The proton-coupled electron transfer process (PCET) plays a crucial role in both natural and artificial photosynthesis, including CO2 fixation chemistry. However, difficulties in capturing the transient intermediates generated during the protonation process impede the clarification of the fundamental mechanism behind photocatalytic CO2 reduction. Herein, we report a general killing two birds with one stone strategy by spatially confining Au nanorods within a typical porphyrin metal-organic framework (MOF). Interestingly, 2.4-fold increase in CH4/CO selectivity and 12-fold increase in CH4 production were observed after loading of Au nanorods, indicative of a strengthened protonation process in the photocatalytic CO2 reduction. More importantly, the plasmonic effect from Au nanorods simultaneously boosted the in-situ Raman signals of *CO and *CHO intermediates on the Au-O-Zr active site. The evident protonation process was further clarified in a control H/D kinetic isotope experiment. This work highlights the significance of successive protonation steps for boosting CH4 production in photocatalytic CO2 reduction.

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MKP0178

Biopolymer production from wood derived sugars based on genetically modified Haloferax mediterranei

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Biomass

Keywords: Sustainable biopolymers, Lignocellulosic biomass, Polyhydroxyalkanoate terpolymer, Haloferax mediterranei, DFT calculation

Abstract Body.

Introduction

Polyhydroxyalkanoates (PHAs) are biodegradable and biocompatible polymers that have been widely recognized as promising alternatives to petroleum-based plastics; however, their large-scale implementation has been constrained by high production costs, limited utilization of low-cost feedstocks, and insufficient control over polymer composition. In particular, the efficient incorporation of 4-hydroxybutyrate (4HB), a monomer critical for improving flexibility, biodegradability, and biomedical performance, has remained a major challenge.

Methods

In this study, a sustainable bioprocessing strategy was developed for the production of high-value P(3HB-co-3HV-co-4HB) terpolymers using lignocellulosic biomass-derived sugars. A genetically engineered Haloferax mediterranei strain (H. mediterranei_zxr1.0) was constructed through the heterologous expression of a codon-optimized 4-hydroxybutyrate-CoA transferase from Cupriavidus necator, enabling enhanced conversion of 4HB precursors into polymerizable intermediates. To replace refined carbon sources, C6-rich wood-derived sugar streams generated from industrial biomass fractionation were systematically evaluated as renewable fermentation substrates. Substrate composition was characterized by HPLC analysis, while genome screening and density functional theory (DFT) calculations were applied to elucidate the metabolic and physicochemical effects of minor constituents, including short-chain organic acids, on microbial growth and PHA polymerization.

Results and discussion

Both shake-flask and batch bioreactor fermentations were performed to assess process performance and scalability. It was demonstrated that C6-rich wood-derived sugars effectively supported cell growth and promoted terpolymer accumulation beyond that achieved with pure glucose. In batch bioreactor operation, a total PHA concentration of 0.42 g L^{-1} was obtained, with the 4HB fraction reaching 25 mol% and the 3HV fraction approximately 9 mol%. This represented a fivefold increase in 4HB content compared with the wild-type strain and a 1.5-fold enhancement in PHA accumulation relative to conventional feedstocks. The formation of a true terpolymer with controlled monomer distribution was confirmed by GC and ^13C NMR analyses.

Conclusion

Overall, a scalable and contamination-resistant platform was established for converting lignocellulosic waste streams into high-value biopolymers. By integrating genetic engineering, molecular modeling, and biomass valorization, a robust framework was demonstrated for sustainable chemical production from renewable resources, supporting the development of next-generation biorefineries for advanced bioplastics.

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MKP0479

Development of end-user property correlations based on polypropylene process modelling results

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Polymerization

Keywords: Polymerization modelling, Polypropylene, Loop polymerization, Polymer properties

Abstract Body.

1. Introduction

Polypropylene is a typical mass plastic with wide fields of application in everyday life as well as in industrial areas. Due to the continuing demand on the market, it is necessary to further develop and optimize the manufacturing processes. To determine the subsequent use of the produced polymer or even to design polymers for specific applications, the polymer properties must be precisely determined. In order to predict the properties of the polymer produced in industrial set-ups and help with optimization tasks, it is possible to model and simulate the process using process simulation software.

2. Methodology and Approach

To obtain simulation-based predictions for the properties of polypropylene produced in the industrial bulk polymerization process, the calculation of the considered properties has to be implemented in the process models. The individual steps taken during model development are shown in the figure below.

Properties which are important for the subsequent applications are for example the average molecular weight, the molecular weight distribution, as well as the tacticity of the polymer chains. These properties are mainly influenced by the concentration of reactants as well as the presence of additional agents that influence polymerization behavior. For example, hydrogen is used as a chain transfer agent and therefore decreases molecular weight. Additionally, an external electron donor can be added to control the stereoselectivity of the polymerization and influence the tacticity of the polymer.

Consequently, further end-user properties can be measured at plants to determine the final use case of the produced polymer. These end-user properties mainly include mechanical properties, which are typically depending on the aforementioned properties. Therefore, the model-predicted properties can be used as reference for developing correlations for the mechanical end-user properties investigated.

3. Results

For developing the polymer properties models, several steps are conducted to decrease complexity in the beginning and investigate the properties one after another. Melt flow rate, molecular weight distribution and tacticity were implemented as a result depending on reaction kinetics and therefore on operational process conditions. When selecting an

application for the produced polymer, additional mechanical properties have to be investigated. It can be helpful to include these properties already in a process model and simulate them for the process conditions. Correlations are based on plant data sets, as well as literature for additional data points and correlation trends. It is possible to get feasible solutions for prediction of end-user properties depending on operational conditions at plant scale.

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MKC0129

The caveats of computational modelling of proton-coupled electron transfer in CO2ER

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Electrochemical

Keywords: DFT, CO2ER, CO_2 valorization, solvation, grand canonical DFT, transition states

Abstract Body.

Introduction. One of the main advantages of electrocatalysis is the use of electric potential to drive reactions under ambient conditions. Precise control over selectivity can be achieved by tuning the catalyst, potential, current, and solvent. A complete reaction mechanism, usually determined using DFT, is essential for optimising the CO2 electroreduction (CO2ER) process. However, proton-coupled electron transfer (PCET) has consistently been avoided at the DFT level due to the many difficulties involved, resulting in an incomplete and unconfirmed reaction mechanism for CO2ER. Recent studies have emphasised the role of solvation [1], which may be key to the successful study of PCET at the DFT level.

Methods. Density Functional Theory (DFT) is an invaluable tool for studying heterogeneous catalysis, providing atomic-level insight into reaction mechanisms. Modelling elementary reactions in electrochemical systems presents unique challenges, such as solvation, the influence of electrode potential, and the presence of charged species, with proton-coupled electron transfer (PCET) being particularly difficult to model. To model CO2 electroreduction (CO2ER) accurately, grand canonical DFT is used to simulate electrode potential. Solvation effects are modelled with JDFTx's LinearPCM Candle model [2]. ASE [3] was used for manipulation of atomic structures and workflow automation.

Results and discussion. This study advances beyond classic DFT reaction mechanism identification by utilising grand canonical DFT combined with the Candle solvation model to calculate PCET energetics, investigated within the framework of CO2ER. The results demonstrate that the use of advanced solvation models is crucial for studying PCET. The calculation setup employs the climbing image nudged elastic band method to identify transition states for both classic and PCET reactions. The resulting reaction energetics, including PCET steps and transition states, are shown to be qualitatively correct across a range of electrode potentials.

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MKC0205

Molecular Origin of Optimal Operando Conditions in Bosch-Meiser Urea Synthesis via Machine Learning Force Field

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Computational

Keywords: Urea synthesis, Bazarov reaction, Machine learning force field, Free energy surface, Reaction mechanism, Enhanced sampling, Bosch-Meiser process, CO_2 utilization

Abstract Body.
Urea is a vital nitrogen fertilizer produced at over 200 million tons annually via the Bosch-Meiser process, serving as the cornerstone of global food security. The industrial synthesis follows the Bazarov reaction: exothermic ammonium carbamate formation from CO_2 and NH_3, followed by endothermic dehydration to yield urea. Industrial processes achieve maximum conversion at 443–493 K and 125-250 bar. Despite over a century of operation, the molecular mechanism governing these optimal conditions has remained unclear, and competing pathways for the rate-determining dehydration step—dehydration-amine addition (DAA), acyl substitution (AS), and concerted (C) mechanisms—remain debated due to experimental limitations under extreme conditions and computational approaches relying on implicit solvation models.

In this study, we developed a machine learning force field based on the deep potential molecular dynamics framework, trained on r²SCAN-level density functional theory data validated against CCSD(T) benchmarks. The training dataset was systematically constructed using the DP-GEN active learning protocol to ensure comprehensive sampling of equilibrium states, intermediates, and transition state regions. We computed the complete two-dimensional free energy surface using on-the-fly probability enhanced sampling (OPES) with PATH collective variables, enabling direct comparison of competing pathways under explicit solvation.

We established the AS pathway as the kinetically dominant mechanism, with activation barriers 20–30 kJ/mol lower than the DAA route at the critical branching point from carbamate to intermediates, while the concerted pathway was confirmed kinetically forbidden. Van't Hoff analysis across 390–530 K revealed that overall reaction free energy exhibited a pronounced minimum at 460–480 K ($\Delta G_{rxn} \approx -35$ kJ/mol), precisely coinciding with industrial conditions. The AS pathway requires both NH_3 collision with the reactive species and the existence of carbamic acid as the reactive form. We found that NH_3 collision rate toward carbamic acid decreases with increasing temperature due to density reduction, while the carbamic acid fraction relative to total carbamate species increases with temperature. The interplay of these two competing factors determines the overall reactivity, creating an optimal temperature window that matches industrial practice.

Our findings provide the first atomistic explanation for the empirically optimized Bosch-Meiser process conditions, resolving a century-old question in industrial chemistry. These

mechanistic insights offer fundamental guidance for rational catalyst design and process optimization in CO_2 utilization technologies toward carbon neutrality.

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MKC0208

Computational Study of Various Organotin Complex Structures in Different Solvents

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Computational

Keywords: Metal oxide, Solution, Machine learning force field

Abstract Body.

Metal oxides, particularly Sn based compounds, are promising photoresists for extreme ultraviolet (EUV) lithography due to their high EUV photon absorption. However, their performance can be affected by stability, for example poor storage stability may inhibit their application in semiconductor manufacturing process, and improved resistance to humidity can increase shelf-life. Therefore, it is important to understand the storage conditions, particularly solvent effects on the organotin compounds, which can be one of the key factor in achieving long shelf-life. Furthermore, microscopic insight between solvent and organotin complex is needed.

In this work, we used a pretrained machine learning force field (MLFF), which combines advantages of density functional theory (DFT) and classical molecular dynamics (MD) simulations, to determine the structures of organotin compound in different solvents. We first evaluated several candidate models for a single organotin compound and selected a model that represents the structure of single molecule well compared to the DFT results. Based on the results, we selected SevenNet-0 for solution systems simulations. MD simulations with SevenNet-0 model in various solvents were performed and detailed structures of the organotin complex were determined. Structural analyses showed structures involving mono-/bi-dentate binding of ligand and solvent coordination to the metal center, although several limitations exist.

These results demonstrate that ligand binding and solvent coordination participate in various organotin structures. Moreover, SevenNet-0, a pretrained MLFF model, enhances microscopic understanding and is expected to provide insights into solvent design for optimizing storage condition of organotin complexes

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MKC0211

Computational Insights into Substrate-Governed Wetting Transparency and Moisture Stability in Monolayer MoSe2

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Computational

Keywords: wetting transparency, moisture adsorption, stability, transition metal dichalcogenides, molecular dynamics simulation, water contact angle

Abstract Body.
Atomically thin transition metal dichalcogenides (TMDCs) readily interact with ambient moisture, which can accelerate degradation and limit device reliability. A key open question is how the substrate governs water interaction with TMDC monolayers. Here we provide computational evidence that substrate surface energy can regulate interfacial water adsorption on monolayer MoSe2 via wetting transparency, suggesting a straightforward route to improve moisture stability by engineering the underlying support.
Molecular dynamics simulations were used to quantify substrate-dependent wetting by modeling a cylindrical water droplet on MoSe2 supported by hydrophilic SiO2 and by hydrophobic alkyl-terminated surfaces; the corresponding bare substrates were also simulated as references. The cylindrical geometry minimizes curvature-induced line tension effects. Contact angles were extracted from two-dimensional density maps using hyperbolic tangent boundary fitting followed by circle fitting. Density functional theory calculations were further used to compare H2O adsorption energetics and associated electronic structure changes for MoSe2 on SiO2 versus alkyl-modified supports.
The simulations show strong substrate imprinting on wettability: bare SiO2 and bare alkyl surfaces yield contact angles of 44.2 and 100.6 degrees, while MoSe2 supported on these substrates yields 62.8 and 96.4 degrees, respectively. Consistent with this wetting trend, computed H2O adsorption is much stronger for SiO2-supported MoSe2 (0.478 eV) than for alkyl-supported MoSe2 (0.043 eV), indicating weaker interfacial interaction on hydrophobic supports. The stronger adsorption on the hydrophilic support is accompanied by more pronounced electronic-structure changes, including a reduced bandgap relative to the hydrophobic support (0.470 versus 0.750 eV).
In summary, the hydrophilic support favors interfacial water adsorption and stronger binding at the MoSe2 interface, whereas the hydrophobic support suppresses both, providing a molecular basis for the experimentally observed contrast in moisture stability between SiO2 and ODTS-treated substrates. This substrate-controlled picture suggests that moisture

adsorption can act as an early gate for subsequent humidity-driven oxidation and performance loss, and that surface-energy engineering of the support is an effective, scalable strategy to mitigate degradation in TMDC-based devices.

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MKC0212

Ionic Liquid–Driven Ion Exchange for High-Performance PEDOT:PSS Films

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Computational

Keywords: PEDOT:PSS, Ionic liquids, Ion exchange,Stretchable conductors, Materials discovery,Conductivity enhancement

Abstract Body.

Introduction.

Poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS) is one of the most widely used conducting polymers owing to its solution processability, optical transparency, and mechanical flexibility. However, pristine PEDOT:PSS films often suffer from limited electrical conductivity and mechanical robustness, restricting their application in stretchable and wearable electronics. Recent studies have shown that ionic liquids (ILs) can significantly modify the microstructure and electronic properties of PEDOT:PSS through ion exchange and secondary doping effects. Despite these advances, a systematic understanding of how the ion exchange capability of ILs governs both mechanical stretchability and electrical conductivity remains incomplete. In this work, we aim to discover ILs that can induce high-performance PEDOT:PSS films by correlating IL-dependent ion exchange behavior with film-level mechanical and electrical properties.

Methods.

A diverse set of ionic liquids with varying cation–anion combinations was selected to span a wide range of ion size, acidity, hydrogen-bonding ability, and ion pairing strength. PEDOT:PSS films were prepared via solution mixing with ILs followed by film casting and thermal treatment. The ion exchange behavior between PEDOT:PSS and ILs was evaluated using spectroscopic and structural analyses. Electrical conductivity was measured using a four-point probe method, while mechanical stretchability was assessed through uniaxial tensile testing. Structure–property relationships were established by correlating IL descriptors with experimentally observed conductivity and elongation behavior.

Results and discussion.

We find that ILs with strong ion exchange capability preferentially remove excess PSS and promote PEDOT chain rearrangement, resulting in enhanced charge transport pathways. Such ILs simultaneously improve film stretchability by inducing a more ductile polymer network. In contrast, ILs with weak ion exchange show limited conductivity enhancement and brittle mechanical behavior. A clear correlation is observed between ion exchange strength and the synergistic improvement of conductivity and stretchability. Based on these trends, optimal IL candidates are identified that maximize both electrical and mechanical performance. This work provides a rational materials discovery framework for designing high-performance PEDOT:PSS films through targeted ionic liquid selection.

Acknowledgments

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MKC0214

Accurate Martini Simulation of Zwitterionic SBMA/DMAAPS Random Copolymers: Focusing on Electrostatic Interactions and Chain Conformations

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Computational

Keywords: Zwitterionic random copolymers, Hybrid CG modeling, Martini force field, Iterative boltzmann inversion, Electrostatic interactions, Chain conformation, SBMA, DMAAPS

Abstract Body.
Zwitterionic hydrogels, such as those based on sulfobetaine methacrylate (SBMA) and 3-[[2-(methacryloyloxy)ethyl]dimethylammonio]propane-1-sulfonate (DMAAPS), have emerged as core materials for advanced biomedical hydrogels due to their exceptional biocompatibility and anti-fouling properties. These hydrogels exhibit unique physicochemical behaviors driven by strong intra- and intermolecular electrostatic interactions. Despite their potential in various fields, accurately capturing these complex coulombic behaviors in a coarse-grained (CG) framework remains a significant challenge due to the high charge density and sensitivity of the zwitterionic groups. In this study, we developed a refined hybrid Martini-IBI (Iterative Boltzmann Inversion) model to precisely simulate the behavior of SBMA/DMAAPS random copolymer hydrogels.
The parametrization process was performed through a multi-step hierarchy. First, bonding parameters, including bond lengths and angle constants, were derived from a comprehensive dataset combining all-atom (AA) molecular dynamics simulations and quantum mechanical calculations via xtb (extended Tight-Binding) for short sequences ranging from monomers to 5-mers. To specifically address the structural complexity of the copolymeric backbone, simulations were performed on various random copolymer sequences with diverse monomeric combinations, ensuring that the fitted backbone constants represent the stochastic nature of the actual hydrogel system. Furthermore, to overcome the limitations of standard harmonic potentials in describing zwitterionic associations, we conbined Iterative Boltzmann Inversion (IBI) to generate tabulated non-bonding and backbone potentials.
The validity of this model was confirmed across multiple scales. At the molecular level, chain conformations such as the radius of gyration) and persistence length showed high consistency with reference data. At the macroscopic level, the model successfully reproduced experimental observables, including swelling ratios and stress-strain relationships provided by experimental collaborators.
In conclusion, this hybrid simulation framework provides a reliable platform for understanding the intricate electrostatic interplay within zwitterionic networks. By bridging the gap between quantum-level accuracy and mesoscale efficiency, this model offers a powerful tool for investigating the structural and mechanical responses of complex charged copolymer systems.

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MKC0241

Automaic Discovery of Interpretable Kinetic Rate Laws via Kolmogorov-Arnold Networks

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Computational

Keywords: Kinetic rate law discovery, Reaction mechanism inference, Kolmogorov–Arnold Networks (KANs), Methanol synthesis, VBF model

Abstract Body.
Purpose: Deriving reliable kinetic mechanisms is a fundamental challenge in chemical engineering, particularly for CO2 hydrogenation where reaction rates exhibit non-monotonic dependence on feed composition. Empirical evidence shows that reaction rates peak at "CO-rich" conditions (CO2 fraction of ~5–10%) due to synergistic effects between intermediate formation and the water-gas shift reaction. Conventional modeling often misses this behavior, while deep learning lacks interpretability. To bridge this gap, we present an explainable AI (XAI) framework that autonomously discovers ODE-based governing equations directly from data.

Methods: Our approach utilizes Kolmogorov–Arnold Networks (KANs), which employ learnable activation functions on edges suitable for symbolic regression. We apply progressive structured pruning to distill these networks into explicit mathematical terms. To strictly validate this capability, we employ a "closed-loop" verification using the Vanden Bussche-Froment (VBF) model as ground truth. We formulated the VBF model—known for physically capturing the CO2 promotional effect—into an ODE system to generate synthetic datasets encoding the critical rate peak. This setup tests whether KANs can "rediscover" the complex physical law solely from data without prior knowledge.

Results: The framework was first validated on standard ODE benchmarks (e.g., Lotka–Volterra, Van der Pol), where it successfully recovered exact governing equations despite data scarcity. Building on this, we applied the pipeline to the synthetic methanol datasets. The results demonstrate that our method is capable of identifying the functional forms of the VBF model. The symbolified KAN accurately reproduced the complex synergistic effects of the CO/CO2/H2 mixture, specifically capturing the local maximum reaction rate at the CO-rich condition. This confirms the network captures underlying physicochemical principles rather than merely overfitting.

Conclusions: This study establishes KANs as reliable tools for deducing physical laws from kinetic data. By validating against the VBF model, we demonstrate the framework's ability to distinguish true mechanistic structures from numerical artifacts. This verification provides a solid foundation for the next phase: utilizing this validated framework to uncover explicit rate laws from noisy, real-world experimental data where true governing equations remain

unknown, thereby accelerating autonomous process development.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

MKC0332

Cracking complexity: multi scale kinetic modeling of mixed plastic pyrolysis for real world recycling

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Computational

Keywords: Pyrolysis, Waste, Plastics, kMC, Circular, Oil

Abstract Body.
Introduction.
Plastics are indispensable to modern life, yet low recycling rates have led to significant environmental accumulation. Conventional mechanical recycling often fails when dealing with contaminated or mixed plastic streams. Pyrolysis offers a promising alternative by thermally decomposing polymers into high-value hydrocarbons. However, the design and optimization of efficient pyrolysis reactors require robust kinetic models capable of handling the immense molecular complexity and diverse reaction pathways associated with polymer degradation.

Methods.
The pyrolysis of polyethylene, polypropylene, and polystyrene was modeled [1 - 4] using the kinetic Monte Carlo (kMC) methodology. This approach provides granular, molecular-level insights by tracking specific chain lengths, branching, and radical positions, yielding high-fidelity product distributions at a higher computational cost.

To represent realistic operating conditions, the kinetic model was coupled with a vapor–liquid equilibrium–based volatilization model. This integration captures the continuous removal of light products from the reactor and accounts for the effects of pressure and gas residence time on conversion. Beyond single-component studies, this research extends the multi-scale approach to simulate the pyrolysis of plastic mixtures, mimicking real-world waste compositions.

Results and discussion.
The models were validated against experimental data from a continuous pilot-scale setup. While currently limited to polyolefins and polystyrene without heteroatom contamination, this integrated modeling approach provides a deep mechanistic understanding of interactive effects in mixed feeds. It serves as a vital predictive tool for the optimization and scale-up of industrial chemical recycling units, effectively bridging the gap between fundamental kinetics and reactor engineering.

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MKC0339

Physics-Informed Machine Learning for Kinetic Modeling: Hydrodeoxygenation of Stearic Acid

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Keywords: Scientific machine learning; Physics-informed machine learning; Kinetic modeling

Introduction. Mechanistic reactor models struggle to accurately model unknown kinetics and side-reactions. To address this limitation, we adopt neural ordinary differential equations (NODEs) as a data-driven framework for learning reactor dynamics. Specifically, stearic acid hydrodeoxygenation kinetics is modelled by approximating the time derivatives with a neural

$_{dc}$ network, f_{θ} such that; $\_\__d = f_{\theta}(\boldsymbol{c}, T, P, w)$, with $\boldsymbol{c}$ denoted as concentration, T as temperature,

P as pressure, w as catalyst weight and $\boldsymbol{\theta}$ as network weights. To ensure physically consistent predictions, we introduce a soft constraint based on an atom balance into the objective function. The mechanistic kinetic model developed by Arora, et al. [1] is used as a benchmark.

Methods. The proposed incorporation of constraints into the objective function is integrated through a self-adaptive approach, in which the strength of the constraint is learned automatically during training. Specifically, the carbon balance is enforced through a regularization term whose weight is a trainable parameter. We build on previous works in the physics-based machine learning paradigm [2], however, previous studies have not incorporated the regularization weights with training of NODEs, particularly where the system dynamics is unknown.

Results and discussion. The physics-informed NODE (PI-NODE) accurately predicts the product distributions as evidenced by Fig. (1), with tight uncertainty bands, indicating low variance across the ensemble predictions. As the figure elucidates, the PI-NODE gives a more accurate description of the product distribution than the kinetic model. The PI-NODE prediction is obtained using deep ensembles, averaging the PI-NODE prediction for 100 independently trained realizations of network parameters. Model generalization is evaluated on a hold-out dataset, on which the PI-NODE exhibits an R^2 of 0.94 compared to 0.80 for the kinetic model.

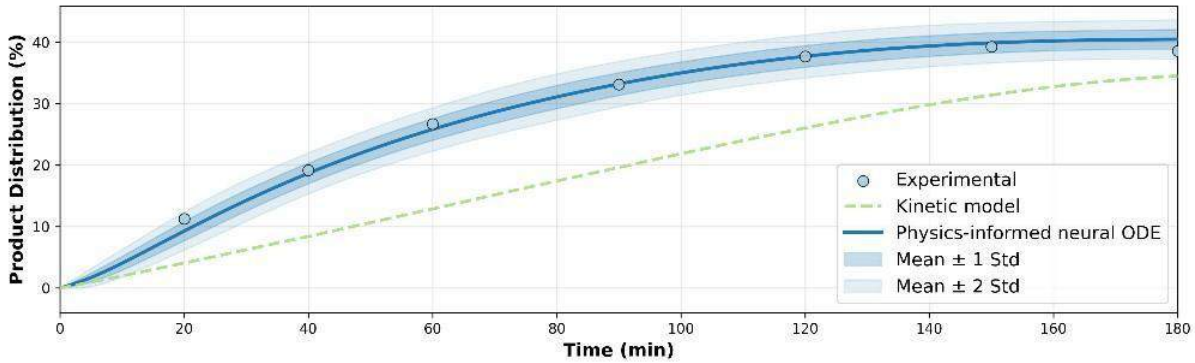

Figure 1. Comparison of PI-NODE predictions with the kinetic model developed by Arora, et al. [1].

Acknowledgments

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MFC0382

Incremental Identification of Reaction Network Structure and Kinetics from Concentration Time-Series Data

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Computational

Keywords: Reaction network identification, stoichiometry inference, data-driven modelling

Abstract Body.
Purpose: Optimization and control of chemical reactions require the knowledge of reaction networks and kinetics. Despite this need, identifying the reaction network and kinetics remains a challenging problem due to the combinatorial nature of the problem. In this work, we present an incremental approach to identify both the reaction network and kinetics directly from concentration time-series data in a model-free manner.

Methods: The proposed method incrementally identifies: (i) reaction candidates, (ii) reaction networks, and (iii) reaction kinetics using the concentration time-series data. Reaction candidate identification is formulated as linear Diophantine equations using the mass-balance constraints [1]. The number of independent reactions is then estimated from concentration data using singular value decomposition (SVD). Candidate stoichiometric matrices are subsequently constructed through an incremental, constraint-driven procedure in which feasible reaction vectors are selected based on (i) the SVD-derived reaction count and (ii) the set of species available at each step, determined from the initial conditions and previously chosen reactions. After each selection, the available-species set is updated, and only vectors consistent with it remain admissible. This sequential pruning yields a tree-structured search that terminates when no further feasible vectors exist or when the required number of reactions has been selected. The resulting stoichiometric candidates are evaluated against the concentration data, and the parameter estimation step identifies [2] the most plausible stoichiometry and the corresponding kinetic model from a set of proposed kinetic structures.

Results and discussions: The proposed methodology is evaluated on two representative systems: biodiesel production and dimethylformamide pyrolysis. In both cases, the underlying stoichiometric structure is recovered, either directly or via a reduced set of reactions that form equivalent linear combinations of the ground-truth stoichiometry. Moreover, the framework also identifies the reaction rate expressions and corresponding kinetic parameters.

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MFC0404

Surface Oxidation-Driven Ethane CO2-ODH Activity-Selectivity Trade-Offs on β-Mo2C Catalysts

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Computational

Keywords: Oxidative dehydrogenation (ODH), light alkanes, Carbon dioxide, Molybdenum carbide, light olefins, Density Functional Theory (DFT)

Abstract Body.
CO2-assisted oxidative dehydrogenation (CO2-ODH) of alkanes offers a promising alternative to the conventional cracking-based methods to produce valuable olefins. Molybdenum carbide (Mo2C) is a potential catalyst due to its high propensity for CO2 activation and alkane dehydrogenation. Experimental studies reveal dynamic structural evolution of Mo2C from carbide to oxycarbide to oxidized phases under CO2-ODH conditions. These structural transformations of Mo2C catalysts essentially govern their catalytic performance. The phase changes dynamically alter the density and nature of active sites, shifting selectivity between the desired ODH pathway ($C_2H_6 + CO_2 \leftrightarrow C_2H_4 + CO + H_2O$) and competing reactions like dry reforming (DR: $C_2H_6 + 2CO_2 \leftrightarrow 4CO + 3H_2$) and reverse water-gas shift (RWGS: $CO_2 + H_2 \leftrightarrow CO + H_2O$). Simultaneous structural evolution and the coexistence of multiple active sites create a complex interplay of reaction pathways, making it extremely challenging to establish well-defined structure-activity correlations of this catalyst for CO2-ODH reaction. Hence, this study explores ethane CO2-ODH over hexagonal β-Mo2C catalysts using density functional theory (DFT) simulations, uncovering mechanistic insights into the dynamic interplay between catalyst phase evolution and reaction performance.
Our simulations indicate that pristine β-Mo2C(101) surface exhibits high first C-H bond activation barriers (~3 eV) in ethane, with thermodynamic preference towards undesired and subsequent C-H cleavages that propagate DR pathways. This aligns with experimental observations of poor ODH selectivity under CO2-free conditions. The favourable kinetics for CO2 dissociation facilitates rapid surface oxidation, achieving 1 monolayer (ML) oxygen coverage under typical ODH conditions (600°C, pC2H4 pH2O/pC2H6 = 2.44×10-5) as predicted by ab initio thermodynamics calculations. The O* species lower first C-H activation barriers to ~2 eV but preferentially steer reaction pathway towards acetaldehyde and further along the DR route. Deeper oxidation to MoO2-like surfaces maintains reduced first C-H activation barriers, while raising CO2 dissociation barriers and suppressing both oxygenate formation and undesired C-H activations. These combined effects improve ethylene selectivity, accompanied by diminished overall activity, consistent with experimental time-on-stream trends.
The work highlights the trade-off between activity and selectivity for ODH governed by surface oxidation depth: – pristine carbide surfaces lack activity; oxygen-covered surfaces enhance activity at the cost of selectivity; and oxidized MoO2 phase improves selectivity –

suggesting that an MoO2 oxide overlayer on Mo2C represents a selective catalyst for CO2-ODH of ethane to give ethylene. These atomic-scale insights provide a mechanistic foundation to guide operational strategies that stabilize selective MoO2-like phases through controlled oxidation depth in CO2-ODH systems.

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MKC0436

Development of a Kinetic Model for Methane Total Oxidation on Iron Beta Zeolite Catalysts

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Computational

Keywords: methane slip, methane oxidation, kinetic modeling, iron beta zeolite

Abstract Body.
Introduction. The new environmental and climate protection policies have introduced stricter regulations on maritime exhaust emissions. Replacing conventional diesel engines with dual-fuel or natural gas systems can greatly reduce pollutant emissions, but methane (CH4) slip remains a significant challenge. Given that CH4 has a higher greenhouse gas intensity than carbon dioxide (CO2), the implementation of CH4 slip reduction technologies, e.g., the application of total oxidation catalysts, is essential. However, despite their excellent catalytic activity in CH4 oxidation, the practical use of precious metal-based catalysts is limited by their high cost and limited availability. As a result, lower-cost alternatives need to be developed, with iron-containing (Fe) zeolites showing strong potential for gas-phase CH4 oxidation reactions. The aim of the present work is to perform kinetic modeling analysis of CH4 total oxidation on the basis of previously proposed reaction mechanisms and further to validate using in-house experimental data over Fe-beta zeolites.
Methods. The mechanistic models, namely Langmuir-Hinshelwood, Eley-Rideal and Mars-van Krevelen (MvK) mechanisms, and a simple power-law (PL) model are implemented. Initially, kinetic fitting is carried out using differential data under dry feed conditions. Next, the models retained from the first discrimination are evaluated by integral kinetic data analysis. Subsequently, the selected models are adapted to account for the inhibition caused by water molecules. All computations are performed using the MATLAB software.
Results and discussion. PL, MvK1 (original) and MvK2 (a variation of MvK1 with the slow product desorption) models were found to adequately describe kinetic data over Fe-beta zeolites after initial model discrimination. However, deeper analysis is required to elucidate potential optimization issues, e.g., low coefficients of determination □2. By integral kinetic data treatment, PL and MvK2 were determined to be the best models with □2 values of 0.877 and 0.913, respectively. MvK2 model was then modified with terms related to water adsorption on reduced or oxidized active sites. While high □2 values of 0.956 and 0.947 were obtained for reduced and oxidized sites respectively, further regression using additional experimental data or advanced optimization techniques is required to fully validate the effect of water inhibition.
Conclusions. The MvK mechanism that considers slow desorption of the reaction products showed superiority in modeling the kinetics of the total oxidation of CH4 on Fe-beta zeolites. Future work will focus on simulating and predicting the observed formation of carbon monoxide.

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MKC0459

Fundamental Understanding of NiO Reactivity as an Oxygen Carrier in Chemical Looping Combustion

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Computational

Keywords: Chemical looping combustion, Oxygen carrier, NiO, Oxygen vacancy, Density functional theory

Abstract Body.
Chemical looping combustion (CLC) has attracted attention as an efficient fossil fuel conversion technology with inherent CO_2 capture capability. However, incomplete oxidation producing CO and H_2 is often observed at low temperatures, while higher temperatures favor full oxidation to CO_2 and H_2O. Since these behaviors are strongly governed by the redox characteristics of oxygen carriers, a fundamental understanding of their reactivity is essential. This study aims to elucidate the role of oxygen vacancies in NiO, one of the most widely used oxygen carriers in CLC. Density functional theory (DFT) calculations were performed to systematically investigate the electronic structure and oxygen migration behavior of NiO with different oxygen vacancy configurations. Particular attention was given to vacancies located in the first and second atomic layers. Although similar overall reaction pathways were identified regardless of vacancy configuration, vacancies in the first layer significantly reduced the electronic energy gap. This effect is attributed to enhanced electron transfer, as indicated by pronounced density-of-states features near the Fermi level. In addition, energy barrier analysis showed that oxygen vacancies in the second layer promote oxygen migration toward the surface layer. The results suggest that while subsurface vacancies facilitate oxygen transport, the large energy requirement associated with vacancy healing makes this process the rate-determining step. These findings provide fundamental insights into the redox behavior of NiO and its performance as an oxygen carrier in chemical looping combustion.

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MKC0465

Adaptive Neural Potentials through Environmental Conditioning

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Computational

Keywords: Atomistic Modeling, Neural Interatomic Potentials, Electronic Sturcture Awareness, Conditional Modeling

Abstract Body.
Improving the adaptability of neural interatomic potentials remains an important challenge in atomistic machine learning, particularly when electronic characteristics vary across molecular systems. Conventional models typically require retraining to accommodate such variations, limiting their flexibility and practical deployment.
In this work, we propose an electron-conditioned modeling framework built upon a fine-tuned Message Passing Atomic Cluster Expansion (MACE) architecture. By incorporating conditional modulation during the fine-tuning process, the model is designed to adapt to changes in electronic properties while preserving a shared structural representation.
As a preliminary study, we focus on molecular systems from the QM9 dataset to examine the feasibility of this approach. Our objective is to evaluate whether electron-aware conditioning can provide a scalable pathway toward more adaptive neural potentials without necessitating fully separate models.
This work aims to establish a foundation for condition-aware atomistic models and to motivate future investigations into transferable neural force fields capable of responding to diverse electronic environments.

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MKC0466

Reaction Pathways for CO_2 Hydrogenation to Methanol on Cu(111): Combined DFT and Microkinetic Study

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Computational

Keywords: CO2 hydrogenation, Methanol selectivity, Indium-modified Cu catalyst, Mechanism-guided catalyst screening

Abstract Body.
CO_2 hydrogenation to methanol offers a sustainable route for carbon utilization. Here, density functional theory (DFT) and microkinetic simulations were combined to elucidate reaction pathways on Cu(111). Three mechanisms—formate, carboxyl, and formyl—were examined for thermodynamic and kinetic feasibility, with CHO and OH intermediates considered as alternative hydrogen sources. DFT suggested comparable favorability for carboxyl and formyl routes, while CHO-assisted hydrogenation lowered barriers in the formate pathway. Microkinetic modeling identified the formate pathway as dominant under steady-state conditions and methanol desorption as the key selectivity-controlling step. Guided by this, catalyst screening revealed that indium doping reduces methanol desorption energy without impairing favorable energetics. Experiments with core–shell $Cu@SiO_2$ and $CuIn@SiO_2$ confirmed that indium enhances methanol selectivity (up to 92.7%) by suppressing CO formation, validating computational predictions. This integrated approach provides mechanistic insight and design guidelines for selective CO_2 -to-methanol conversion over Cu-based catalysts.

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MKC0506

Experimental and theoretical studies of furfural hydrogenation to furfuryl alcohol

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Computational

Keywords: furfural; furfuryl alcohol; CFD modelling; catalytic reactions

Abstract Body.
Introduction.
Furfural hydrogenation is an important process for bio-production of high-value added biofuels and chemicals, with application in energy storage systems and chemical engineering industry. Computational fluid dynamics (CFD) simulations are an efficient tool for evaluating the performance of reactors during the time that the reaction occurs. In this work, we focused on the development of CFD models to study the effect of a range of parameters, such as temperature, concentration, and catalyst amount, on furfural conversion. The data regarding the system was observed via both experiments and literature [1].
Modelling Methodology.
The model was developed using COMSOL Multiphysics version 6.2, with Chemical Reaction Engineering physics and a time-dependent study, to validate experimental data of furfural hydrogenation to furfuryl alcohol in batch system. The reaction occurs in the presence of a rhodium (Rh) catalyst and hydrogen was generated in situ via isopropanol decomposition. The kinetic model was based on Langmuir-Hinshelwood mechanism, while the mass transfer of the species was explained via convection-diffusion equations. Hypotheses that both gas and liquid phases are ideal and that the volume is constant are assumed in the development of the zero-dimension (0D) model.
(Selected) Results and discussion.
Figure 1 represents the comparison between experimental data and COMSOL simulations results on the effect of temperature on furfural conversation as a function of reaction time. A range of temperatures between 120 °C and 150 °C was examined showing that the increase of temperature leads to higher conversion and increased reaction rates. A deviation of 0.7-11.2% between experimental and COMSOL simulation results is observed, showing good model validation and a good description of furfural hydrogenation in a batch reactor. Ongoing research includes sensitivity analysis, development of 2D models, evaluation of more parameters' effect, further use of furfuryl alcohol for production of more valuable products, as well as the study of both in situ hydrogen production and addition hydrogen supply to the system, aiming to optimize the reaction.

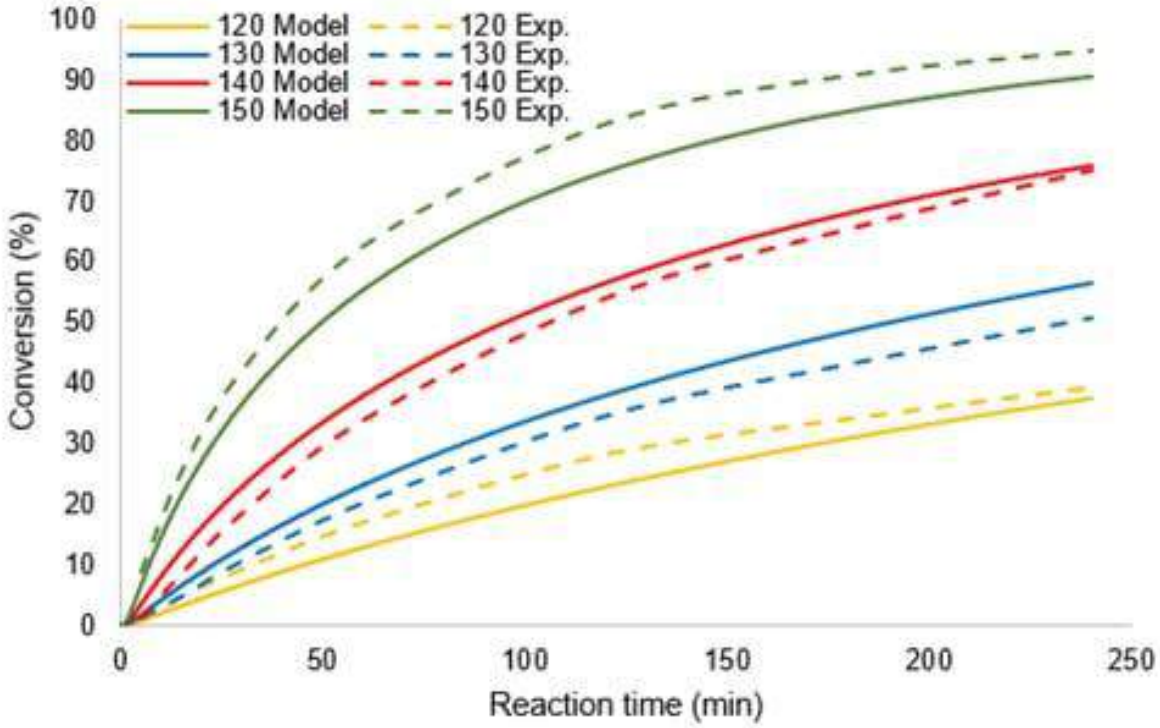

Figure 1. Comparison of furfural conversion (%) between experimental data and model results.

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MKC0531

Zn-Promoted Ni/$MgAl_2O_4$ Catalyst for Dry Reforming of Methane

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Computational

Keywords: Dry reforming of methane (DRM), Zn, DFT calculations, $MgAl_2O_4$ support

Abstract Body.
Methane (CH_4) and carbon dioxide (CO_2) are major greenhouse gases, and rising atmospheric concentrations of these species are accelerating global warming and climate change. As a potential mitigation strategy, the dry reforming of methane (DRM) reaction has attracted significant attention. DRM is an environmentally friendly process that simultaneously utilizes two greenhouse gases to produce syngas (H_2 + CO), yielding an H_2/CO ratio of approximately 1, which is suitable for downstream Fischer–Tropsch synthesis or methanol production. However, because DRM is typically operated at high temperatures, catalyst deactivation remains a critical challenge due to carbon deposition (coking) and sintering of Ni particles.
In this study, the DRM reaction mechanism over a Zn-doped Ni/$MgAl_2O_4$ (Zn–Ni/$MgAl_2O_4$) catalyst was investigated using density functional theory (DFT). Calculations were performed with VASP employing the PBE exchange–correlation functional and PAW potentials to evaluate CH_4 and CO_2 dissociation on Ni(111) and $MgAl_2O_4$ (100) surfaces. Transition states and activation barriers were determined using the nudged elastic band (NEB) method. The results show that CH_4 dehydrogenation proceeds preferentially on the Ni surface, whereas the $MgAl_2O_4$ surface exhibits a high energy barrier for CH_4 dissociation, indicating substantially lower activity than Ni. In contrast, CO_2 dissociation is much more facile on $MgAl_2O_4$ than on Ni, as evidenced by a significantly lower dissociation barrier on $MgAl_2O_4$. This suggests that $MgAl_2O_4$ can act as an oxygen supplier: the generated oxygen can diffuse to Ni and oxidize surface CH species, thereby suppressing coking.
Microkinetic simulations further indicate that the reaction order with respect to CH_4 partial pressure is close to zero, while the reaction is first order in CO_2. In addition, increasing the Ni loading leads to an increase in the apparent activation energy, and the CO_2 dissociation step was identified as the rate-determining step (RDS) of the overall DRM reaction. In conclusion, Ni is favorable for CH_4 activation, whereas $MgAl_2O_4$ is advantageous for CO_2 dissociation and oxygen transfer. The interfacial synergy between these components can suppress coking and improve the stability of DRM catalysis.

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MKC0538

Tree Based Kinetic Monte Carlo Modeling of Polypropylene Pyrolysis Under Intrinsic Conditions

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Keywords: Pyrolysis, plastic waste, Ziegler-Natta polypropylene, kinetic Monte Carlo **Introduction.** Poor recycling of solid plastic waste (SPW) has led to massive amounts of it ending up in the environment, triggering a worldwide crisis. It can only be solved if recycling methods are developed that can handle contaminated, mixed SPW, often rich in polypropylene (PP) [1], like pyrolysis. Optimizing pyrolysis processes requires fundamental insight into the kinetics, which can be obtained only through detailed kinetic models. **Methods.** The pyrolysis of Ziegler-Natta PP (ZNPP) is modeled using tree-based kinetic Monte Carlo (*k*MC), previously applied to polystyrene and polyethylene [2, 3]. ZNPP chains possess distinct head ($\mathcal{H}$) and tail ($\mathcal{T}$) carbons (Figure 1a), and the tree-based kMC framework explicitly captures this molecular structure, enabling improved prediction of product distributions and deeper mechanistic insight into ZNPP pyrolysis. This approach describes the kinetics in full detail, tracking specific chain lengths, individual reactions, and radical positions. Hence, the impact of the methyl side groups on the pyrolysis kinetics could be investigated by differentiating the rate coefficients for relevant reactions. More generally, the model considers the different reactivity of secondary and tertiary carbon atoms in the PP backbone. Furthermore, the model features novel, compact data structures to track the PP backbone's structure throughout its degradation. The model is validated against experimental data obtained using a micropyrolyzer operating under intrinsic kinetics. Thermal pyrolysis experiments were performed at 500, 600, and 700 °C. Products were analyzed using GC × GC with FID and ToF-MS detectors.

Results and discussion. The model successfully predicts naphtha production (C5-10 & C520 in Figure 1b) from ZNPP pyrolysis, the formation of key products, and the substantial C_9 and C_{15} oligomers across a wide range of temperatures. The constructed kinetic model thus provides deep mechanistic insights into ZNPP pyrolysis and acts as an important tool for the accurate and efficient design and optimization of industrial pyrolysis plants. The modeling framework has proven to be easily adaptable to other polymers, thereby enhancing their potential for chemical recycling and advancing a solution to the worldwide SPW crisis.

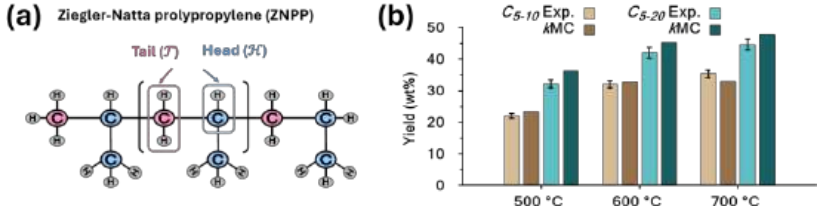

Figure 1. (a) Explicit representation of head and tail carbons in ZNPP and (b) agreement between experimental and predicted product yields for $C_{5\text{-}10}$ and $C_{5\text{-}20}$ fractions over a wide temperature range.

Acknowledgments *This research forms part of the MADPY project (#856) of DPI. DW acknowledges support by the Fund for Scientific Research Flanders (FWO) through fellowship 1SHAM24N.*

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

MKC0564

Selective Oxidation of Ethane to Value-Added Products on RhO2(110)

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Computational

Keywords: RhO2(110); Selective Conversion; Micro Kinetic; DFT;

Abstract Body.
Selective oxidation of light alkanes remains difficult due to their strong tendency toward deep oxidation. In ethane oxidation, facile C–H activation often results in poor ethylene selectivity through the formation of CO and CO2. Catalysts with moderate reactivity have been proposed to balance activity and selectivity, yet the mechanisms governing ethylene formation and suppression of overoxidation on oxide surfaces remain unclear. Clarifying the competition between product desorption and further oxidation is therefore essential for selective catalyst design.
Density functional theory (DFT) calculations were used to investigate ethane oxidation pathways on the RhO2(110) surface, including C–H activation, dehydrogenation, and oxidation steps. Temperature-programmed reaction spectroscopy (TPRS) simulations were performed based on DFT energetics to link theoretical predictions with reaction behavior. The results show that the intermediate reactivity of RhO2(110) favors ethylene formation through a reformation-driven desorption pathway. Following initial C–H activation and partial dehydrogenation, C2H4 desorption competes effectively with further oxidation, leading to enhanced ethylene selectivity. TPRS simulations support this mechanism, exhibiting distinct C2H4 desorption features preceding deep oxidation. In contrast, although similar desorption pathways exist on the more reactive IrO2 surface, stronger overoxidation tendencies reduce ethylene selectivity. These findings demonstrate that while reformative desorption mechanisms can operate on active transition metal oxides, selectivity is strongly governed by intrinsic surface reactivity. Overall, this study highlights a catalytic design strategy in which tuning oxide reactivity enables control over the balance between product desorption and overoxidation, thereby improving ethylene yields from ethane oxidation.

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MKC0605

The H2O-assisted Oxidation Half-Cycle of Low Temperature NH3-SCR over Cu-CHA

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Computational

Keywords: NH3-SCR, Operando UV-Vis, MCR, DFT, H2O-dissociation path, H2O2 oxidation

Abstract Body.
H2O/O2 is reported to accelerate the oxidation half-cycle (OHC) of the NH3-SCR reaction, leading to higher rates as compared to oxidation with sole O2. However, the detailed Cu-oxidation pathway remains unclear. Here, we combine operando UV–vis spectroscopy and DFT calculations with transient reactor methods to elucidate the mechanistic role of H2O in the OHC, providing a kinetically-consistent mechanism of the NH3-SCR catalytic cycle under realistic conditions.
The methods adopted consist in a packed bed microreactor filled with 148 mg of Cu-CHA (Si/Al=25, Cu=1.77%) is coupled with an Exemplar Plus BTC655N spectrometer to measure UV/Vis DR spectra during OHC transients (8% O2/ 2% H2O v/v) at 200 C°, after pre reduction with 500 ppm NO/NH3. Concentration profiles of Cu(I) during oxidation are quantified by Multivariate Curve Resolution. Spin-polarized density functional theory (DFT) calculations and statistical thermodynamic formalism are adopted to study reaction intermediates and free energy pathways in the OHC within a hexagonal CHA unit cell.
Figure 1a shows the UV–vis DR spectra collected during O_2 /H_2 O transients at 200 °C. The dashed line corresponds to fully reduced Cu(I), characterized by a d^{10} closed-shell configuration and the absence of d–d transitions. Upon introduction of H_2 O and O_2 , Cu(I) is oxidized to Cu(II), developing the features in the 25 000–45 000 cm^{-1} range (final state: light-blue curve). MCR analysis is applied to assess the quantitative evolution of the Cu(II) fraction during the oxidation transient: the comparison with experiments with O_2 feed are reported in Figure 1b, showing enhanced OHC rates in the presence of H2O (rate constant = 61.0*10-3 s-1 for O2/H2O vs. 21.0*10-3 s-1 for O2). DFT-derived free energies are then computed to describe the evolution of Cu species along the OHC, see Fig. 1c. They reveal that H_2 O preferentially dissociates on the peroxo complex forming a hydroperoxo species and H_2 O_2 , which can diffuse to a second cage and oxidize additional Cu(I) pairs.
To conclude, the role of H_2 O in the OHC of NH_3 -SCR is investigated combining operando UV/Vis spectroscopy and DFT calculations. UV–vis spectra show that H_2 O accelerates OHC rates compared to sole O_2 feed and free-energy calculations indicate that H_2 O follows a dissociation pathway to form H_2 O2. These results clarify the Cu-oxidation pathway and explain the observed promotional effect of water from a mechanistic point of view, providing a kinetically-consistent mechanistic of NH_3 -SCR under realistic conditions.

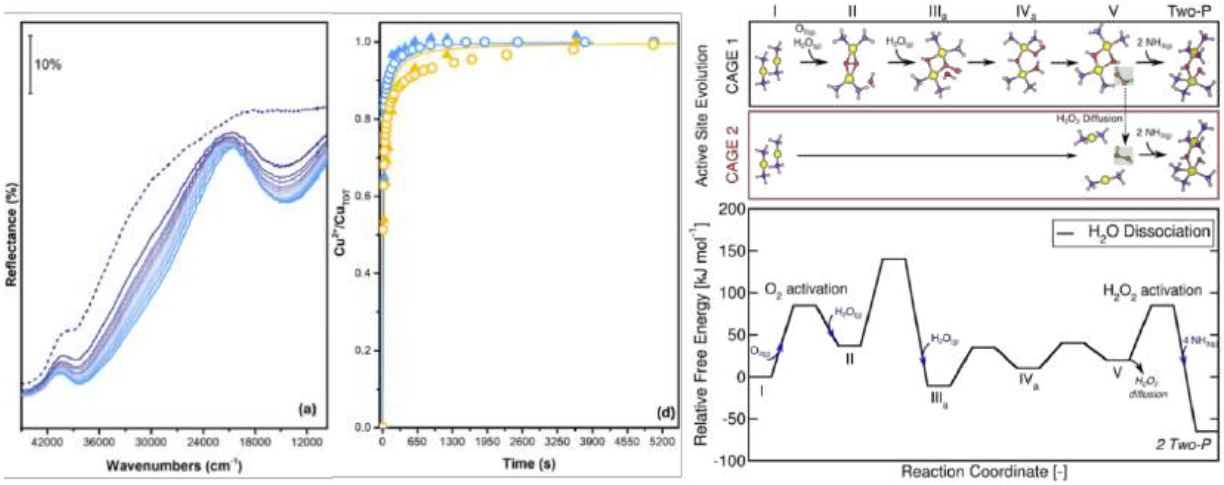

Figure 1: (a) UV/Vis DR spectra (8% O2/2% H2O) (b) Cu(II) oxidation dynamics (c) H2O-dissociation at 200 °C.

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MKC0695

DFT Study on Metal Dopant Effects in Methanol-to-BTX Conversion over ZSM-5 Catalyst

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Computational

Keywords: Zeolite, Stability, Dopant, Metal, DFT **Abstract**

Body.

The conversion of CO_2 into BTX represents a promising strategy for simultaneously mitigating greenhouse gas emissions and producing high-value chemicals. Among various approaches, the stepwise CO_2 → methanol → DME → olefin → BTX pathway is industrially attractive, yet its efficiency strongly depends on how active sites are modulated during the methanol-to-olefin stage. In this work, density functional theory (DFT) calculations were employed to systematically investigate the effects of metal dopants on ZSM-5 zeolites, with particular emphasis on the electronic structure of Brønsted acid sites (BAS). All dopant candidates were evaluated under identical computational criteria to isolate intrinsic dopant effects. The results indicate that metal incorporation can alter the electronic environment of BAS, thereby influencing key reaction steps such as DME formation and subsequent aromatization. Notably, Mo doping was found to effectively tune BAS reactivity, leading to reduced activation barriers along these pathways and suggesting a potential enhancement in BTX selectivity. These findings provide fundamental insights into dopant-driven active site modulation and offer guidance for the rational design of ZSM-5-based catalysts for efficient CO_2 conversion.

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MKC0728

Hydrogen Sulfide Splitting via the Iodine Thermochemical Cycle for Hydrogen Production: Mechanism Insights and Catalytic Enhancement with Deep Eutectic Solvents

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Computational

Keywords: Quantum chemistry, Transition State Theory, Sulfur recovery, Gas phase, Aqueous phase

Abstract Body.
Hydrogen sulfide (H_2S) is a hazardous yet abundant byproduct of the oil& gas industry that has gained attention as a hydrogen carrier. In this perspective, the H2S-Iodine (H_2S–I_2) thermochemical cycle offers a solution for both H_2S treatment and hydrogen production. This cycle involves the production of hydrogen iodide (HI) from H_2S and I_2 at high H_2S concentrations, or from H_2S, I_2, and water at low H_2S concentrations. In a second step, the produced HI can be decomposed into hydrogen. This study provides a detailed computational analysis of stepwise mechanisms, aiming to elucidate reaction mechanisms and to explore catalytic strategies to address kinetic challenges, using quantum chemistry and kinetic calculations at the M06-2X/def2-TZVP level of theory with Gaussian 16, Gaussrate 17, and Polyrate.
Gas-phase calculations reveal that the H_2S–I_2 thermochemical cycle is strongly kinetically and thermodynamically hindered. Under high H_2S concentrations, the rate-limiting step corresponds to the first addition of an –SH group to HSI, with a Gibbs free energy barrier of 91.84 kcal·mol^{-1}. At low H_2S concentrations, the analogous reaction involving water is even more unfavorable, exhibiting a barrier exceeding 105 kcal·mol^{-1}. In both regimes, the overall reaction free energies are positive, confirming that the gas-phase mechanisms are intrinsically unfavorable.
Given the practical relevance of aqueous environments, solvent effects were investigated. Attempts to stabilize the gas-phase transition states in water were unsuccessful, leading instead to the identification of alternative aqueous-phase mechanisms that yield similar products. However, the aqueous mechanisms remain highly hindered, with rate-limiting barriers of 88.79 kcal·mol^{-1} at high H_2S concentration and 104.67 kcal·mol^{-1} at low H_2S concentration, indicating that water alone does not improve the kinetic or thermodynamic limitations of the cycle.
To address these challenges, three deep eutectic solvents (DESs) were evaluated as catalytic media. Among them, the alcohol-based DES, e.g., ChCl:2EG, showed the highest catalytic activity. Extensive conformational explorations revealed significant stabilization of key transition states through double hydrogen bonding. As a result, free energy barriers were reduced by up to 29 kcal·mol^{-1} for the high-concentration rate-limiting step, and 57

kcal·mol^{-1} for the low-concentration pathway.

This study provides the first quantitative demonstration that deep eutectic solvents, particularly flexible alcohol-based systems, can substantially lower kinetic barriers in the H_2S–I_2 thermochemical cycle. The findings establish a mechanistic foundation for DES-assisted H_2S valorization and provide clear design principles for catalytic media that enable simultaneous sulfur recovery and low-carbon hydrogen production.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

MKC5685

DEVELOPMENT OF A SURFACE-REACTION CHEMICAL REACTOR NETWORK (CRN) METHOD AS A TOOL FOR SIMULATING DRY REFORMING OF METHANE IN FLUIDIZED BEDS

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Computational

Keywords: Dry reforming of methane, chemical reactor network, fluidized bed reactor, catalysis, OpenSMOKE++, model validation.

Abstract Body.

Dry reforming of methane (DRM) is a promising route to convert waste CO_2 and CH_4 into valuable syngas, but the highly exothermic reaction and rapid coking demand efficient catalyst- bed reactors and advanced models. Fluidized- bed reactors (FBRs) offer excellent mixing and heat transfer for DRM, yet predicting their behavior is challenging. Conventional CFD models of gas–solid multiphase flows often require simplified chemistry (reduced kinetic schemes) due to computational cost, limiting their accuracy for detailed reactions. In contrast, a CRN approach divides the reactor volume into idealized elements (plug- flow and well- mixed zones) and solves coupled mass and energy balances with complete chemistry[1]. This approach greatly simplifies mixing while allowing full inclusion of catalytic DRM kinetics. We have developed a novel multiphase CRN tool using the OpenSMOKE++ framework (NetSMOKE++ solver[2]) that explicitly represents surface-reaction interactions in a bubbling FBR. Specialized reactor modules are introduced to model catalyst pellets and back-mixing effects.

In our CRN, each zone (core, bubble, jet, etc.) is treated as a PFR or CSTR whose volumes and flow splits are tuned to match measured residence times. NetSMOKE++ (a C++ CRN solver built on OpenSMOKE++ libraries) integrates detailed Ni-catalyzed DRM kinetics and heat transfer. Because the network is solved as a set of ordinary differential equations, full microkinetic mechanisms can be used without the prohibitive cost of 3-D CFD[3]. This yields a rapid, high-fidelity model that captures the interplay of transport and chemistry more effectively than conventional CFD in many cases.

The multiphase CRN model was validated against laboratory FBR data. For example, a Ni/FCC catalyst tested at 800 °C and superficial gas velocity U_0 =0.1 m/s in a bubbling FBR gave ~57% CO_2 conversion and 41% CH_4 conversion (H_2 /CO ≈0.67)[4]. Our CRN prediction of syngas composition and conversion closely matched these values, and the trend of lower overall conversion (relative to a packed bed) due to bubble- induced bypassing was correctly captured. In general, the CRN results agreed with literature within experimental uncertainty, comparable to high-fidelity CFD studies[4]. Importantly, the CRN captured kinetic effects (e.g. CO_2 /CH_4 reaction order, reverse Boudouard coking kinetics) that are difficult for coarse CFD models to resolve.

Overall, the NetSMOKE++ multiphase CRN represents a powerful new simulation tool. It achieved >100× speed- up over detailed CFD while retaining detailed chemistry. The model

provides a computationally efficient way to explore design and operating conditions for catalytic FBR-DRM.

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Poster Presentation

Reactor Modeling and Design

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2026 / SEOUL, KOREA

DFN0203

Deactivation Kinetic Modelling and Industrial Multi-Stage Adiabatic Reactor Design for Deacon Process Using Cu-K-La Catalyst

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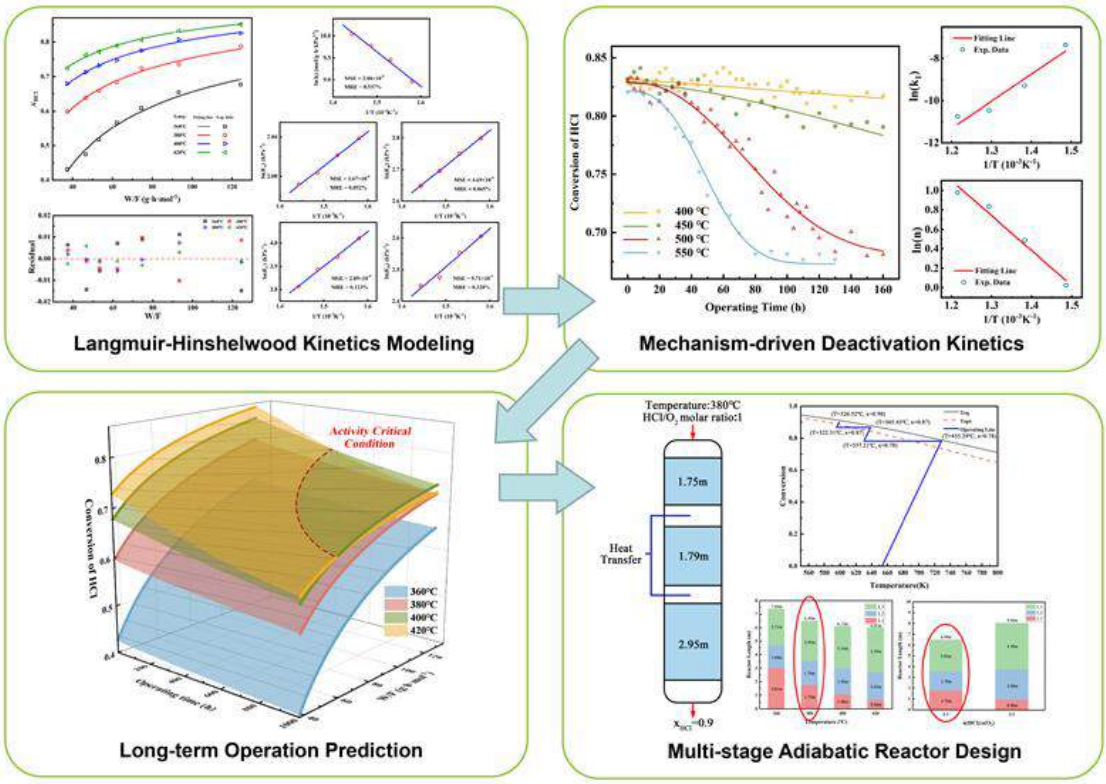
Abstract Category: Reactor Modeling and Design - Reactor Design - Fundamental

Keywords: Microkinetic modelling; Deactivation kinetics; Multi-stage adiabatic reactor.

Abstract Body.
Introduction.
The Deacon process provides a sustainable route for Cl2 production from HCl. Compared to expensive fixed beds or low-conversion fluidized beds, Cu-based catalysts in multi-stage adiabatic reactors (MSAR) offer a high-performance, low-cost alternative. However, high adiabatic temperature rises, particularly in the first stage, accelerate catalyst deactivation. This study aims to develop a deactivation kinetic model to predict long-term activity and optimize MSAR design for efficient industrial operation.
Methods.
Using a Cu-K-La/γ-Al2O3 catalyst, deactivation experiments were performed across 400–550 °C. A Langmuir-Hinshelwood microkinetic model served as the foundation, with selective deactivation functions established for model fitting. Kinetic modelling was solved in lsqnonlin, MATLAB, and the MSAR design was solved via a custom MATLAB subroutine utilizing 4th-order Runge-Kutta and Hooke-Jeeves methods.
Results and discussion.
The complete mechanism-driven deactivation kinetic has been established. The selective deactivation model yielded the best fit, enabling 1,000-hour activity predictions. Optimization results confirmed that MSAR outperforms ideal PFR and CSTR models with higher conversion and reduced bed height. The optimal first-stage operating temperature is recommended between 360–420 °C, with a 1:1 HCl/O2 feed ratio to maintain manageable bed heights. Additionally, variants of MSAR have been developed for specific application scenarios. This integrated framework provides a robust foundation for the industrial-scale implementation of Cu-based Deacon processes.



Integrated industrial process development: From microkinetic modeling to deactivation kinetics and multi-stage adiabatic reactor design.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

DFN0273

Enhancing Hydrodynamic Uniformity in Stirred Tanks Using an H-Like Fractal Impeller

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Abstract Category: Process Intensification - 선택 없음

Keywords: Fractal impeller, Stirred tank, Mixing, LES

Abstract Body.

The stirred tank reactor is a fundamental unit operation for mass transfer, momentum exchange, energy transport, and chemical reactions in fluids. It has wide applications in the petrochemical, fine chemical, biomedical, and metallurgical industries. However, conventional impellers often create uneven distributions of flow parameters, e.g., velocity and turbulent kinetic energy (TKE), and suffer from performance loss during scale-up. This study aims to address these issues by applying fractal theory to design a novel H-like fractal impeller (HLF series) for more uniform hydrodynamics and improved energy efficiency.

A self-similar fractal impeller was designed. Its performance was compared with the widely used Rushton Turbine (RT) using Time-Resolved Particle Image Velocimetry (TR-PIV) and Large Eddy Simulation (LES) to analyze flow patterns, vortices, TKE distribution, and power consumption. The flow characteristics were analyzed in standard baffled tanks with aspect ratios (H/D) of 1.0, 1.5 and 2.0.

Under equal specific power input (P/V), the fractal impellers generated significantly more uniform velocity and TKE fields than the RT impeller. Quantitatively, the standard deviation of the velocity field was reduced by approximately 11.4% for HLF-1 (primary fractal) at a standard aspect ratio (H/T=1.0). For higher aspect ratios (H/T=1.5, 2.0), the secondary fractal design (HLF-2) further improved uniformity, reducing the standard deviation by 10-20% compared to multiple RT impellers and effectively mitigating stagnant zones. Notably, the power number of the fractal impellers was lower than or comparable to their RT counterparts, demonstrating superior energy utilization.

In summary, the fractal impeller design successfully enhances hydrodynamic uniformity and mixing intensity while reducing energy consumption, particularly in tanks with high aspect ratios. This work validates fractal theory as an effective strategy for advanced impeller design, offering a promising solution to overcome scale-up challenges and improve efficiency in stirred tank reactors.

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DFN0321

Bayesian Optimization of Integrated Intercooling Systems in Rotating Packed Beds for Enhanced Carbon Capture Scale-up

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fundamental

Keywords: Rotating packed bed, CO2 absorption, Process intensification

Abstract Body.

Introduction

The Rotating Packed Bed (RPB) is a promising technology for post-combustion CO2 capture, as its high centrifugal force allows for the use of concentrated monoethanolamine (MEA > 70%). However, the reaction between MEA and CO2 is highly exothermic. These high concentrations generate excessive heat, raising the reactor temperature and reducing the driving force for mass transfer. This thermal degradation of efficiency intensifies as the reactor is scaled up. To mitigate this, we propose an intercooling system. This study simulates a pilot-scale RPB equipped with a heat exchanger and optimizes the design such as the location and size of the intercooler to maximize CO2 capture capacity.

Methods

A first-principle model of laboratory and pilot-scale RPBs, comprising an inner packing zone and an outer cavity zone, was developed and validated against experimental data [1]. A Bayesian optimization framework was employed to determine the optimal configuration for maximizing CO2 capture. The optimization variables included the inner and outer radius of the packing, packing height, and the spatial positioning and effective length of the intercooling system. Finally, a techno-economic assessment was conducted to evaluate industrial viability by comparing the CAPEX and OPEX.

Results

As illustrated in Figure 1, the intercooled RPB exhibits significantly higher relative efficiency compared to conventional systems, particularly at lower L/G ratios. In conventional RPBs, high MEA concentrations trigger an exothermic surge that hinders mass transfer However, the intercooling system effectively suppresses this temperature rise, preserving the driving force.

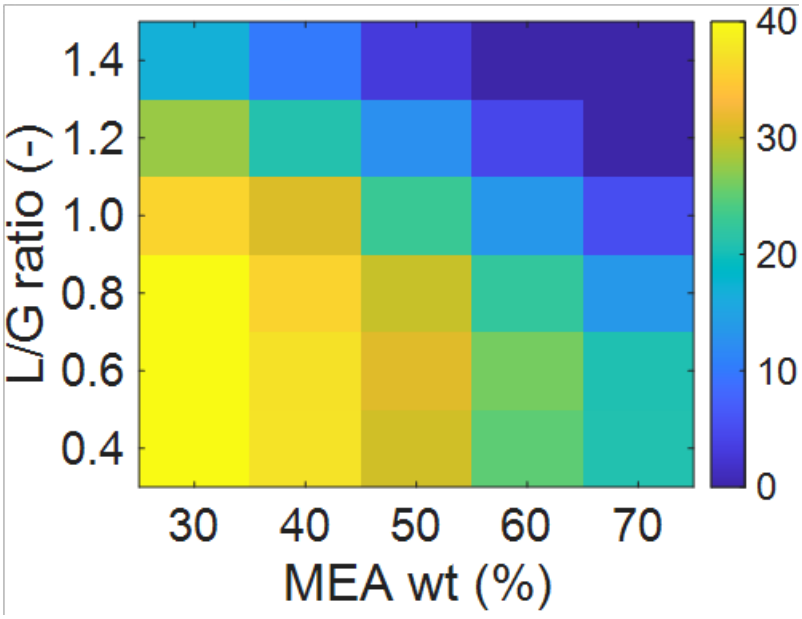

Figure1. relative efficiency for the intercooled RPB at 1150RPM compare to conventional RPB

The optimization reveals that optimal design points shift as the scale increases. While lab-scale units may tolerate certain thermal profiles, pilot and industrial-scale units require more strategic intercooler placement due to the increased path length and cumulative heat generation. The Bayesian framework identified these shifting optimizations, ensuring maximum capture capacity is maintained even during scale-up.

Conclusions

This study demonstrates that integrating an intercooling system within an RPB is a highly effective strategy for overcoming the thermal limitations of high-concentration MEA solvent systems. This research provides a robust design methodology for the next generation of industrial-scale, high-efficiency RPB absorbers in carbon capture applications.

[1] M. Akram et al. Fuel 388, 2025, 134484

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2026 / SEOUL, KOREA

DFN0557

On the importance of hard physical constraints in neural networks for kinetic mechanism discovery and accelerated reactor simulations

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fundamental

Keywords: Physics-informed neural networks, Catalysis, Physical hard-constraints, Surrogate modelling, Chemical kinetics, Mechanism discovery

Abstract Body.
Introduction. Machine learning has emerged as an important tool in chemical mechanism discovery, reduction, and acceleration [1]. In particular, neural networks have been used to discover reaction mechanisms from integral reactor data [2, 3], accelerate detailed reactor simulations [4], and directly predict the outcome of reactor simulations to allow for real-time evaluations [5]. All these applications have in common that they massively profit from the inclusion of hard physical constraints into the neural network structure. Here, we analyze and quantify the importance of these constraints (e.g., atom conservation and thermodynamic consistency) to improve model accuracy and robustness, demonstrating their key role in machine-learning assisted mechanism discovery and reactor surrogates.
Methods. We focus on two examples showing the effect of hard constraints on neural networks for chemically reactive systems. First, we modeled an externally cooled NiAlOx-catalyzed 1-D pseudohomogeneous CO2 methanation reactor [6] over a wide range of feed conditions (H2/CO2 = 2-10, 20% N2, T0 = 495–555 K) with a Physics-Informed neural network (PINN) and proposed the inclusion of atomic and energy conservation for surrogate accuracy and consistency. Second, we simulated 20 isothermal concentration profiles for 50 s with a reversible variant of the Searson trimerization mechanism [2] at different feed compositions. For the first time, we implemented thermodynamic consistency into Chemical Reaction Neural Networks (CRNNs) through De Donder constraints to allow for robust mechanism discovery.
Results and discussion. For the acceleration of CO2 methanation reactor simulations, the implementation of atom and energy conservation into PINNs does not only guarantee physically plausible solutions but also reduces the required amount of reactor data and strongly increases the reliability for extrapolation scenarios. The resulting model predicts temperature and composition at any point in the reactor within 5 % error and evaluates 28-times faster than ODE solvers. For mechanism discovery, the implementation of De Donder constraints into CRNNs strongly increases their robustness towards noisy data. While the standard CRNN cannot discover the correct trimerization kinetics, the thermodynamically consistent variant identifies the correct mechanism and kinetic parameters even when up to 50 % noise is added to the data. As the consistent model makes use of the intrinsic connection between forward and reverse reactions, it has at least 50 % fewer parameters to learn. Overall, we provide an extensive overview on the effect of hard physical constraints on neural networks for kinetic mechanism discovery and accelerated reactor simulations, highlighting their importance for robust, consistent and accurate results.

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2026 / SEOUL, KOREA

DFN0753

Multidimensional Modeling of Fixed-Bed Reactors for CO_2-Assisted Propane Oxidative Dehydrogenation

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fundamental

Keywords: Oxidative dehydrogenation of propane(ODPC), Fixed-bed reactor modeling, Reactor scale-up

Abstract Body.

Conventional propane dehydrogenation (PDH) processes suffer from high energy consumption and substantial CO2 emissions, which limit their sustainability. As an alternative, oxidative dehydrogenation of propane with CO2 (ODPC), which utilizes CO2 as a mild oxidant, has been proposed. In this study, an integrated fixed-bed reactor modeling and scale-up strategy for the ODPC process is presented, incorporating reaction kinetics, reactor geometry, and heat- and mass-transfer effects.

First, a reaction kinetics model based on the Mars–van Krevelen (MvK) mechanism was developed using 27 experimental cases obtained from a differential reactor, and the kinetic parameters were estimated. A hybrid optimization framework combining Monte Carlo simulation, particle swarm optimization, and the interior-point method was employed to determine the pre-exponential factors and activation energies. The estimated kinetic parameters reproduced the experimental results with a root-mean-square deviation (RMSD) of 3%, confirming the reliability of the developed model.

Based on the reaction-rate expression, a one-dimensional fixed-bed reactor model was constructed in MATLAB and validated by incorporating heat- and mass-transfer equations, assuming pelletized catalyst particles. Subsequently, optimal operating conditions maximizing CO2 conversion and propylene yield.

To account for radial temperature gradients and heat-supply limitations during scale-up, a two-dimensional fixed-bed reactor model that accounts for axial and radial directions was further developed. Using a predefined reactor volume and optimal operating conditions, the reactor length-to-diameter ratio (L/D) was selected as the key geometric variable, and reactor performance was systematically compared to identify configurations that simultaneously optimize reaction performance and heat-transfer efficiency.

In addition, sensitivity analyses were performed by varying the reactor diameter while maintaining the optimal L/D ratio, thereby identifying a critical reactor size beyond which heat transfer limitations and performance deterioration become significant. The effects of catalyst shape and particle size on reactor performance were also evaluated from a heat- and mass-transfer perspective. Finally, the reactor model was extended to computational fluid dynamics (CFD) simulations to further analyze heat transfer characteristics in multitubular reactor systems.

In summary, this study establishes an integrated modeling framework for the ODPC process by combining an experimentally validated MvK-based kinetic model with one- and two-dimensional fixed-bed reactor models that account for heat and mass transfer effects.

The framework enables the systematic evaluation of optimal operating conditions, reactor geometry, and scale-up limitations, and provides a reliable basis for reactor scale-up and thermal optimization of ODPC processes.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

DFN5689

Modeling and Simulation of a Fixed Bed Reactor for Fischer-Tropsch Reaction Using Hierarchically Porous MFI Zeolites Supported by Metal Nanoparticles

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fundamental

Keywords: Fischer-Tropsch, e-Fuel, Modeling and Simulation, Hierarchically Porous MFI Zeolites, Metal Nanoparticle Catalysts

Abstract Body.
Introduction.
Fischer–Tropsch (FT) synthesis in fixed-bed reactors has gained renewed interest as a viable pathway for producing sustainable aviation fuel (SAF) and e-fuels. Hierarchically porous MFI zeolite-supported metal nanoparticle catalysts are particularly attractive due to their acidic properties, which promote secondary hydrocarbon cracking and modify product selectivity. However, conventional FT kinetic models are primarily formulated for synthesis-dominated systems and do not explicitly account for catalyst-induced cracking reactions. As a result, their predictive capability is limited when product distribution and thermal behavior are strongly influenced by coupled synthesis–cracking pathways.
Methods.
In this study, an established Fischer–Tropsch synthesis kinetics framework is extended to incorporate hydrocarbon cracking reactions occurring on acidic catalyst sites. The FT synthesis rate is described using a Langmuir–Hinshelwood–Hougen–Watson (LHHW) formulation combined with a chain-growth probability to consistently predict hydrocarbon distribution and reaction heat. Kinetic parameters for the synthesis reaction are adopted from the literature and refined using experimental data. Hydrocarbon cracking is modeled as a set of parallel secondary reactions to FT synthesis. Cracking kinetics are represented using Arrhenius-type rate expressions with chain-length-dependent activation energies, reflecting the enhanced reactivity of long-chain hydrocarbons on acidic zeolite sites. This approach enables temperature-dependent competition between chain growth and cracking reactions while preserving the intrinsic FT reaction mechanism. The combined kinetic model is implemented in a fixed-bed reactor model developed in gPROMS, where reaction kinetics are fully coupled with mass and heat transfer. The model captures the complex thermal and compositional interactions arising from simultaneous synthesis and cracking under practical operating conditions.
Results and discussion.
The validated reactor model reproduces experimental trends in CO conversion and hydrocarbon product distribution, capturing the temperature-dependent competition between chain growth and catalyst-induced cracking that governs SAF and e-fuel selectivity. By extending conventional Fischer–Tropsch kinetics with Arrhenius-type cracking reactions, the proposed framework links catalyst-level reactivity to reactor-scale performance. This capability enables quantitative evaluation of selectivity and thermal behavior under varying operating conditions, providing a practical basis for the design, optimization, and scale-up of

fixed-bed FT reactors for carbon-neutral fuel production.

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DFL0055

Electrifying Fluidization: Particle-Resolved Modeling of Direct Resistive Heating in Electrothermal Fluidized Beds

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fluidization/Multiphase Flow Reactors

Keywords: Electrification; Electrothermal fluidized bed reactors; CFD-DEM; Direct resistive heating

Abstract Body.
Electrification is reshaping the chemical industry, with power-to-heat (P2H) strategies using green electricity emerging as a compelling route for sustainable process intensification. Electrothermal fluidized bed reactors (e-Beds) are particularly promising, combining the ~100% efficiency of direct resistive particle heating with the excellent mixing and transport characteristics of fluidization. Yet industrial deployment remains limited due to an incomplete understanding of their complex multiscale multiphysics behavior. State-of-the-art studies of direct resistive particle heating fail to capture the physical phenomenon of these reactors. This work presents the first particle-resolved modeling framework for electrical conduction and Joule heating in e-Beds, providing fundamental insights into their coupled thermo-electro-hydrodynamic physics. Computational Fluid Dynamics (CFD) coupled with the Discrete Element Method (DEM) is used to model gas and particle dynamics in e-Beds, respectively. Conductive electrical pathways are identified using a resistor-network approach that builds evolving particle-contact networks with DEM neighbor lists and employs a label-propagation search algorithm from graph theory to track current-carrying connections. Assuming ohmic behavior at particle contacts, conservation laws of current density and charge are then used along each pathway to compute electric potentials, from which electric current and Joule heat generation follow. Beyond fluidization in e-Beds, this methodology also provides a new framework for studying electricity transfer in granular flows. At high temperatures where radiative transfer dominates, a Monte Carlo ray-tracing method is used. Model predictions agree well with electrically heated fixed-bed experiments, accurately capturing I-V and power-temperature profiles. Electrostatic and electric-field effects on hydrodynamics are incorporated by solving the Laplace equation for the electric potential and applying electrostatic contact-force models with spatially resolved electric fields, verified against analytical solutions. Electrical conductivity is treated as temperature-dependent. Simulations of a prototype 2D e-Bed with a central electrode reveal dynamic localization of Joule heating near the electrical source and preferential current transport along the shortest low-resistance pathways. As bubbling rearranges the particle contact network, the formation and disruption of conductive pathways cause reactor-scale Joule power to oscillate at the characteristic bubbling frequency. A systematic parametric study under constant-voltage conditions further shows that the heating rate does not increase linearly with the applied voltage, and that smaller particles heat faster due to higher conductive contacts. This model, along with these findings, establishes the scientific basis for designing next-generation

electrically heated fluidized bed reactors for catalytic and thermal processes.

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DFL0346

Modeling and Optimization of Gas Flow Distribution in Blast Furnace Charging under Hydrogen-Rich Conditions for Carbon-Neutral Steelmaking

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fluidization/Multiphase Flow Reactors

Keywords: blast furnace; burden distribution; gas flow; hydrogen-rich; CFD-DEM

Abstract Body.

Transitioning blast furnace operation toward hydrogen-rich conditions has become a key focus for achieving carbon-neutral steelmaking. This study aims to investigate the influence of hydrogen-enriched gas atmospheres on gas flow distribution within the burden bed in blast furnace throat and explore optimization strategies for burden distribution under such conditions. Coupled CFD-DEM (Computational fluid dynamics - Discrete element method) simulations were conducted to model gas flow patterns and burden distribution in the blast furnace throat at varying hydrogen concentrations. The DEM method simulated the realistic burden bed distribution under actual charging conditions, while CFD calculated the gas flow behavior through the particulate bed. The effects of hydrogen enrichment on velocity fields, pressure distribution, and flow uniformity within the charging zone were systematically analyzed. Simulation results indicate that increasing hydrogen concentration significantly modifies gas flow behavior, causing notable changes in velocity profiles and pressure gradients. These alterations impact the uniformity of burden distribution, which is critical for maintaining stable and efficient furnace operation. Quantitative analysis provides insight into how hydrogen enrichment affects internal flow dynamics. This study underscores the importance of considering hydrogen-enriched gas properties in blast furnace operation. The findings guide optimization of charging strategies to improve burden distribution under hydrogen-rich conditions, contributing to the development of low-carbon steel production technologies. The approach supports the broader objective of carbon neutrality in the steel industry.

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DFL0371

Markov chain assisted Monte Carlo model for direct air capture in fluidized bed system

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fluidization/Multiphase Flow Reactors

Keywords: Direct air capture (DAC), Metal-organic framework (MOF), HKUST-1, Monte Carlo, Computational fluid dynamics (CFD)

Abstract Body.

Rising global CO_2 emissions from human activities have accelerated the development of carbon capture, utilization, and storage (CCUS), and have also positioned direct air capture (DAC) as a necessary pathway for mitigating distributed and hard-to-abate emissions. However, capture processes optimized for high-CO2 point sources face inherent limitations under ultra-dilute atmospheric conditions (~400 ppm), including higher specific regeneration energy associated with cyclic desorption, and performance degradation driven by mass-transfer resistances. In this study, we developed a dynamic model for interpreting time series data on direct air capture system operating in fluidized bed, applied HKUST-1 as a CO2 sorbent. Particularly, a particle-resolved Monte Carlo simulator was developed to retain particle-specific state variables, residence-time variability, and cumulative adsorption-desorption cycle history while enforcing reactor-scale mass balances. The developed model was then validated with the computational experimental data driven by the computational fluid dynamics (CFD) simulation. The framework improves fidelity relative to deterministic, averaged models and enables mechanistic attribution of performance variability to dominant stochastic drivers, particularly particle-size-dependent diffusion scaling and residence-time distributions. Overall, the results highlight the need for integrated equilibrium-kinetic-flow coupling to achieve reliable design and scale-up of MOF-based DAC systems, and provide a computational basis for performance prediction and process optimization under realistic atmospheric capture conditions.

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DFL0428

A User-Defined Electrothermal Fluidized Bed Reactor Model for Direct Joule Heating with Application to Non-Oxidative Coupling of Methane

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fluidization/Multiphase Flow Reactors

Keywords: Methane conversion, Electrified reactors, Two-phase fluidization modeling

Abstract Body.
Electrothermal fluidized bed reactors (EFBRs) are promising for high-temperature gas–solid endothermic reaction systems, including methane coupling, because of their high heat-transfer rates and precise temperature control. Within EFBR designs, direct Joule heating delivers electrical energy by passing current through electrically conductive bed particles, generating heat internally through electrical resistance. This enables uniform bed temperatures and high electrical heating efficiency. However, there is no built-in reactor model available in commercial process simulators for electrothermal fluidized bed reactors with direct Joule heating. Consequently, a user-defined EFBR reactor model is required to enable realistic process-level assessment of EFBRs with direct Joule heating.
Within the CAMELEON project, a preliminary one-dimensional reactor model for an electrothermal fluidized bed reactor with direct Joule heating is being developed. The model is based on an axially resolved two-phase bubble–emulsion description of the fluidized bed. The governing equations describing mass and energy transport in the fluidized bed are implemented and solved in MATLAB. The model is designed to be coupled with Aspen Plus as a CAPE-OPEN–compliant user-defined unit operation, enabling the exchange of material and energy streams at the flowsheet level. Application to a non-oxidative methane coupling (NOCM) system is considered as a case study, using gas-phase chemistry described by the AramcoMech 3.0 mechanism and surface reactions based on established literature models. The model provides detailed axial profiles for the bubble and emulsion phases, capturing the impact of interphase mass transfer on methane conversion and product selectivity. The framework calculates the axial energy requirement of the reactor, quantifying the electrical power needed to sustain the endothermic NOCM reaction, with preliminary reactor-level results indicating an energy demand of approximately 19.1 kJ per mol of methane feed. In addition, it provides a predictive tool to assess how variations in superficial gas velocity and electrical input affect reactor efficiency.
Overall, this work presents a process-oriented modeling framework for directly Joule-heated electrothermal fluidized bed reactors that can be integrated into industrial process simulation environments. The proposed approach provides a foundation for assessing and further developing electrified fluidized bed concepts for NOCM applications, as well as for future techno-economic and sustainability studies.

Acknowledgment
This work was performed in the framework of the Moonshot clusterSBO project CAMELEON (HBC.2023.0551 “Electrified catalytic non-oxidative methane coupling for separated hydrogen and ethylene production"), with the financial support of the European Recovery Fund and VLAIO (Flemish Agency for Innovation and Entrepreneurship) via the Flemish spearhead cluster Catalisti.

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DFL0474

Modeling Mass Transfer-Reaction in a Single Diesel Hydrotreating Particle via CFD-VOF-PMM

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fluidization/Multiphase Flow Reactors

Keywords: CFD-VOF-PMM model, Diesel hydrotreating process, Single porous particle, Dynamic liquid distribution

Abstract Body.
Although early studies often assumed that catalyst particles were in a fully wetted state, various factors during actual reaction processes can lead to the formation of unwetted regions inside the particles. To investigate the dynamic liquid distribution within a particle, this study established a multiscale CFD-VOF-PMM model and incorporated a capillary force model to describe liquid flow inside the pores. The method was first validated in the AMS hydrogenation system, where the simulated flow patterns showed good agreement with experimental observations. Subsequently, for a heterogeneous diesel hydrotreating system, the apparent reaction was decomposed into five key steps, coupling liquid flow with mass transfer, heat transfer, evaporation, and reaction processes. The study found that when evaporation was neglected, variations in different physical parameters generally resulted in liquid holdup values above 0.8. However, after introducing the evaporation effect induced by strongly exothermic reactions, increased temperature and gas velocity led to a significant decrease in liquid holdup. Enhanced evaporation triggers gas-liquid two-phase displacement inside the particle, which substantially reduces the effectively wetted area and limits reactant contact, thereby becoming a key mechanism restricting the overall reaction process. This research clarifies that internal phase change and flow driven by evaporation represent the core microscopic processes affecting trickle-bed reactor performance, providing a new theoretical basis for catalyst design.

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DFL0484

Fluidization of Bed Material and Catalyst Mixture for Optimizing Methane Pyrolysis

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fluidization/Multiphase Flow Reactors

Keywords: Hydrogen Production, Methane Pyrolysis, Fluidized-bed Reactor, Computational Particle Fluid Dynamics (CPFD), Multiphase Particle-In-Cell (MP-PIC)

Abstract Body.

Methane pyrolysis is a promising route for CO2-free hydrogen production because it directly converts methane into hydrogen and solid carbon, eliminating CO2 separation while enabling carbon recovery. For large-scale operation, packed-bed reactors can experience clogging and severe flow restriction due to carbon deposition, whereas fluidized-bed reactors can better handle deposited carbon and sustain catalyst activity through continuous catalyst renewal [1]. However, burner-heated fluidized beds often suffer from temperature non-uniformity, which can induce catalyst sintering at hot spots and reduced activity, poisoning, and coking in colder regions. This study numerically investigates the mixing behavior of the bed material and catalyst mixture in a fluidized-bed reactor and verify the results by a lab-scale cold-bed reactor designed for visualization. Bed hydrodynamics were simulated using the multiphase particle-in-cell (MP-PIC [2]) method in Barracuda CPFD [3], employing an Eulerian description of the gas phase and Lagrangian tracking of solid parcels to represent semi-dense multiphase flows efficiently. The bed was composed of spherical particles (460 μm diameter, 2,650 kg/m3 density) with an initial bed height of 10 cm and an initial in-bed gas volume fraction of 0.43. The results show relatively mild bed fluctuations near the minimum fluidization condition (0.3 m/s), while more active particle motion and pronounced bubbling are observed at 0.45 and 0.6 m/s. Across the tested range, the bed remains in the bubbling regime without transition to slugging or turbulent regimes, and the predicted particle behavior agrees well with observations from a lab-scale pilot reactor. The proposed MP-PIC-based workflow enables efficient evaluation of operating-condition-dependent fluidization behavior and provides derived scale-up metrics, including vertical voidage profiles, surface-to-volume ratio, and space velocity, to optimize reactor design and operating strategies toward stable industrial-scale CO2-free hydrogen production.

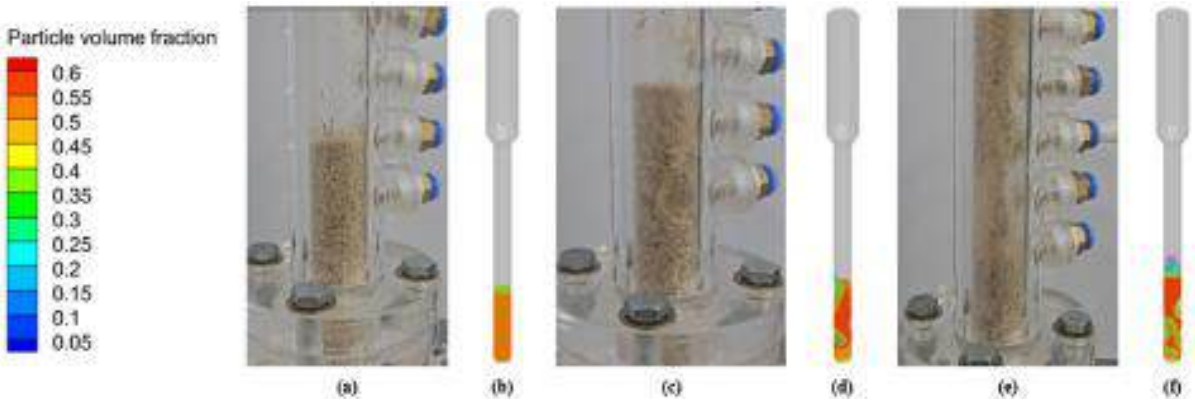

Figure 1: Cold-bed experiments for three inlet gas velocities (a, c, e) and corresponding MP-PIC simulations (b, d, f)

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DFL0525

Mixing Characteristics of Binary Particles in a Fluidized Bed of Carbon Nanotubes

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fluidization/Multiphase Flow Reactors

Keywords: Carbon nanotube, Solid mixing, Binary mixture, Fluidized bed

Abstract Body.
Introduction. Carbon nanotubes (CNTs) are widely used in various applications due to their excellent physical, thermal, and electrical properties [1]. Fluidized bed catalytic chemical vapor deposition (FBCCVD) has been extensively adopted for the continuous and large-scale production owing to its high heat and mass transfer efficiency [2]. In continuous CNT production process, effective mixing between catalyst particles and synthesized CNTs is critical for maintaining stable bed operation [3]. A quantitative understanding of solid mixing behavior is essential for the design and optimization of continuous CNT fluidized-bed reactors [3].
In this study, the fluidization behavior of CNT beds with the catalyst was investigated using a borescope probe, and the degree of mixing was quantified by image processing and a solid segregation index under various operating conditions.
Methods. The cold-flow fluidized bed consists of a transparent Plexiglas main column (0.15m-i.d. by 2.0m) and a tuyere-type gas distributor. Vertically aligned multi-walled carbon nanotubes (MWCNTs) and Geldart A catalyst particles were employed as bed materials, with catalyst volume of 0.04 to 0.10. Local mixing behavior was measured using a borescope probe (25mm-i.d.) installed 40mm above the distributor, which could be traversed horizontally. The degree of mixing was determined using image processing of captured particles behavior.
Results and discussion. The minimum fluidization velocity of the mixtures (Umf,M) was found to be between the Umf values of the CNT and the catalyst particles. The Umf,M was decreased with increasing the volume fraction of catalyst particle because the motion of catalyst particles disrupted the CNT network formed by strong interparticle forces. The local volume fraction of catalyst particles increased radially from the center to the wall due to wall effect, whereas increasing gas velocity reduced the radial gradient in local concentration, resulting in a more uniform mixing. The local segregation index, ranging from -1 to 1, approached zero from negative values as the gas velocity increased, indicating an improvement toward complete mixing. It decreased with increasing the volume fraction of the catalyst particle due to their accumulation at the bottom by the large density difference between the CNTs and the catalyst particles.

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DFL0555

A dynamic FBR framework for CH4 pyrolysis over Fe/Al2O3

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fluidization/Multiphase Flow Reactors

Keywords: Keywords: CH4 pyrolysis, Dynamic modelling, Iron catalyst, Activity decay, Carbon growth

Abstract Body.

Please, refer to the attached PDF file; I am reporting the abstract body text due to impossibility to go on with the submission.

Introduction: Catalytic CH4 pyrolysis is a promising bridging technology for low-C hydrogen production without direct CO2 emissions [1]. In this work, the dynamic macroscopic model of a pyrolysis fluidized bed reactor (FBR) using Fe-based catalyst is developed, deepening the understanding of the effect of C-accumulation on fluid dynamics, kinetics, deactivation and integral reactor performance, true challenge towards industrial reactor design.

Methods: The model is based on the three-region Kunii–Levenspiel fluidized bed framework [2]. It predicts the axial and temporal evolution of gas-phase composition, while solid carbon deposition is described through dedicated mass balance equations. Independent correlations, linking the rate of reaction and the particle properties to the evolving carbon loading (obtained by dedicated experimental campaigns) were herein embedded to predict the axial and temporal evolution of conversion, bed height, and fluidization behavior, ultimately providing a comprehensive tool to describe the reactor dynamic performance.

Results & discussion: Simulations of a bench-scale FBR (ID 2.55 cm) show that CH4 concentration and gas mass flowrate decrease along the reactor height due to conversion and C-deposition. With time, C-growth reduces activity and modifies the particle size and density, resulting in reduced conversion, increased bed height, and evolving fluidization characteristics. A parametric analysis varying temperature and methane concentration highlighted the impact of operating conditions on performance: reducing inlet methane concentration promotes higher conversion and slower deactivation, although limiting hydrogen productivity (Fig 1a). Conversely, higher temperatures result in higher initial conversions and hydrogen yields, but accelerate carbon deposition and consequent deactivation, hindering catalyst lifetime (Fig 1b). The proposed dynamic framework allows the simulation of CH4 pyrolysis in FBRs under realistic operating conditions. It enables the interpretation and analysis of experimental data and the identification of operating windows where chemical regime dominates. Therefore, it highlights key controlling parameters and trade-offs in performance indicators, ultimately making the FBR a reliable tool for the kinetic investigation of this complex process. Overall, by describing the evolving kinetics and solid properties, this framework not only allows for the design and simulation of lab-scale reactor and operation, but also for the analysis and scale-up of industrial reactors.

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DFL0583

Modified two-phase theory (MTPT)-based reactor network model for a bubbling fluidized bed co-gasifier coupled with particle population balances

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fluidization/Multiphase Flow Reactors

Keywords: Reactor network model, Co-gasification, Modified two-phase theory, Discretized population balance

Abstract Body.
Rapid and expeditious phasing-out of coal is impractical, particularly in developing nations, as coal is still the largest individual energy source for electricity production worldwide. In light of coal-only utilization being the primary concern for global climate change, co-utilization of coal with biomass allows for its continued use for the integrated production of electricity, heat, fuels/chemicals through co-gasification-based polygeneration framework potentially resulting in carbon neutrality when paired with carbon capture, utilization, and storage. Fluidized bed technology offers exceptional fuel flexibility compared to other gasifier types and thus, is more amenable for the co-gasification of diverse, low-quality, and opportunistic fuels alongside coal. Classical two-phase theory (TPT) based semi-mechanistic reactor network models are widely applied to simulate bubbling fluidized bed gasifiers by splitting the bubbling zone into solids-free bubble and emulsion phases. Original version of this theory assumes that all the excess is transferred to the bubble phase such that incipient fluidization conditions are maintained in the emulsion phase; this has been reported to be an overestimation of visible bubble flow. In this work, we present a novel one-dimensional steady-state reactor network model for a bubbling fluidized bed co-gasifier coupled with particle population balances that includes bulk mass transfer terms in species conservation equations to compute the flow split between phases using locally evolving hydrodynamic correction factors in accordance with modified TPT (MTPT). Moreover, considering the intrinsic differences in chemical structures, compositions, and thermal behaviour between coal and biomass and the consequent effect on devolatilization mechanisms and yields, up-to-date multi-step devolatilization kinetic models have been employed to predict yields and composition of devolatilization products (light gases and tars) including residual char. Non-isothermal treatment of bubble and interstitial emulsion gases, heterogeneous kinetics accounting for pressure and product inhibition effects, homogenous and secondary tar conversion chemistry and discretized particle population balances for coarse and fine chars to compute char inventory and distribution in the bed considering hybrid thermal fragmentation, reaction-enhanced attrition, and volumetric char–gas reactions are additional features of the model. The predicted major gasification performance metrics such as syngas composition and carbon conversion reasonably match with published co-gasification experimental data. This comprehensive model may be used for the scale-up and optimization of co-gasification process.

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DFL0596

A hybrid Eulerian-Lagrangian multiphase CFD approach for gasification of high-ash coal under oxygen-enriched conditions in a pilot-scale bubbling fluidized bed

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fluidization/Multiphase Flow Reactors

Keywords: High ash coal, Hybrid Eulerian-Lagrangian, DPM, CFD, Oxygen-enrichment, Bubbling fluidized bed

Abstract Body.
Gasification of high-ash coal (ash content >30%) in a bubbling fluidized bed (BFB) reactor presents significant operational and technical challenges due to the complex interactions between gas-solid phases and the influence of ash on fluidization behavior. Accurate prediction of bed hydrodynamics and coal particle conversion under reactive conditions is essential for optimizing reactor performance and syngas yield. To address these challenges and support indigenous technology development, a 1.5 Tonnes Per Day (TPD) pressurized fluidized bed gasification (PFBG) pilot plant has been developed and successfully installed and commissioned at CSIR–Central Institute of Mining and Fuel Research (CIMFR), Dhanbad, India. The pilot facility is designed to process coal/biomass at a feed rate of 1.5 TPD, operating at pressures up to 10 kg/cm² and temperatures up to 1050 °C, using air/oxygen and steam as gasifying agents. Along with experimental investigations, Computational Fluid Dynamics (CFD) provides a powerful tool for understanding and simulating these multiphase, multiscale processes with high spatial resolution.

In this study, a 3-Dimensional Hybrid Eulerian-Lagrangian multiphase modeling approach is employed to simulate air/oxygen/steam-blown gasification of high-ash coal in a pilot-scale BFB reactor. The gaseous phase (gasifying agents) and the inert bed material (representing ash) are modeled using an Eulerian and Eulerian-granular framework, respectively. Meanwhile, the coal particles are tracked using the discrete phase model (DPM) in a Lagrangian framework to account for particle-scale physics. The model incorporates sub-processes such as coal injection, heating, drying, devolatilization, and heterogeneous char gasification. The simulation predicts the spatial and temporal evolution of coal particle temperature, conversion, and gas product composition (CO, H2, CO2, CH4). Volume fraction distributions of gas, and solid phases are monitored to evaluate bed fluidization quality. The performance parameters and syngas yield are also predicted under oxygen-enriched environments.

The developed CFD framework offers physically consistent insights into the coupled hydrodynamic–reaction behavior of high-ash coal gasification in fluidized beds and serves as a robust tool for process optimization, operational stability assessment, and scale-up of

indigenous pressurized fluidized bed gasification systems.

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DFL0648

Fluidized bed thermocatalytic processing of liquid feedstocks: the case of steam reforming of biomass-generated pyrolytic bioliquids

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fluidization/Multiphase Flow Reactors

Keywords: fluidized bed, liquid feeding, biooil, steam reforming, biomass

Abstract Body.
Fluidised bed reactors are widely used in chemical engineering as heterogeneous, gas-phase thermocatalytic converters. When the feedstock is available in liquid form, operating the reaction by directly injecting liquid reactants into the fluidised bed may be preferable to feeding reactants in vapour form. Direct feeding of liquid feedstock eliminates the need for a pre-evaporation stage. Furthermore, hot-spot formation at the reactant feed point can be effectively moderated by the endothermic phase change that follows liquid injection. However, direct liquid feeding requires careful consideration of clogging and flow instability issues.
This study examines key aspects of thermocatalytic processing of liquid feedstocks in fluidised beds with direct liquid injection, focusing on steam reforming of pyrolytic bio-oils generated from biomass. First, a mechanistic framework was established, the key aspects of which are: a) the interaction of the liquid feedstock with the fluidised solids, driven by pressure, viscous and interfacial forces; b) the formation of liquid-particle agglomerates; c) the vaporisation of the liquid phase; d) the formation of 'endogenous' vapour bubbles; e) the dispersion of agglomerates away from the feeding point, promoted by the motion of the fluidised solids. A key variable is the liquid loading established at steady state as a result of the balance between liquid feeding and vaporisation. The latter depends on the heat transfer rate from the bulk of the bed to the region occupied by the liquid, which is driven by the motion and circulation of the fluidised solids. This complex framework underpins the set of reactions responsible for the chemical conversion of the feedstock, driven by the cooperative/competitive effects of thermally activated homogeneous reactions in the liquid and vapour phases, interphase mass transfer between bubbles and the emulsion phase of the bed, and catalysed heterogeneous reactions on the solids.
The general validity of the proposed framework has been verified in experiments conducted under non-reactive conditions, by feeding water to a 78 mm ID hot bubbling fluidised bed reactor through a refrigerated injection nozzle, operated with or without liquid gas atomisation. The extent of liquid loading in the bed as a function of the liquid feeding rate was characterised using a purpose-designed experimental setup and technique at temperatures up to 500 °C and with different combinations of gas superficial velocity and liquid feed rate. The results have been analysed and discussed to provide guidelines for the

optimal design and operation of liquid-fed fluidised bed thermocatalytic converters.

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DFL0674

Particle Breakage and Aggregation in Fluidized Bed Gasification: An Integrated Experimental and Population Balance Modelling Approach

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fluidization/Multiphase Flow Reactors

Keywords: Particle breakage; particle aggregation; population balance modelling; fluidised bed; cold flow study

Abstract Body.
Uncontrolled particle breakage and aggregation present significant operational challenges in fluidized bed gasifiers. While breakage generates fines that elutriate and reduce carbon conversion efficiency, aggregation can lead to bed de-fluidization and eventual system shutdown. Together, these phenomena induce polydispersity, resulting in unpredictable bed hydrodynamics. Consequently, a fundamental understanding of the particle-scale dynamics governing these processes is critical for stable operation. This study integrates cold-flow batch experiments with population balance equation (PBE) modeling to characterize evolving particle size distributions. Using silica gel and silica sand as experimental analogues for breakage and aggregation respectively, we employed inverse modeling via genetic algorithms to determine governing kernel functions. Key parameters, such as breakage frequency, daughter particle distribution, and aggregation frequency, were precisely quantified. As a cold-flow experimental mock up, a fluidized bed of silica gel (dp=1.85 and 1.55 mm) and silica sand (dp=0.3675 and 0.23 mm) were used for mimicking particle breakage and aggregation, respectively.
Results indicate that breakage is best described by a power-law model with a tri-modal log-normal distribution, while aggregation frequency follows an exponent of the sum of inverse particle sizes. Figures 1 (a) and (b) show the temporal evolution of the Sauter mean diameter for one run of particle breakage and aggregation, respectively. These findings establish a robust framework for predicting particle behaviour and defining safe operational regimes in gasification systems.

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DFL0677

Solid Flow-Pattern in a Sidewall Injected High Temperature Gas-Solid Fluidized Bed Using Radioactive Particle Tracking Technique

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fluidization/Multiphase Flow Reactors

Keywords: Radioactive particle tracking, Fluidized Bed, Gas-solid, High Temperature, Velocity Measurement, Sidewall Nozzle

Abstract Body.
Introduction Nozzles assisted gas solids fluidized bed has wide applications in chemical process industries for various processes like fluid coking, coating, thermal denitration, drying etc. In all these processes some precursors/reactants are added to the gas-solids fluidized bed reactor in atomized form through side nozzle injections. The excess gas that is injected through side nozzles to assist atomization increases the bed voidage in the vicinity of the injection. This leads to severe gas bypassing and poor gas-solids contacting. Further, most of these processes requires high temperature, which further modifies the mixing characteristics of the bed. In lack of reliable experimental data, most of these reactors are still designed and scaled up by using some heuristic rules. The current work aims to develop a detailed understanding of nozzle assisted high temperature gas-solids fluidized bed by using radioactive particle tracking (RPT) technique. Experiments are performed for different gas inlet velocities, bed temperature and side wall nozzle injection flowrates in a specially designed high temperature gas-solid fluidized bed and solid flow field is measured by using RPT.
Methods In RPT, velocity field of a single radioactive tracer particle, which is the marker of the flow (in current case solid), is tracked by using an array of scintillation detectors. Experiments are performed in a 3-inch diameter and 1.5 m long gas-solid fluidized bed reactor. The solid velocity fields are measured at different gas inlet velocities (U/Umf: 2, 2.5 and 3), temperatures (50-200 ℃) and side wall nozzle injection flowrates (10-100 LPM). The total bed mass is kept constant (3.6 kg) in all the experiments. Data was acquired at a frequency of 50 Hz.
Results and discussion The results indicate that for no sidewall nozzle injection, solids were moving up at the center and down near the wall for all the temperatures. The solid velocity increases with increase in bed temperature as the gas density is reduced which enhances the gas volumetric flowrate. Further, it was observed that the solid velocity field becomes asymmetric with sidewall nozzle injection and now the solid moves upward towards the nozzle injection wall and downwards near the opposite wall. This was mainly due the low-pressure zone created due to the nozzle injection which led to migration of gas bubbles

coming through the bottom of the column towards the nozzle injection wall. The detailed quantitative results for all the experimental conditions will be presented in the final contribution.

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DFL0751

Hydrodynamic Analysis and Correlation of Solids Circulation in Pressurized High-Temperature CFB

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Abstract Category: Reactor Modeling and Design - Reactor Design - Fluidization/Multiphase Flow Reactors

Keywords: Circulating fluidized bed; Solids circulation rate; Hydrodynamics; MP-PIC

Abstract Body.
Calcium looping has been extensively studied as a carbon capture technology for high-temperature CO2 capture in circulating fluidized bed systems. In circulating fluidized bed–based CaL processes, the solids circulation rate (Gs) is an important hydrodynamic indicator influencing gas–solid contact and particle residence time during operation. Previous studies on Gs have mainly focused on high-temperature atmospheric conditions or cold-flow pressurized systems. However, practical CaL operation is typically conducted under combined high-temperature and high-pressure conditions, where gas–solid hydrodynamics can differ substantially. Accordingly, the applicability of existing solids circulation correlations to realistic operating conditions remains limited. This study derives a Gs correlation under representative high-temperature and high-pressure conditions.

Hydrodynamic simulations were performed using the Barracuda Virtual Reactor based on the MP-PIC method. A circulating fluidized bed configuration representative of a calcium looping system was analyzed under high-temperature and high-pressure conditions by varying the superficial gas velocity to account for pressure-dependent changes in gas properties and characteristic velocities. The solids circulation rate was evaluated under steady-state conditions based on the simulation results.

Under high-temperature and high-pressure conditions, Gs exhibits a nonlinear dependence on gas velocity. Based on the simulation results, a hydrodynamics-driven correlation for predicting solids circulation rate was derived, capturing the influence of gas velocity under pressurized operation. The proposed correlation provides a practical basis for estimating Gs in calcium looping systems operated under realistic conditions and supports reactor design and scale-up considerations.

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DFL0778

A Cyclic Molten Metal Process for F-gas Decomposition and Metal Fluoride Regeneration Enabling Fluorine Recovery

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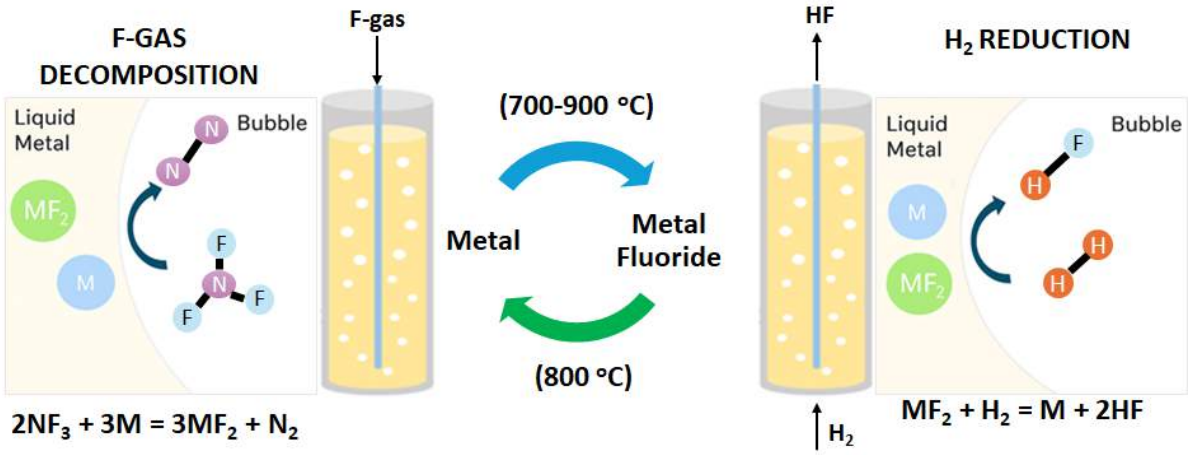
Keywords: F-gas decomposition; Molten metal; Fluorine recovery; Hydrogen reduction

Introduction. The semiconductor industry relies on F-gases (e.g., CF_4, NF_3) for plasma processes, but their strong C-F bonds lead to extremely high global warming potentials and long atmospheric lifetimes [1]. As emissions increase with industry expansion, advanced technologies are needed to both mitigate these gases and recover fluorine. Existing abatement methods including combustion, plasma treatment, and catalytic pyrolysis are constrained by high energy demand [2], secondary wastewater generation, catalyst deactivation [3], and the lack of fluorine recovery. To overcome these limitations, this study proposes a molten metal based catalytic system that enables efficient F-gas decomposition with simultaneous fluorine recovery via hydrogen reduction of metal fluorides.

Methods. Lab-scale experiments were conducted in a molten metal bubble column reactor using molten tin. F-gases were injected into the molten tin layer through a nozzle at 500-1000 °C, where they reacted to form tin fluorides. The fluorinated tin was then treated with hydrogen at 700-900 °C to regenerate metallic tin and produce HF. The outlet gas stream was analyzed using Fourier-transform infrared spectroscopy (FTIR) and non-dispersive infrared (NDIR) analysis to evaluate both decomposition and regeneration performance. FTIR was used to quantify the concentrations of F-gases and HF in the outlet stream, while NDIR was used to measure the H_2 concentration.

Results and discussion. Lab-scale experiments confirmed that molten tin effectively decomposes F-gas, with performance strongly dependent on gas species and temperature. SF_6 and NF_3 exhibited high destruction efficiencies, exceeding 90% above 500, while CF_4 showed significantly higher resistance to decomposition, requiring temperatures ≥1000 °C due to the strong C-F bond stability. Hydrogen reduction was essential for converting tin fluorides into recoverable HF. NF_3 demonstrated the most efficient HF formation at 700-800 °C, indicating favorable fluorine release from tin fluorides. SF_6 generated HF at 800 °C; however, HF yield saturated beyond a certain H_2 flow rate, suggesting partial fluorine retention in molten tin. CF_4 produced only limited HF even at ≥800-900 °C and high H_2 ratios, although HF formation was qualitatively confirmed by pH indicators.



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DPL0199

Ozone production from electrolysis by-product oxygen on Wastewater Treatment Plants – An operating model-based feasibility study

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Keywords: oxygen utilization; ozone generator; plasma reactor modeling; wastewater treatment plant; water electrolysis

Introduction. Wastewater treatment plants (WWTPs) will soon require a mandatory fourth treatment step, e.g., via ozonation, after generating ozone via dielectric barrier discharge [1]. Traditionally, the feed gas of ozone generators (OZG) is liquid oxygen (LOX), which must be purchased and transported to the WWTP first. Water electrolysis at the WWTP offers potential advantages: green oxygen is produced on-site without delay and hydrogen can also be used, e.g., to valorize CO_2 from digestion towers. However, oxygen from electrolysis (EL-O_2) contains significant amounts of H_2 and H_2O, which diminish the ozone production [2]. As there is up-to-date no systematic investigation of this phenomenon, we propose a steady-state model of an OZG to study the effect in more detail and assess the feasibility on WWTPs.

Methods. To this end, a stationary plug flow model of an OZG [3] formulated for a pure O_2 feed is extended to consider the effects of H_2 and H_2O by adding relevant kinetic equations from the literature. Using the modified reaction system, it is possible to study conversion and yield under varying feed composition, and to determine whether hydrogen peroxide (or other components) are likely by-products, as, e.g., hydrogen peroxide is produced at higher H_2 concentrations in plasma applications [4].
To test the influence of the EL-O_2 on ozone production and energy consumption, three different scenarios of the gas inlet stream composition are investigated: The first one is LOX as standard feed. The second one mimics the unpurified EL-O_2 with a corresponding amount of H_2 and H_2O. The third one models (partly) purified EL-O_2 via a systematic reduction of the impurities of EL-O_2 until pure oxygen quality. The purification encompasses catalytical removal of H_2 and cooling and adsorption drying for removal of H_2O. Based on these findings, the economic feasibility of these alternatives is assessed via the operating cost of a fixed ozone demand. Through adapting the operating parameters volume flow and power input, the costs of ozone production of each alternative are minimized and then compared.

Results and discussion. Preliminary findings show that the presence of H_2 and H_2O in EL-O_2 increases energy consumption by 1 % and 68 %, respectively. Both gases react with single oxygen atoms, which reduces the selectivity towards ozone. Moreover, economic feasibility depends strongly on the production costs of oxygen and the operating parameters. Purification of EL-O_2 offers an interesting opportunity to increase the lower ozone yield while keeping the advantages of on-site oxygen production.

Acknowledgments

The authors gratefully acknowledge the financial support of the German Federal Ministry of Economic Affairs and Energy of Germany for the project E-MetO (project number 03EI3093C).

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DPL0746

CFD-Based Evaluation of Nozzles for plasma based H_2O_2 Production in Microgravity

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Abstract Category: Reactor Modeling and Design - Reactor Design - Plasma **Keywords:** Nozzle, Mixing performance, Computational fluid dynamics, Multiphysics modeling

Abstract Body.

Introduction. For long-term space exploration, in-space propellant production with easily storable and accessible resources has emerged as a key direction for next-generation spacecraft systems. Plasma reactors are particularly attractive for producing hydrogen (H2) and hydrogen peroxide (H2O2) without cold-start limitations, enabling instantaneous operation [1]. Even if H2O2 concentrations are promising, efficient chemical conversion requires good plasma-liquid contact [2]. Moreover, the reported synthesis mostly takes place under earth gravity.

Therefore, in this work, we develop and investigate nozzle geometries with enhanced mixing performance within the reactor. Since experimental validation of nozzle performance under microgravity environment is costly and time-intensive, computational fluid dynamics (CFD) is employed to evaluate and compare the mixing performance of different nozzle configurations.

Methods. A three-dimensional CFD model is developed to evaluate mixing performance using single-phase and multiphase flow models under gravity and microgravity conditions. The simulations are implemented in COMSOL MultiphysicsTM[3], which couple the Reynolds-averaged Navier-Stokes (RANS) equations with phase transport equations for two-phase flow.

The critical parameters in nozzle configurations are diameter, tip shape, and orifice position.

A two-step simulation strategy is adopted: first, single-phase flow simulations are used to perform preliminary screening of nozzle designs based on residence time and flow field analysis. Subsequently, multiphase flow simulations are performed for selected designs to analyze mixture fraction distribution and concentration and export mixture data for future reactive and plasma simulations.

Results and discussion. Variations in the tip shape led to distinct velocity, fields, directly affecting fluid residence time, as can be seen in Figure 1. The open-ended nozzle produces a direct flow toward the reactor bottom, while the closed-ended nozzles extend residence time by modifying the internal flow pattern. The sharp-tip nozzles configurations exhibit the strongest impact on the overall flow field, suggesting superior mixing performance.

In contrast, the effect of orifices position is less distinguishable in single-phase simulations. Consequently, two-phase flow models are introduced to evaluate volumetric mixture fraction and concentration as additional quantitative measures for evaluating mixing performance.

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DMB0183

Virtual Prototyping and Experimental Validation of a Membrane Reactor for Enhanced Once-Through Yield in Methanol Synthesis.

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Abstract Category: Reactor Modeling and Design - Reactor Design - Membrane reactor

Keywords: Power-to-Methanol, Membrane Reactors, CFD Modeling, Optimization

Abstract Body.
For a prospective carbon-neutral future, carbonaceous fuels and chemicals will need to be synthesized using recycled or captured carbon. A widely discussed option is the catalytic hydrogenation of carbon dioxide in power-to-X processes. However, due to the formation of water during the synthesis and the emergence of a chemical equilibrium, synthesis yields are limited. To overcome this yield restriction, membrane reactors can be applied to remove the undesired side product from the reaction zone, thereby shifting the chemical equilibrium to higher yields and resulting in reduced recycle ratios and required recompression power.
In this study, we focus on the application of a membrane reactor in a power-to-methanol process incorporating a NaA zeolite membrane at pressures up to 100 bars. After designing a suitable membrane reactor based on literature, a sophisticated CFD model was developed for virtual prototyping, incorporating the Maxwell-Stefan approach for permeation that considers the complex behavior of pervaporating water-alcohol mixtures [1]. After validating the model based on literature values, a comprehensive full-factorial design of experiment was conducted to identify key constructive and operating parameters. Two general categories of parameters influencing the conversion and yield in the membrane reactor were identified. The first parameter is the ratio between reaction and permeation, as permeation appears to be the rate-determining step influenced by the GHSV, as well as the ratio between the surface area of the membrane and the volume of the reaction zone. Second, the partial pressure difference is a key parameter, as the driving force for permeation, being influenced by both the total pressure difference as well as the sweep velocity. Based on these findings, the first design of the membrane reactor was optimized and adopted for manufacturing conditions.
Subsequently, we are validating the CFD model with a focus on permeation kinetics, as experimental data is scarce in literature. This will enable us to utilize our virtual prototyping model in various applications where the use of selective water-permeable membrane reactors is discussed. After validating the CFD model, the membrane reactor is characterized to identify optimal operating conditions for methanol synthesis and to assess the benefits of a membrane reactor compared to a traditional reactor. These results will be used for a third design optimization that will finally be analyzed in the validated virtual prototyping CFD model.

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DMB0417

Novel e-Membrane Reactor for NH3 Decomposition

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Abstract Category: Reactor Modeling and Design - Reactor Design - Membrane reactor

Keywords: Hydrogen, Ammonia, Electrified reactor, Membrane reactor.

Abstract Body.

Introduction.

The two main challenges for scale-up of NH3 decomposition are achieving effective heat transfer and addressing the strong H2 inhibition that affects best performing Ru-based catalysts [1]. We propose the design of a novel electrified membrane reactor (eMR) for NH3 decomposition. The introduction of a Pd-based membrane dramatically increases reaction rate by removing H2 from the catalyst surface, and electrification improves coupling of heat supply and demand, approaching the ideal performance of an isothermal reactor.

Method.

A mathematical model was developed to design an eMR. The model represents a packed SiSiC foam reactor [2] containing Pd membrane through mass, energy and momentum balances. The kinetics of Franchi et al. [3] and the membrane parameters of Ongis et al. [4] were implemented. The reactor performance is quantified considering two KPIs: NH3 conversion and Hydrogen Recovery Factor (HRF=H2perm/(3/2*NH3in)).

Results and discussion.

Figure 1 reports NH3 conversion (A) and HRF (B) as function of inlet temperature for isothermal packed bed (isoT-PB), and isothermal and electrified membrane reactors (isoT-MR and eMR), with different power distribution at GHSV=6 Nm3/h/kgcat, pret.=20 bar, pperm.=1 bar, and with a membrane surface to catalytic bed volume ratio SV,m=60 1/m. isoT-MR reaches the equilibrium conversion of conventional isoT-PB at a T nearly 100 °C lower and complete conversion and almost unitary H2 recovery at 500 °C. Moreover, H2 removal shifts thermodynamic equilibrium allowing MR to overcome the PB equilibrium conversion. The KPIs decrease considering realistic electrification because of the mismatch along the axial coordinate between variable heat demand (proportional to reaction rate) and constant volumetric power input (qv) generated due to Joule effect with a single resistive element. By tailoring the resistive element and/or its power supply, it is possible to obtain a variable (segmented) qv along the reactor axial coordinate (Figure 1C). qv segmentation results in a better coupling of heat demand and supply, improving both conversion and HRF. In the simulated conditions, the 4-segments eMR approaches the ideal case of isothermal reactor with NH3 conversion of 95% and HRF=85% at Tin=500 °C.

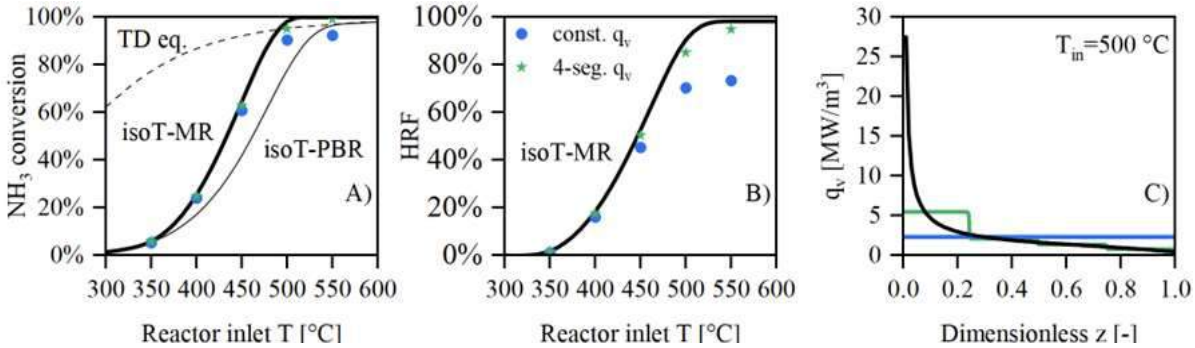

Figure 1: simulated NH3 conversion (A), HRF (B), and qv distributions (C).

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DMB0532

Computational Study of CO2 capture with Deep Eutectic Solvents in a Tube-in-Tube Teflon AF2400 Membrane Reactor

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Abstract Category: Net-zero CO2 Technologies - 선택 없음

Keywords: CO2 Capture; DES; AF2400; Tube-in-Tube, Membrane Reactor; CFD

Abstract Body.

Introduction.

Conventional amine-based solvents like monoethanolamine (MEA) are widely used in industry for post-combustion CO2 capture, but face limitations, such as volatility and high regeneration requirements, which Deep Eutectic Solvents (DES) can overcome. This study introduces Choline Chloride (ChCl) based DES as alternative absorbents combined with a tube-in-tube membrane reactor with an AF2400 inner tube, aiming to intensify gas-liquid mass transfer and avoid wetting issues that heavily affect the performance and longevity of membrane systems [1]. The objectives of this work are to study the CO2 potential of different DES compared to amine solutions (i.e. MEA) and optimize and scale up the process.

Methods.

The Absorption model is set up at ambient conditions with a 20/80 vol% CO2/N2 post-combustion simulated gas and solvents supplied concurrently in the shell and lumen side, respectively. The Computational Fluid Dynamics (CFD) model was developed in COMSOL Multiphysics 6.2. The diffusivity of CO2 in the AF2400 was calculated following the solution-diffusion mechanism and the absorption of CO2 in the solvent was simulated using solvent specific absorption reaction kinetics. The following mass balance equation was adapted with appropriate boundary conditions to describe the concentration profiles in each of the gas, liquid and membrane domains:

$$v_r \frac{\partial C_i}{\partial r} + v_z \frac{\partial C_i}{\partial z} = D_i \left[\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial Ci}{\partial r} \right) + \frac{\partial^2 Ci}{\partial z^2} \right] + R_i \qquad (1)$$

Results and discussion.

The results demonstrate a higher capture efficiency from the ChCl:MEA DES compared to 10 wt% aqueous MEA. Ongoing work includes theoretical and experimental evaluation of different solvents, further operating parameter optimization, and study of potential configurations and dimensions for process scale-up.

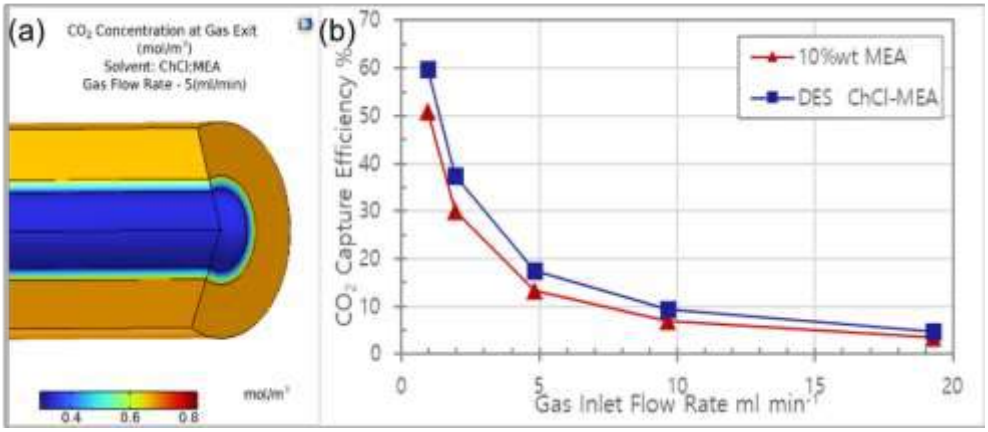

Figure 1:(a) CO2 Concentration profile of tube-in-tube reactor's exit (b) CO2 capture efficiency of 10wt% MEA and ChCl:MEA DES at different Flow Rates

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DER0263

Pressure-driven enhancement of CO2 to C2+ conversion on copper electrocatalyst

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Abstract Category: Reactor Modeling and Design - Reactor Design - Electrochemical Reactors

Keywords: Electrochemical CO2 reduction, Copper catalyst, High pressure, H-type cell.

Abstract Body.
Electrochemical carbon dioxide reduction reaction (CO2RR) is a promising approach to mitigate CO2 concentration and generate carbon feedstock. Copper has been widely explored for the CO2RR owing to its tendency to form hydrocarbons but low faradaic efficiency (FE) for C2+ products, which highlights the CO2RR dependence and sensitivity to the surface of Cu catalysts. CO2RR faces several challenges, including high hydrogen evolution reaction (HER) and low current density, which limit C2+ selectivity. In this study, we designed a copper oxide catalyst that can effectively overcome the reaction barrier to improve kinetics and FE. Furthermore, the competent HER and mass transfer limitations have been enhanced under high-pressure CO2 conditions. Herein, the effect of high-pressure conditions over CuOx was studied, which increased the CO2RR activity significantly in H-type cells and maintained the selectivity of C1 and C2 at low overpotential. The impact of CuOx at higher pressure, activation mechanism, and formation of C1 and C2 from CO2RR are elucidated by experimental studies. Several parameters were compared through comprehensive analyses, including HPLC analysis, and various ex-situ analyses (HR–TEM, XRD, XPS, and SEM). It is challenging, but the selectivity towards C2+ was maintained at ~ 17.8% at 10.0 MPa. This work not only offers fundamental insight into the structural transformation of electrocatalysts under high-pressure reaction conditions but also enables the rational design of efficient and low-cost catalysts towards CO2RR for commercialization.

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DER0265

Reactor Design for Ammonia Cracking Using Induction Heating

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Abstract Category: Reactor Modeling and Design - Reactor Design - Electrochemical Reactors

Keywords: Induction heating reactor, Ammonia decompositon, Reactor design

Abstract Body.
Conventional furnace or burner heating suffers from large thermal inertia and heat-transfer limits, leading to slow start-up/shut-down, strong temperature gradients, and local overheating that reduce efficiency and raise safety and durability concerns. This study develops an induction-heated ammonia cracking reactor that generates heat directly in the tubular workpiece to enable rapid electrified operation and precise, localized heating. We quantify eddy-current and hysteresis losses, impedance, and power factor using electromagnetic simulations, then couple Maxwell–Fluent to transfer these losses as heat sources for thermo-fluid and reaction modeling. Key design variables include frequency and current, coil–tube gap, tube thickness/material, and flow rate (GHSV), and performance is assessed under the conversion–hydrogen yield trade-off. Increasing frequency/current and strengthening coupling increase tube heating and wall temperature, improving conversion, while higher GHSV reduces hydrogen yield despite higher throughput. The results provide practical design and operating guidelines and motivate multi-objective optimization for balancing conversion, yield, and electrical efficiency.

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DER0562

Degradation analysis of electrode materials for durability test of anion exchange membrane-unitized regenerative fuel cells

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Abstract Category: Reactor Modeling and Design - Reactor Design - Electrochemical Reactors

Keywords: AEM-URFC, fuel cell, water electrolyzer, degradation

Abstract Body.
An integrated fuel cell/water electrolysis system using an anion exchange membrane (anion exchange membrane-unitized regenerative fuel cells, AEM-URFC) consists of a fuel cell (FC), which generates electricity using hydrogen, and a water electrolyzer (WE), which produces hydrogen using electricity. However, when cycling between FC and WE, the magnitude and direction of the voltage applied to each electrode change, accelerating the degradation of the electrode materials. This study aims to analyze how electrode materials degrade when cycling between FC and WE modes, and to what extent this degradation affects durability. To perform the analysis under conditions identical to those of the AEM-URFC, half-cells were constructed with separate cathodes and anodes, and cycling tests were performed. The electrode catalyst used was platinum on carbon black (40% Pt/C) for the hydrogen electrode and iridium black for the oxygen electrode. The method for manufacturing a catalyst-coated gas diffusion electrode is as follows: first, a catalyst, ionomer, and solvent are appropriately mixed to prepare a catalyst ink, which is then sprayed onto the gas diffusion layer until the desired loading amount is achieved. The manufactured electrode was mounted on a cell frame, and 0.7 V and 1.9 V were applied for 2 hours each for cycling in FC and WE mode in a 0.1 M KOH solution. The change in current according to the number of cycles was measured, and the degree of degradation of the catalyst, conductive material and ionomer according to the number of cycles was analyzed. The catalytic activity gradually decreased with repeated cycling, and this phenomenon was particularly severe at the oxygen electrode. We developed a method to quantitatively measure the degree of material degradation according to the number of cycles and presented the results. In the case of the oxygen electrode, it is exposed to a significantly high oxidation potential environment in the WE mode, which accelerates the oxidation of the catalyst and reduces the catalytic activity. Unlike the oxygen electrode, the hydrogen electrode has a significantly high overpotential for the oxidation reaction (FC mode) and the generation reaction (WE mode) of hydrogen in an alkaline solution. This high overpotential may be a major factor in lowering the performance of the overall system. However, since the potential range of the hydrogen oxidation and generation reactions does not affect the catalyst deterioration, the deterioration of the hydrogen electrode material was significantly

lower than that of the oxygen electrode material.

ISCRE29 & APCRE11
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DER0563

Mass Transfer Analysis in the Catalyst Layer for Electrochemical Reduction of CO_2

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Keywords: CO_2 electrolyser; Porous electrode; Flooding; Mass transfer limitations, CFD

Introduction: Electrochemical utilization of CO_2 has great potential to convert it into valuable chemicals such as CO. In recent years, significant progress has been made in the design of gas diffusion electrodes (GDEs) for the electrochemical reduction of CO_2. However, the multiscale, multiphase, and multiphysics nature of the porous catalyst layer (CL) makes accurate modelling a challenge. A transition from a kinetic to a mass-transfer-controlled regime has been observed as the applied potential increases. However, the quantitative representation of the CO_2 (gas)-electrolyte (liquid) distribution as a function of surface tension, wettability, and porous structure remains poorly understood. In this study, we develop a 1D model for a GDE for CO2 conversion, validate it against literature experiments, and probe the impact of mass transfer rate on the GDE performance. Moreover, pore-scale Volume of Fluid (VOF) simulations are performed to examine the gas-liquid distribution for different material properties and their influence on the mass transfer in the catalyst layer.

Methods: A 1D model of a microfluidic CO_2 electrolyzer with an Ag GDE is developed and validated against the experiments [1,2]. The simulations are performed at 1 atm and 0.5 M $KHCO_3$ electrolyte, with a reduction potential varying from -0.5V to -2V (V vs. RHE). The model is implemented in *COMSOL Multiphysics* using the *transport of concentrated species*, the *tertiary current distribution*, and *chemistry* modules. The CO_2 (gas)-electrolyte (liquid) distribution in the pore-resolved catalyst layer is investigated using VOF in ANSYS Fluent.

Results and discussion: The developed 1D model is analyzed for two wettability conditions in the catalyst layer (CL): (i) Wetted – electrolyte forms a thin film and wets the CL; (ii) Flooded – electrolyte floods the pores of CL. Figure 1(a) shows the influence of the gas-liquid mass transfer coefficient on the CO partial current density obtained from the 1D model. Figure 1(b) shows the gas-liquid distribution obtained from VOF simulations for two contact angles (50° and 70°). These results demonstrate that the CL is always flooded at an operating pressure of 1atm. These observations show that thin-film-based mass transfer assumptions may not be appropriate under typical operating conditions, and flooding-dominant transport provides a realistic description of gas-liquid distribution in CL.

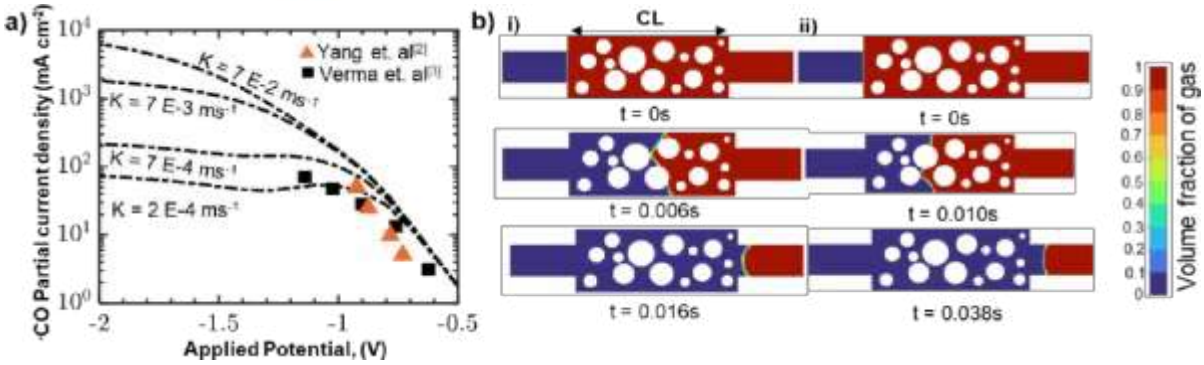

Figure 1: a) Effect of the mass transfer coefficient on CO partial current density; b) Gas-liquid distribution in a modeled CL at contact angles: i) 50° and ii) 70°.

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2026 / SEOUL, KOREA

DER0747

Anode vs Cathode water feed operation in PEMWE: Simulation-based analysis of performance gains and operational limits

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Keywords: PEM water electrolysis; PEMWE feed configuration; Hydrogen production

Introduction. Proton exchange membrane water electrolysers (PEMWE) are increasingly recognized as efficient and flexible technologies for sustainable hydrogen production, a key vector in the transition to clean energy systems. While significant research has advanced catalyst activity, membrane conductivity, and overall operational efficiency [1], the optimization of water feed strategies remains relatively underexplored [2]. Conventionally, PEMWE systems introduce liquid water at the anode, facilitating oxygen evolution, while hydrogen is generated at the cathode without direct water feed. This study investigates an alternative operational configuration: feeding water into the cathode and air into the anode. This approach is claimed to deliver improvements in efficiency, safety, and system compactness, which are critical for industrial deployment and scale-up [3].

Methods. To rigorously assess the impact of this innovative feed strategy, high-fidelity simulations were performed using gPROMS Process 2025.2.0 [4] and the Electro Chemical Reactor libraries. These models, based on first-principle equations, enable a detailed comparison between traditional and cathode water feed configurations, capturing the complex interplay of transport phenomena, electrochemical kinetics, and membrane behavior.

Results and discussion. Simulation results reveal that the cathode water feed layout yields notable gains in both efficiency and safety. Efficiency improvements are primarily attributed to the use of thinner separation membranes, which reduce ohmic losses and enhance proton conductivity. Safety is improved by introducing air at the anode, which dilutes the oxygen stream and mitigates risks associated with hydrogen crossover—a critical consideration for operational reliability. However, the analysis also identifies operational boundaries, particularly concerning the minimum feasible membrane thickness and the potential for air components to permeate into the cathode compartment, which could affect hydrogen purity and system integrity.

This work demonstrates the value of advanced modeling in guiding the design and optimization of PEMWE water feed strategies. The cathode feed configuration offers clear advantages in terms of efficiency and safety, though further research is needed to address membrane design constraints and gas crossover phenomena. These findings contribute to the ongoing development of robust, high-performance PEMWE systems for large-scale hydrogen production, supporting the broader goals of chemical

reaction engineering and sustainable energy transition.

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DER0756

Mass-Transfer Coefficient Correction for Improved CO Prediction in a Low-Temperature AEM CO2 Electrolyzer Implemented in Aspen Custom Modeler (ACM)

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Abstract Category: Reactor Modeling and Design - Reactor Design - Electrochemical Reactors

Keywords: CO2 electrolysis, low-temperature electrolyzer, mass-transfer coefficient, Aspen Custom Modeler (ACM), anion-exchange membrane (AEM)

Abstract Body.
Closing the carbon cycle for sustainable aviation fuel (SAF) requires low-temperature CO2 electrolysis models that reliably predict carbon products, because syngas quality—especially CO yield and H2/CO control—dictates recycle, separation, and conversion targets in downstream Fischer–Tropsch (FT) synthesis and hydrocracking. Here, an anion-exchange-membrane (AEM) CO2 electrolyzer is modeled in Aspen Custom Modeler (ACM) to support computationally efficient, process-integrated Power-to-Liquid (PtL) assessments. CO prediction accuracy is critical for net-zero PtL design, where carbon utilization and hydrogen make-up are strongly coupled to carbon-product selectivity and overall system efficiency.
We build on a published semi-empirical ACM framework trained on lab-scale data (5 cm2) and validated against pilot-scale operation (800 cm2 single cell and 10 × 800 cm2 stack). In the baseline formulation, cathodic CO was substantially overpredicted, with deviations increasing from ~180% at 75 mA/cm2 to ~330% at 150 mA/cm2. The main cause is an optimistic representation of CO2 availability at the cathode, where the driving bulk CO2 concentration was approximated as the arithmetic mean of inlet and outlet concentrations.
To improve physical consistency while retaining a reduced-order description, CO2 delivery to the reaction interface was reformulated using two coupled modifications. First, the net mass-transfer coefficient was revised to include additional diffusion resistance through the catalyst layer (CL) by explicitly accounting for CL thickness and porosity within the gas diffusion electrode (GDE) transport pathway. Second, Henry's law was imposed at the cathode gas–liquid interface to map gaseous CO2 to dissolved CO2 available at the reaction interface. These updates reduced the maximum CO prediction error from ~330% to ~140% across 75–150 mA/cm2 and lowered the 75 mA/cm2 deviation to ~2%, indicating that interfacial CO2 availability is a primary determinant of cathodic CO fidelity in this ACM framework.
Scale-up from lab to 800 cm2 still shows increasing mismatch, likely reflecting additional factors beyond transport and ohmic losses (e.g., spatial non-uniformity and catalyst-related performance changes). A limited sensitivity check found that adding an explicit ohmic-loss term beyond the published baseline produced minor changes in cathodic CO, whereas the calibrated transport/Henry treatment governed the predictive shift; comprehensive scale-up closure remains future work.
The resulting potentiostatic ACM model supports parametric evaluation and direct coupling with Aspen-based FT and hydrocracker simulations for integrated PtL optimization under realistic CO2-to-syngas constraints. Overall, enforcing physically admissible interfacial CO2

delivery—rather than further detailing of ohmic losses—emerges as the principal requirement for improving cathodic CO predictability within reduced-order, process-integrated electrolyzer models.

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DPR0733

CFD modeling of 300 mL multi-zone LDPE reactor for the prediction of molecular weight distribution

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Keywords: LDPE polymerization; CFD; Probability generating function transform; Molecular weight distribution

Introduction. Accurate molecular weight distribution (MWD) prediction in a polymerization reactor requires detailed analysis of the MWD in the presence of non-ideal mixing. Previous studies often exhibited a trade-off between MWD and hydrodynamic details. Studies with detailed MWD analysis typically assume ideal mixing (e.g., CSTR or CSTR in series), while CFD-based, hydrodynamically detailed studies often simplify the MWD as a Flory-Schulz distribution. To bridge this gap, this study developed an integrated detailed analysis of the MWD with CFD to predict MWD produced in a 300 mL multi-zone LDPE reactor. This approach enables precise MWD prediction by accounting for complex hydrodynamic effects.

Methods. Kinetic parameter validation was performed by comparing experimental data from a singlezone 100 mL reactor with CSTR simulations under various operating conditions [3]. Three literature-based kinetic parameter sets [1-3] were evaluated based on monomer conversion and MWD, which was computed using the Method of Moments and the probability generating function (PGF). The selected parameter set was then applied to a CFD-based analysis of an LDPE polymerization reactor. For this study, a 300 mL multi-zone reactor geometry [4] was used to consider the multi-zone characteristics of industrial reactors.

Results and discussion. The kinetic parameters reported in Pladis et al. [2] were selected based on their numerical stability and agreement with experimental data. In CFD simulations, the predicted monomer conversion showed a relative error of 4.89 % compared to experimental data, while reactor temperature distributions showed relative errors of 8.62 % across the different reactor zones. However, notable discrepancies were observed in MWD predictions. These deviations were attributed to assumptions regarding unreported operating conditions and numerical constraints arising from PGF–CFD coupling. The proposed framework establishes a quantitative link between reactor hydrodynamics and detailed MWD analysis under spatially non-uniform conditions.

Acknowledgments

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ISCRE29 & APCRE11
2026 / SEOUL, KOREA

DNR0432

EMERALD: A novel eReactor with Radial Current and Centrifugal Gas Flow for the Intensification of Endothermic Catalytic Processes

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Abstract Category: Reactor Modeling and Design - Reactor Design - Novel Reactors

Keywords: Electrification, Process Intensification, Innovative Reactor Design

Abstract Body.
Introduction. Electrification of Steam Methane Reforming (eSMR) is a promising route towards the decarbonization of H2 production; in this work we address a major topical challenge of SMR: tuning the heat supply to the varying heat demand of the reaction, so to enhance the reactor performance (e.g., reduced cold spot). To this scope, we propose a novel Joule heated eSMR reactor configuration based on radial electric current and centrifugal gas flow in an annular packed foam (Figure 1 B, EMERALD configuration) [1].
Methods. Comparative simulations were carried out for packed foam reactors with axial and radial centrifugal configurations, employing a hybrid heterogeneous hierarchical approach [2]: 3D CFD simulation results were used to derive correlations and parameters for 1D and 2D porous media models [3] and then compared with the experimental results collected in a lab-scale prototype reactor (Vcatalytic bed = 0.1 l).
Results and discussion. Figure 1 compares simulations of the axial (A) and the EMERALD (B) configuration. In both cases SiSiC foams (10 PPI) loaded with Rh-based catalyst particles (dp = 1 mm), operating at the same inlet temperature (773 K), outlet pressure (7 bar), feed composition (H2O:CH4 = 2.5:1), GHSV (20 Nl/h/gcat), reactor volume (21.4 l), and power supply (234 kW) were considered. The axial configuration results in a cold spot at the reactor inlet (Figure 1 A). In the radial EMERALD configuration, the cold spot is substantially eliminated (Figure 1 B) thanks to a specific power input (Figure 1 B, solid black line) that is maximum at the entrance of the catalytic bed and decreases with 1/r2 (assuming constant electrical resistivity), closely matching the reaction heat demand. Furthermore, the pressure drop is drastically reduced. Implications for the optimal eSMR reactor design will be discussed.

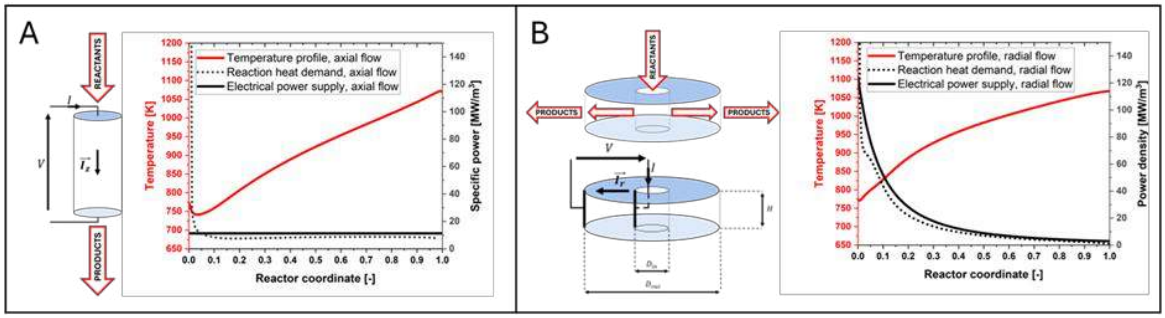

Figure 1. Simulation results: A) Axial configuration B) EMERALD (radial) configuration [1].

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DNR0444

CFD modeling of a bench-scale reactor for mixed reforming of methane

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Keywords: CFD; mixed reforming of methane; reactor modeling

Introduction. Mixed reforming of methane, which combines steam and dry reforming, stands out as a sustainable hydrogen production process due to its CO_2 utilization and coke suppression by the presence of steam [1]. Computational fluid dynamics (CFD) has been widely employed for reformer design and analysis for effective thermal management within the catalytic bed [2, 3]. In this study, a CFD model for a Bayonet-type reactor was developed based on bench-scale experimental data for the mixed reforming of methane.

Methods. The experiments were conducted under varying space velocity (SV) and furnace temperature conditions. Additional experiments were carried out to investigate the effect of mixing inert materials with catalysts in the upper region of the catalytic bed. Kinetic parameters for the CFD model were derived from experiments. To improve model accuracy, heat transfer coefficients and effective thermal conductivity were estimated to match experimental conditions.

Results and discussion. Model validation was performed by comparing simulation results with experimental data. The mean absolute relative residuals (MARR) for CH_4 conversion, CO_2 conversion, H_2/CO molar ratio and the temperature at the end of the catalytic bed were 0.84%, 7.77%, 3.70%, and 3.20%, respectively, while the corresponding relative standard deviation errors (RSDE) were 1.02%, 5.10%, 2.40%, and 2.67 (cf. Figure 1). Low MARR (< 8%) and RSDE (< 6%) demonstrate the effectiveness of the developed CFD model.

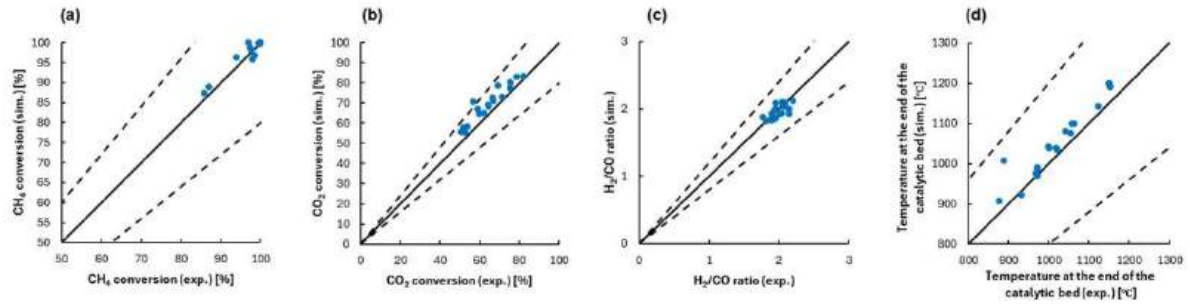

Figure 1. Parity plots between experimental data and simulated results for (a) CH_4 conversion, (b) CO_2 conversion, (c) H_2/CO molar ratio, and (d) temperature at the end of the catalytic bed. Dashed lines represent ±20% errors.

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2026 / SEOUL, KOREA

DNR0530

Microwave-Assisted Acetylation of Glycerol to Triacetin over Tungstophosphoric Acid Supported on Activated Carbon

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Abstract Category: Heterogeneous/Homogeneous Catalysis - 선택 없음

Keywords: Triacetin, Glycerol acetylation, Microwave, Glycerol valorization

Abstract Body.
Triacetin production via acetylation of glycerol with acetic acid was investigated using tungstophosphoric acid supported on activated carbon (TPA/AC) as a heterogeneous acid catalyst under microwave-assisted heating. The effects of catalyst loading, glycerol-to-acetic acid molar ratio, reaction temperature, and heating mode on glycerol conversion and product distribution were evaluated. The results showed that increasing TPA loading and catalyst dosage enhanced glycerol conversion and promoted consecutive acetylation, shifting selectivity from monoacetin toward diacetin and triacetin. Under the optimized conditions using 40 wt.% TPA/AC at a catalyst dosage of 25 wt.% relative to glycerol, near-complete glycerol conversion (>99%) was achieved. At a glycerol-to-acetic acid molar ratio of 1:12, microwave-assisted heating reached near-complete conversion within 30 min at 110 °C, whereas conventional heating required a longer reaction time of approximately 60 min. Product selectivity under microwave irradiation consisted of 67.7% diacetin and 26.6% triacetin, with 5.7% monoacetin formation. In comparison, conventional heating resulted in a lower triacetin selectivity of 17.7% under similar conditions after 30 min. The enhanced performance under microwave irradiation is attributed to accelerated reaction kinetics and more effective progression of the stepwise acetylation pathway. These results demonstrated that microwave-assisted acetylation using TPA/AC catalysts is an efficient and energy-effective route for glycerol valorization to triacetin.

Poster Presentation

Process Intensification

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

PTL0061

Zeolite-Assisted Sorption-Enhanced CO2-to-Methanol on Cu/ZnO/Al2O3

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Abstract Category: Process Intensification - Process Intensification / TEA / LCA

Keywords: CO_2 hydrogenation; methanol synthesis; sorption-enhanced catalysis; zeolites; fixed-bed reactor

Abstract Body. Introduction
Methanol synthesis from CO2 proceeds via CO2 + 3H2 ⇌ CH3OH + H2O. In fixed beds the formed water accumulates, lowers the effective H2 activity and drives the equilibrium back to CO2, so that conversion and CH3OH yield remain limited.1 Sorption-enhanced methanol synthesis (SEMS) counteracts this by removing H2O in situ with a solid sorbent.2 Fixed-bed data are scarce, this study examines how zeolite type and regeneration temperature influence the magnitude and stability of SEMS. Methods
A commercial Cu/ZnO/Al2O3 catalyst (CZA) was tested in a tubular reactor at 250 °C, 40 bar, H2/CO2 = 3 and WHSV = 15,000 mL g-¹ h-¹. As reference, CZA was measured without sorbent. SEMS beds were prepared by dry mixing CZA with molecular sieve 3A (MS3A) or 4A (MS4A) at a catalyst-to-sorbent mass ratio of 1:8. After H2 pre-reduction, samples underwent repeated reaction-regeneration cycles. Regeneration was performed in Ar at 1 bar and 270 to 330 °C. The outlet was analyzed online by GC (CO2, H2, CO, CH3OH, H2O). Sorbent texture before and after cycling was probed by N2-physisorption (77 K).
Results and discussion
Compared with CZA alone, SEMS gave a clear initial uplift. With MS3A, CO2 conversion, CH3OH yield and CO yield increased by about +153, +162 and +176 %, respectively. MS4A also enhanced performance but less strongly (≈ +70 % for all quantities). For MS3A, the enhancement decayed to the CZA baseline after roughly 90 to 110 min, for MS4A it vanished after about 60 to 80 min. Regeneration at 270 °C restored only a small fraction of the effect. At 300 °C peak heights increased but the enhancement window shortened, whereas 330 °C produced the highest CH3OH peaks and the longest cycles. N2physisorption showed slightly higher surface area and pore volume for 3A, supporting its larger transient capacity.

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PTL0251

CFD Validation of n-Butane Oxidation Kinetics to Maleic Anhydride and Optimization of Milli-Fluidic Mixers

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Abstract Category: Process Intensification - Process Intensification / TEA / LCA

Keywords: n-butane oxidation; maleic anhydride; Müller kinetics; ANSYS Fluent; UDF; Tesla mixer

Abstract Body.

Introduction: Maleic anhydride (MA) is an important industrial intermediate used in polymer resins and specialty chemicals. The selective oxidation of n-butane to MA involves parallel oxidation pathways and is highly sensitive to reaction kinetics, transport, and upstream feed preparation [1,2]. Predictive CFD tools with reliable kinetic models are essential for design and scale-out of intensified milli-scale oxidation reactors. In addition, effective premixing of n-butane and air is a key upstream requirement for stable operation and safe handling. This work reports (i) CFD implementation and validation of a detailed n-butane oxidation kinetic model and (ii) a separate CFD-based design assessment of milli-fluidic mixers for improved n-butane–air premixing.

Methodology: A detailed n-butane oxidation kinetic model from Müller et al. [1], including MA formation and parallel CO/CO_2 pathways, was implemented in ANSYS Fluent using a custom UDF coupled with multicomponent transport in a porous VPO catalyst bed. The reactor was modeled as an MFBR domain with inlet/outlet sections and a porous reaction zone (Fig. 1c), and the model was validated against experimental n-butane conversion and MA selectivity over temperature (Fig. 1b). In parallel, plain, static, and Tesla-type milli-fluidic mixers were designed for n-butane–air premixing and assessed using the uniform mixing index and pressure-drop penalty for internal diameters of 2–5 mm (Fig. 1a).

Results and Discussion: For the Tesla-type mixer (selected for high mixing efficiency with a low pressure-drop penalty), the uniform mixing index increased monotonically with mixer length for all internal diameters, approaching unity under optimized conditions (Fig. 1a). Smaller diameters achieved near-complete mixing within shorter lengths, whereas larger diameters required longer channels (Fig. 1a). The Fluent–UDF implementation of Müller kinetics reproduced the experimental temperature dependence of n-butane conversion and MA selectivity, confirming reliable predictive capability for MFBR simulations (Fig. 1b). The validated porous-bed reactor framework (Fig. 1c) enables systematic design screening, while detailed contour-based analysis and parametric mapping will be presented in the fulllength manuscript.

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PTL0259

Numerical Study of a Modified Splitting Distributor for Uniform Flow in Parallel Microchannels

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Abstract Category: Process Intensification - Process Intensification / TEA / LCA **Keywords:**

Two-phase flow; phase-field; bubble splitting; microchannels; flow uniformity.

Abstract Body.

Introduction. Uniform gas-liquid distribution remains a major bottleneck in the numbering-up of microreactors, where even slight hydrodynamic asymmetries at successive T-junctions can amplify into severe maldistribution. Width-reducing distributors (half-width concepts) offer an attractive pathway to reduce pressure drop while retaining acceptable uniformity [1]. In this work, we present a systematic numerical investigation of gas-liquid splitting in a modified multi-stage half-width distributor, incorporating geometry features that actively suppress asymmetry and accelerate stable splitting. The predictions are validated against experimental observations [2] to establish robust design rules for reliable parallelization.

Methods. A 2-D Phase-Field model (COMSOL Multiphysics) was developed to simulate twophase flow through a half-width distributor comprising three successive splitting stages. Four T-junction configurations were investigated: (i) plain, (ii) wedge, (iii) flow-focusing, and (iv) combined wedge + flow-focusing. Simulations were conducted for a kerosene–air system at a fixed gas flow rate of 3.09 mL min^{-1} and liquid flow rates ranging from 4 to 12 mL min^{-1}. Model predictions were validated against experimental observations in terms of bubble formation dynamics, slug length, and splitting behavior, including downstream obstructed/partially obstructed regimes. A 3-D schematic of the half-width distributor is shown in Fig. 1a.

Results and discussion. The combined wedge + flow-focusing configuration delivered the fastest splitting response and the best flow uniformity over a wide operating range, outperforming the plain, wedge-only, and flow-focusing-only junctions. The Phase-Field simulations reproduced the squeezing and transition regimes at the first T-junction and showed good agreement with experiments. Downstream obstructed and partially obstructed splitting regimes were also captured, and Fig. 1b compares experimental observations with numerical predictions for the obstructed regime. Predicted gas-slug lengths were validated against experiments across multiple flow-rate ratios (FR = 0.26, 0.31, 0.39, 0.52, 0.77 mL min^{-1}), as shown in Fig. 1c. The aggressive scaling (2 → 1 → 0.5 mm) produced longer daughter slugs, widening the stable operating window. Further analysis of symmetry index/maldistribution and the ANN-based slug-length prediction model (trained on >1500 datapoints using Ca, Re, and geometric descriptors) will be included in the full-length manuscript.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

PTL0323

Sustainable bio-oil production: Experimental and process modelling studies

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Waste Valorization

Keywords: liquefaction, pyrolysis, bio-oil, process modelling, energy optimisation

Abstract Body.
Introduction.
The thermal treatment of waste biomass such as sewage sludge can contribute to the utilisation of waste materials into useful product generation. Liquefaction and pyrolysis are two well-known processes where organic materials are thermally degradated into bio-gas, bio-oil and bio-char, which can afterwards be upgraded to fuels and chemicals [1]. In this work, an integration of a liquefaction and pyrolysis process is designed using Aspen Plus software, validating experimental results obtained from sludge liquefaction and subsequent solid residue pyrolysis, in order to obtain bio-polyols and phenolic bio-oil to be used for polyurethane (PU) and phenol-formaldehyde (PF) materials production. Further studies were conducted using a heat exchnager (HEX) to optimise the energy efficiency of the process.
Methods. The feedstock was liquefied at 110 oC for 1h, where the solid reside was afterwards pyrolysed at 500 oC with holding times of 30 minutes. Aspen Plus was used to model the integrated system using the Soave-Redlich-Kwong equation of state. A conversion reactor was used for liquefaction where the sludge biomass was modelled as non-conventional component and a plug-flow reactor for pyrolysis where the solid reside was modelled as a pseudo-component with an assumed power-law reaction rate.
(Selected) Results and discussion.
Using the developed model, the different components of bio oil derived experimentally were validated, with the power law kinetic rate approach successfully predicting the concentration of several components within the bio-oil mixture (Figure 1). The utilisation of a HEX, where the hot stream of pyrolysis was used to heat the feedstock before entering the pre-heating step, resulted in reduced heating load by 13 kW.

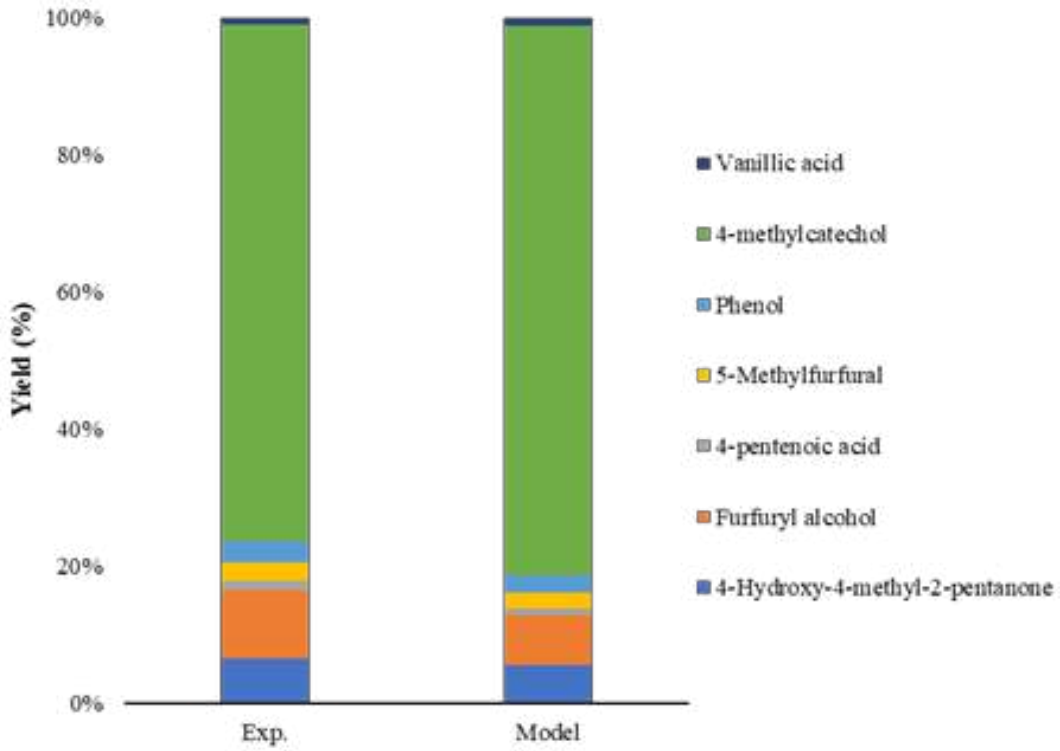

Figure 1. Composition of bio-oil: Experimental and computational comparison.

Acknowledgments
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PTL0354

Techno-economic and Environmental Assessment of Biohydrogenated Diesel Production from Palm Fatty Acid Distillate using Alternative Hydrogen Donors

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Abstract Category: Process Intensification - Process Intensification / TEA / LCA

Keywords: Bio-hydrogenated diesel; Palm fatty acid distillate; Hydrogen donors; Technoeconomic analysis; Environmental assessment

Abstract Body.

Introduction. Bio-hydrogenated diesel (BHD) produced via the deoxygenation of Palm Fatty Acid Distillate (PFAD) offers superior fuel properties compared to conventional biodiesel [1]. However, traditional hydro-processing relies on high-pressure external hydrogen, presenting safety and economic barriers. This study investigates the techno-economic and environmental feasibility of utilizing glycerol and acetic acid as alternative in-situ hydrogen donors. The purpose is to evaluate whether these alternatives can bridge the gap between laboratory kinetics and industrial sustainability.

Methods. A process simulation was developed in Aspen Plus V.14. Reaction kinetics were validated against experimental laboratory data for palmitic acid deoxygenation [2], achieving a Mean Absolute Error of <9% for product selectivity. The model was scaled to a 50-ton/day PFAD feed capacity operating at 270°C and 34 bar. Process synthesis included a Heat Exchanger Network (HEN) design using Pinch Analysis to minimize utility consumption. The study evaluated technical performance (mass yield), environmental impact (Global Warming Potential - GWP), and economic feasibility (NPV, ROI) over a 20-year plant life. Results and discussion. Simulation results demonstrated that glycerol is the superior hydrogen donor in terms of yield, achieving 86.93% compared to 76.40% for acetic acid. Energy integration significantly improved sustainability, reducing utility costs by approximately 45% for the glycerol process. Environmentally, both pathways drastically reduced the carbon footprint compared to petroleum diesel (0.638 kg CO2eq/L); acetic acid resulted in the lowest GWP (0.194 kg CO2eq/L), followed closely by glycerol (0.237 kg CO2eq/L). Economically, production costs continue to be a challenge. The break-even selling prices were calculated at $1.017/L for glycerol and $1.040/L for acetic acid, both exceeding the current diesel retail price of $0.940/L. Sensitivity analysis identified the PFAD feedstock price as the most critical variable affecting NPV. In conclusion, while glycerol offers

technical efficiency and acetic acid offers marginal environmental gains, commercial success requires supportive policies to offset production costs.

Acknowledgments
The authors acknowledge the support of the Faculty of Engineering, King Mongkut's University of Technology North Bangkok.

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PTL0396

Transport-Permeation Coupling in Plate-Type Membrane Reactors for Hydrogen Production via Methanol Steam Reforming

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Abstract Category: Process Intensification - Process Intensification / TEA / LCA

Keywords: Hydrogen, CFD, Plate membrane reactor, Methanol steam reforming, Concentration Polarization

Abstract Body.
On-board hydrogen production from methanol steam reforming offers a compact and safer alternative to compressed hydrogen storage for fuel-cell-based transportation. Membrane reactors are particularly attractive for this application, as selective hydrogen removal enhances conversion by shifting reaction equilibrium. While most membrane-assisted reforming studies focus on tubular packed-bed reactors, plate-type membrane reactors provide higher membrane-area-to-volume ratios, compactness, and scalability through stacking. However, transport–permeation interactions and concentration polarization effects in plate geometries remain insufficiently understood.
In this work, a two-dimensional model of a plate-type membrane reactor for methanol steam reforming is developed to systematically analyze reaction–transport–permeation coupling under realistic operating conditions. The model couples laminar flow, multicomponent species transport, heterogeneous surface reaction kinetics, and selective hydrogen permeation through a Pd membrane governed by Sieverts' law. Methanol steam reforming, methanol decomposition, and water–gas shift reactions are described using Langmuir–Hinshelwood kinetics, while multicomponent diffusion is modeled using the Maxwell–Stefan formulation. Reactor performance is evaluated over a wide range of temperatures, feed flow rates, and channel heights representative of milli- and sub-millimeter plate reactors. The results reveal that transverse mass-transfer resistance near the membrane surface leads to pronounced concentration polarization under reacting multicomponent conditions, significantly limiting effective membrane utilization. Channel height is identified as a critical design parameter: reducing the channel height to 1 mm minimizes diffusion resistance, suppresses concentration polarization, and enhances hydrogen recovery and methanol conversion. In contrast to tubular reactors, increasing flow rate in plate-type configurations intensifies polarization effects, reducing separation efficiency despite higher reactant throughput.
These findings provide quantitative design guidelines for compact, stacked plate-type membrane reactors and highlight the importance of explicitly accounting for transport–permeation coupling when developing scalable on-board hydrogen generation systems.

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PTL0412

CO2 capture and utilization via physical absorption and catalytic hydrogenation

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: CO2 capture, Physical absorption, CO2 hydrogenation, Process integration

Abstract Body.

Carbon capture and conversion technologies have emerged as critical pathways toward achiving carbon neutrality. In this context, we conducted in-depth investigations into the CO2 absorption performance of linear carboxylic esters with varying chain lengths, combining experiments and molecular simulations. Results indicated that carboxylic ester with longer carbon chains exhibit weaker absorption, with the length of carbon chain on the alkoxy side significantly affecting CO2 solubility. CO2 molecules tend to distribute near carbonyl group and closer to alkoxy side at absorption equilibrium. Increasing carbon chain length introduced greater steric hindrance, thereby affecting CO2 absorption. These findings provide insights for designing efficient physical absorbents for CO2 capture processes. Moreover, we prepared efficient catalysts to promote the deep conversion of CO2 into liquid fuel and high-calorie SNG. A series of KFeAl catalysts were modified with transition metal promoters and FeOx/zeolite tandem catalysts for CO2 hydrogenation to liquid fuel. we prepared a series of KFeAl catalysts modified with transition metal promoters and FeOx/zeolite tandem catalysts to promote the deep conversion of CO2 to liquid fuel. The C5+ selectivity of the catalyst coupled with HZSM-5 was greatly improved compared with the K/FeCoAl catalyst. By modulating the Co content, we further tailored the Fe-Co interaction between catalytic activity and C1-C4 selectivity for producing high-calorie SNG.

Based on the commercial Cu-based catalyst, the reaction kinetic model for methanol synthesis was developed, which is suitable for various CO2/CO ratios in syngas. A pseudohomogeneous reactor model was developed to evaluate the impact of structural parameters on reactor performance and material cost under different industrial scenarios. Novel CO2 hydrogenation technologies for producing clean fuel, methanol, DME, and olefins are proposed. Meanwhile, these carbon-neutral technologies were efficiently integrated with various industrial processes.Techno-economic and environmental analyses demonstrated that the integrated schemes showed significant promise for the efficient utilization of waste carbon resources, offering a practical pathway towards sustainable fuel/chemical production.

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Acknowledgments

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PTL0427

Pathways to Low-Carbon Hydrogen Economy: A Life Cycle Assessment of Centralized and Distributed Systems

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Abstract Category: Process Intensification - Process Intensification / TEA / LCA

Keywords: Hydrogen, LCA, Distributed production, Methanol, Glycerol

Abstract Body. Introduction
Hydrogen is a promising clean energy carrier for fuel-cell applications, yet its low volumetric density presents significant storage challenges, particularly for vehicles with limited tank volume. Distributed, small-scale hydrogen production near end users offers an alternative solution to high-pressure tanks and liquefied hydrogen infrastructure. On-board production, enabled by intensified technologies such as thermally balanced membrane reactors, can reduce or eliminate the need for costly compression and storage. Various hydrocarbons can serve as hydrogen carriers; although reforming them releases CO_2, these carriers can be synthesized from renewable biomass or CO_2-derived e-fuels, thereby enabling a closed carbon cycle.
This study evaluates the cradle-to-H_2 greenhouse gas emissions of multiple distributed production pathways using life-cycle assessment (LCA). Distributed routes are compared with current centralized benchmarks, natural-gas steam methane reforming (SMR) and large-scale solar-powered electrolysis.
Methods
Life-cycle inventories (LCIs) for centralized and distributed systems were developed using the GREET 2024 model. Methane (natural gas), methanol (from natural gas, biomass, and e-fuel routes), ethanol (from biomass and e-fuel), and glycerol (a biodiesel by-product) were assessed as hydrogen carriers for on-board generation. The cradle-to-H_2 system boundary includes feedstock extraction, carrier production and processing, distribution, and on-board hydrogen generation. Centralized SMR includes natural-gas extraction, transmission, reforming, purification, compression or liquefaction, distribution to refuelling stations, and final delivery to vehicles. Solar-powered electrolysis was modelled using analogous system boundaries for comparison.
Results and discussion
Figure 1 summarizes the resulting GHG emissions. In centralized hydrogen, compression and, especially, liquefaction dominate total emissions due to their high energy intensity. In contrast, distributed pathways substantially reduce, and in some cases eliminate, the emissions associated with compression and long-distance transport. Fossil-derived carriers emit the most, while renewable carriers offset a large portion of upstream impacts. E-fuel routes are energy-intensive synthesis, leading to elevated emissions in the e-methanol and e-ethanol pathways. Biomass-derived carriers, particularly methanol and glycerol, emerge as the most favourable options. Glycerol benefits from low upstream burdens due to its allocation with biodiesel production. Biomethanol synthesis via autothermal pyrolysis

requires minimal external energy input, further reducing emissions. Both bio-methanol and bio-glycerol achieve emissions significantly below those of centralized SMR and approach those of solar electrolysis.

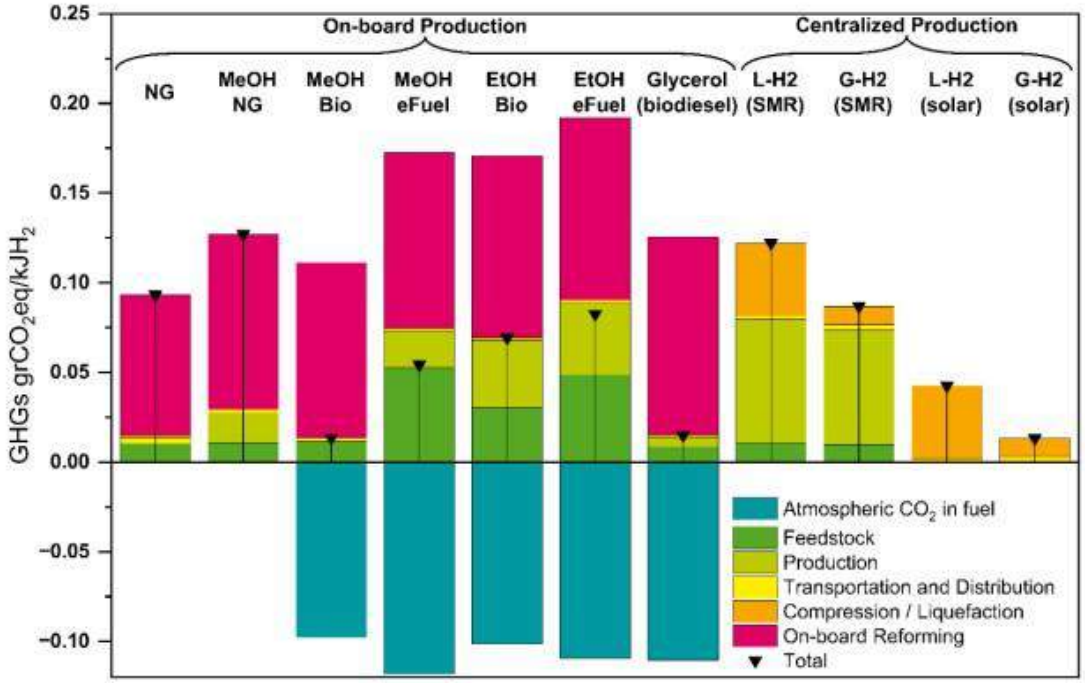

Figure 1: LCI analysis results for the different hydrogen carriers and pathways.

Conclusions

The analysis highlights the strong potential of distributed hydrogen production as a processintensified strategy for reducing lifecycle emissions in transportation. Biomass-based carriers, notably methanol and glycerol, appear particularly promising due to their low production carbon intensities and compatibility with compact onboard reforming technologies.

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2026 / SEOUL, KOREA

PTL0460

Drawdown and suspension of corn straw in the non-Newtonian fluid in stirred tank

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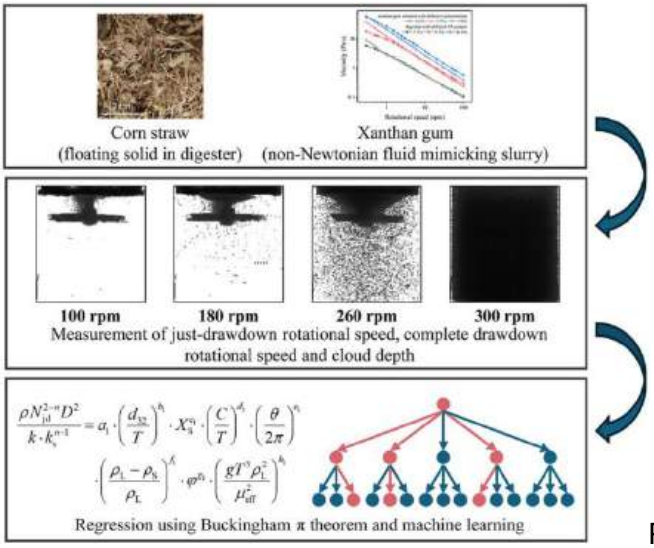
Abstract Category: Process Intensification - Process Intensification / TEA / LCA

Keywords: Solid-liquid mixing, Just-drawdown rotational speed, Cloud depth, Anaerobic digester, Non-Newtonian fluid

Abstract Body.



Purpose: Anaerobic digestion (AD) has emerged as a popular approach to realize the efficient utilization of corn straw (CS). During the AD process, straw particles tend to accumulate on the top of the anaerobic digester, forming a “scum layer” due to the low density, hydrophobic nature, and flotation caused by biogas generation, deteriorating the bioconversion efficiency and process stability. At present, researches on the drawdown and suspension of floating solids focused on regular solids in Newtonian fluid. Nevertheless, the solid (CS) - liquid (slurry) mixing system still has unique characteristics. On the one hand, the anaerobic slurry has been proved to be a shear-thinning non-Newtonian fluid, and its rheological characteristics result in complex flow field around the impeller and non-ideal flow behavior in the rest of the stirred tank. On the other hand, straw particles are usually irregular, exhibiting a wide range of diameter, aspect ratio, and sphericity. Considering the non-Newtonian fluid behavior and particle irregularity, the drawdown and suspension of straw particles in the anaerobic digester represents a novel area of research and has not been sufficiently investigated.
Methods: The experiment was carried out in a flat-bottom transparent polymethyl methacrylate cylindrical vessel with an inner diameter (T) of 0.105 m. This paper investigated the effect of particle size, liquid viscosity, solid phase mass fraction, impeller type and off-bottom distance on the just-drawdown rotational speed (Njd), complete

drawdown rotational speed (Ncd) and cloud depth (CD) of dry and wet straw particles in the stirred tank.

Results: The results showed that the distribution of dry and wet straw in the stirred tank significantly differed. The models built by dimensional analysis and machine learning were suitable for accurate predictions of specific variables. Based on the model analysis, the Njd of dry straw was mainly affected by the liquid viscosity, impeller type and off-bottom distance, as these factors determined the flow field of liquid phase for its drawdown. Njd of wet straw was related to the liquid viscosity and Ncd was influenced by impeller off-bottom distance. The CD of dry and wet straw particles were both affected by rotational speed, impeller type, and liquid viscosity, which were related to the mean flow and turbulence intensity in the tank.

Conclusions: This study not only provides deep insights into the mixing dynamics of floating CS in non-Newtonian fluid but lays a foundation for the development of efficient mixing system for anaerobic digesters of lignocellulosic feedstock.

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2026 / SEOUL, KOREA

PTL0493

Hybrid GA-RL Optimization Framework for Natural Gas Liquefaction Under Compositional Variability

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Abstract Category: Process Intensification - Process Intensification / TEA / LCA **Keywords:**

Reinforcement learning, Natural gas liquefaction, Adaptive optimization

Abstract Body.
Natural gas liquefaction processes face compositional variability across feedstock sources, requiring repeated re-optimization that is computationally prohibitive for real-time operations. Traditional optimization methods like genetic algorithms (GA) achieve near-optimal solutions but demand extensive computational resources, often requiring thousands of process simulations per cycle, which makes them impractical for adaptive control under frequently changing feedstock conditions.
This study proposes a baseline-enhanced reinforcement learning framework that integrates evolutionary algorithms and reinforcement learning approaches for efficient adaptive optimization. The methodology consists of two phases: baseline establishment and adaptive fine-tuning. Genetic algorithms first systematically explore the design space across diverse natural gas compositions to generate high-quality reference solutions. These GA-optimized baselines serve as informed starting points for subsequent adaptation.
The key innovation is a baseline-deviation action formulation where the reinforcement learning agent learns relative adjustments from GA-optimized references rather than absolute operational values. This reformulation transforms the learning problem: instead of exploring the entire unbounded action space, the agent focuses on small corrective adjustments within feasible operational regions. The reinforcement learning algorithms enable stable policy gradient learning through variance reduction, while the continuous action space accommodates precise process adjustments.
Trained on diverse natural gas compositions spanning industrial feedstock ranges, the framework demonstrates significant computational efficiency gains compared to repeated GA optimization while maintaining near-optimal energy performance. The baselineenhanced approach also exhibits improved generalization to unseen compositions compared to standalone reinforcement learning methods. The baseline-deviation formulation ensures constraint satisfaction by restricting exploration to regions near feasible GA solutions, eliminating constraint handling challenges that plague conventional RL approaches in process optimization.
This work provides a practical solution for adaptive optimization under varying feedstock conditions, enabling near-real-time process adaptation without the computational burden of full re-optimization, particularly valuable where feedstock composition changes occur more frequently than traditional optimization cycles can accommodate.

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PTL0496

Multi-Objective Optimization of CO_2-LT-MED Integrated System for Carbon Capture and Desalination

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Abstract Category: Process Intensification - Process Intensification / TEA / LCA

Keywords: CO_2 utilization, CO_2 hydrate, Multi-effect desalination, Multi-objective optimization

Abstract Body.

This study proposes an innovative hybrid process that integrates CO_2 liquefaction and hydrate formation with low-temperature multi-effect desalination (LT-MED) to simultaneously enhance energy efficiency and economic viability. The system utilizes CO_2 captured from thermal power plants and processes it through two parallel pathways: liquefaction and hydrate formation. The core mechanism lies in strategic heat integration, where waste heat inevitably generated during CO_2 compression and phase-change processes is recovered and converted into thermal energy essential for operating the LT-MED system. This approach establishes direct thermal synergy between carbon management and desalination processes, fundamentally reducing the external energy requirements that conventional thermal desalination systems demand.

To evaluate the integrated system's performance, a multi-objective optimization framework was employed. Key operational parameters including the split ratio between liquefaction and hydrate pathways, seawater feed flow rate, and vapor fraction in individual evaporation stages were systematically adjusted. The optimization aimed to simultaneously maximize the Gained Output Ratio (GOR), a thermodynamic indicator of heat reuse efficiency, while minimizing the Unit Production Cost (UPC), which represents the economic competitiveness of freshwater production.

The integration of CO_2 capture and utilization (CCU) technology with freshwater production dramatically reduces the substantial external thermal energy demand inherent in conventional thermal desalination processes. The incorporation of hydrate technology not only presents a novel pathway for carbon management but also contributes to the overall thermal stability of the system. By strategically leveraging waste heat from CO_2 processing, this research demonstrates an environmentally sustainable solution through significant carbon emission reduction. Furthermore, the potential commercialization of CO_2 hydrate products is expected to generate additional revenue streams, enhancing the overall economic viability of the integrated system beyond conventional desalination operations

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

PTL0501

Techno-economic evaluation of hydrothermal liquefaction for chemical recycling of synthetic textile waste

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Abstract Category: Process Intensification - Process Intensification / TEA / LCA

Keywords: Hydrothermal liquefaction, Chemical recycling, Techno-economic assessment, Synthetic textile waste

Abstract Body.
Synthetic textile waste, largely composed of polyester (PET) and Nylon (PA6), is an attractive feedstock for chemical recycling due to its high climate impact, limited recycling options, and growing volumes linked to fast fashion. Subcritical hydrothermal liquefaction (HTL) enables direct monomer recovery from mixed condensation polymers [1], but its techno-economic feasibility at industrial scale remains unexplored.
The techno-economic assessment is based on eight HTL conditions performed in laboratory on a PET/PA6 (75/25 wt%) textile blend by varying dry matter content (10–20 wt%), residence time (10–30 min), and temperature (300–340 °C). Mass and elemental balances were closed by combining the experimental product yields with literature information through a Monte Carlo based MATLAB model. The resulting yields were then implemented in Aspen Plus® to simulate an industrial plant with a feed capacity of 5 ktdry/y. The general process layout is represented in Figure 1. Several alternative process configurations were modeled to compare separation and valorization strategies for terephthalic acid (TPA), ethylene glycol (EG) and ε-caprolactam (CL), each evaluated with and without internal process recirculation, including distillation, liquid–liquid extraction, eutectic freeze crystallization, and direct wastewater treatment.
The most significant energy demand for the PET/PA6 HTL process is associated with heat requirements, which range between 2 and 5 MW, making heat integration essential for process feasibility. Among the scenarios evaluated, the 20% d.m.–30 min–340 °C reaction condition emerged as the most favorable due to its high monomer yields. For TPA, the analysis showed that optimizing the separation strategy based on its solubility across thermodynamic conditions is critical to monomer valorization potential. Direct caprolactam separation via eutectic freezing, combined with aqueous phase recirculation to concentrate ethylene glycol up to 37 wt%, enabled economically viable downstream distillation and resulted in overall monomer prices potentially competitive with current market values (TPA: 0.7-1.1 $/kg, EG: 0.5-0.7 $/kg, CL: 1.5-2.00 $/kg).

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PTL0566

CFD simulations of an electrically heated steam methane reforming reactor

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Abstract Category: Process Intensification - Process Intensification / TEA / LCA **Keywords:**

Internal Joule heating; Electrified SMR; Power profiles; Green hydrogen

Abstract Body.
Introduction: The increasing availability of affordable renewable electricity offers a significant opportunity to decarbonize energy-intensive chemical processes. Among the various technologies for converting electricity into heat, Joule heating—using direct electric current—has emerged as a promising option due to its higher thermal efficiency and faster thermal response. While several experimental studies have demonstrated the feasibility of electrically heated catalytic reactors, extending this technology to different design frameworks and industrial scales remains challenging. To tackle these challenges, highfidelity computational models are essential for capturing the system's multiphysics behavior and enabling systematic, in-depth analysis. This study investigates the impact of internal heating element design on the performance of an electrically heated reactor.

Methods: A 2-D axisymmetric computational fluid dynamics (CFD) model is developed to analyze the coupled electro-thermal-species behavior for the electrically heated steam methane reforming (SMR) reactor. Variable-density fluid flow, electric current, heat transfer, and species transport are solved in COMSOL Multiphysics. The reaction kinetics are based on the kinetic model proposed by Xu and Froment[1]. Both cold-flow and reactive simulations are performed, providing insights into heat and mass transfer and their coupling with catalytic reactions. Various internal heating element placements are explored, including helical wire, rod, mesh, and chord. Additionally, the optimization of the axial power distribution is examined to provide insights into the system's thermal and species behavior.

Results and discussion: The developed CFD model is validated against experimentally measured axial temperature profiles for an electrified SMR by Wismann et al.[2]. Three different axial power profiles, constant power, linearly increasing power, and linearly decreasing power, are studied. Regarding the potential for process intensification, the simulations show that a linearly decreasing power profile produces nearly uniform temperature distributions along the reactor length. This enhances reaction rates and hydrogen yield. Importantly, the same level of methane conversion achieved in a full-length reactor can be obtained using only 50% of the reactor length under a linearly decreasing power input. A similar analysis is done for SMR under non-equilibrium conditions.

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PTL0603

Investigating Ni-Co/Al2O3-based structured foam catalyst for both exothermic and endothermic reactions

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Abstract Category: Process Intensification - Process Intensification / TEA / LCA

Keywords: Process intensification, Structured catalyst, Metal foam, Flue gas reforming of methane (FGRM), CO2 methanation

Abstract Body.

Introduction. Packed-bed reactors are often constrained by pressure drop and transport limitations, which can hinder performance in strongly exothermic reactions (e.g., CO_2 methanation) and endothermic processes (e.g., methane reforming). Open-cell metal foams offer high geometric surface area, low pressure drop, and enhanced transport properties, making them potential candidates for intensified reactor operation. Here, we develop a Ni–Co/Al_2O_3 washcoated Ni-foam structured catalyst and evaluate its relevance for FGRM and CO_2 methanation, with a specific focus on identifying the efficacy of using such type of structured catalyst.

Methods. A 10 wt% Ni3Co/Al2O3 catalyst was synthesized by incipient wetness impregnation method [1], and characterized using BET, XRD, SEM, and TEM. The catalyst was deposited on a commercial Ni foam (20 ppi, ~95% porosity) by dip coating using an optimized aqueous slurry, followed by calcination at 600 °C. The coated catalyst is referred to as catpowder. To probe mass-transfer transport effects, catpowder was tested as pellets with three average sizes (5.2, 275, 300 μm) in a fixed-bed quartz reactor in setups reported elsewhere [1], [2]. FGRM was performed at 600 °C and 800 °C (Wc = 10.9 mg; Ft/Wc = 5,50,459 mL g^{-1} h^{-1}), while CO_2 methanation was performed at 300 °C and 350 °C (Wc = 50 mg; Ft/Wc = 30,000 mL g^{-1} h^{-1}).

Results and discussion. BET analysis gives a surface area of 105 m^2 g^{-1}. EDX mapping confirms the targeted 10 wt% metal loading in catpowder, and XRD evidence shows Ni–Co alloy formation. Dip coating produced reproducible, homogeneous washcoat layers on the foam with a uniform thickness of ~8 μm. Figure 1 shows that CH4 conversion in FGRM at both 600 °C and 800 °C depends strongly on particle size, indicating clear transport limitations at both temperatures. For CO_2 methanation, transport limitations become evident for particle sizes ≥ 275 μm, with the activity penalty more pronounced at higher temperature for both reactions. Furthermore, a Ni–Co/Al_2O_3@Ni-foam structured catalyst with a uniform coating is synthesized and is currently being tested for the two reactions.

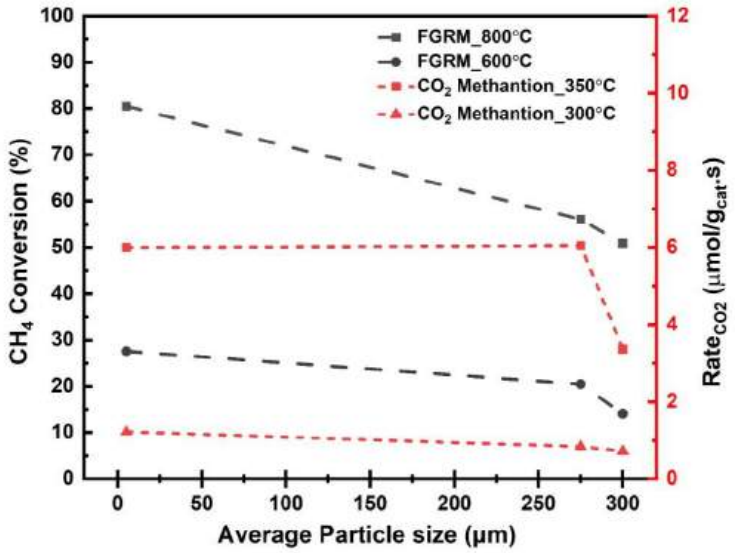

Figure 1. Effect of average particle size of Catpowder on activity for FGRM reaction and CO2 methanation at their specified reaction conditions.

Conclusions. Catalyst particle size introduces transport limitations in both FGRM and CO_2 methanation, particularly at higher temperatures and for larger particles (≥275 μm in methanation). Ongoing work focuses on establishing the benefits of using structured catalysts for improved activity and long-term stability under the respective FGRM and CO_2 methanation conditions.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

PTL0610

Effect of nonlinear fluid rheology on gas-liquid flows in milli/microchannel distributors

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Abstract Category: Process Intensification - Process Intensification / TEA / LCA

Keywords: microchannel distributor, T-junction splitting, phase-field model, non-Newtonian rheology, kerosene – air, flow uniformity

Abstract Body.

Introduction. Numbering-up of milli/microreactors can raise throughput while preserving microscale transport advantages, but only if gas-liquid flow is uniformly distributed across parallel channels. Small maldistribution quickly magnifies into large variations in bubble/slug length, junction pressure drop, and residence-time distribution. In distributor networks, this behavior is largely set by breakup and phase splitting at T-junctions, governed by the balance of capillarity, viscous stresses, and transient pressure fluctuations. Most prior studies assume Newtonian liquids [1], however, many practical fluids are shear rate dependent. This aspect changes the effective resistance and capillary number at the junction, thus affecting formation/ breakup time scales and split ratios. The role of such nonlinear rheology in optimized uniformity-focused distributors remains insufficiently quantified, motivating this study.

Methods. For the present study we utilize our earlier distributor design for Newtonian silicone oil – air system [2] featuring wedge-assisted, flow focusing and successive square-root reduction of channel widths. A model case of kerosene (Newtonian) – air system is chosen to establish baseline splitting behavior at a T-junction and to validate phase-field simulations against experiments. For simulations, power-law is chosen to describe fluid rheology. Liquid and gas flow rates are selected to match stable segmented flow operation, and splitting is analyzed using formation/splitting time, relative slug/bubble lengths, and pressure-drop trends. (Rheological model with parameter estimation will be presented in the full-length manuscript.)

Results and discussion. Figure presents transient images of bubble splitting at the T-junction for the model case at QL, QG = 10, 3.09 mL/min. The experimentally observed sequence of bubble growth, necking, and breakup agrees well with phase-field simulations, confirming that the model captures the key interfacial evolution and splitting time scales, including partially-obstructed splitting behavior. We have further investigated non-Newtonian rheological effects (e.g., power-law index and consistency) on formation/splitting times, sluglength asymmetry, and hydraulic resistance in the distributor network. The corresponding model validation and detailed analysis will be included in the full-length manuscript.

Acknowledgments. The authors acknowledge the kind support provided by the host institution for lab space and equipment.

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PTL0671

Process-Level Assessment of Sustainable Aviation Fuel Production via RWGS Packed-Bed Membrane Reactor Integration

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Abstract Category: Process Intensification - Process Intensification / TEA / LCA

Keywords: Membrane reactor, process simulation, SAF production, LCA analysis, Aspen Plus

Abstract Body.

Introduction Current environmental and energy challenges require effective CO_2 mitigation strategies in the aviation sector. Because full electrification is impractical for long-distance air transport, sustainable aviation fuel (SAF) is considered as a key decarbonization pathway. Among available routes, low-temperature Fischer–Tropsch (LTFT) synthesis is promising, in which renewable H_2 and CO_2 are converted to syngas via the reverse water gas shift (RWGS) and subsequently to hydrocarbons [1,2]. However, due to the endothermic and equilibrium-limited nature of RWGS, the reactor typically requiring high operating temperatures (600–900 °C) that cannot be readily supplied by renewable heat. To address this limitation, packed-bed membrane reactors (PBMRs) equipped with hydrophilic membranes are investigated as a process-intensification strategy, enabling lowertemperature operation through water removal [3]. This work assesses the energy and environmental benefits of integrating an RWGS PBMR relative to a conventional RWGS process.

Methods A PBMR model is implemented in MATLAB and coupled with Aspen Plus via an Excel interface for process simulation. The RWGS PBMR is integrated into a full SAF production flowsheet and compared to conventional RWGS-based process, including RWGS, FT synthesis, hydrocracking, and autothermal reforming. The environmental impact of SAF production is quantified through life-cycle greenhouse gas (GHG) emissions using the GREET model developed by Argonne National Laboratory. Results and discussion The KPIs for comparison are shown in Table 1.

	Conventional case	PBMR case
Energy efficiency	42.4%	43.2%
Mass yield	25.1%	25.2%
Well-to-gate GHG, g/MJ-SAF	-84.1	-97.1

Table 1: KPIs for SAF production:

PBMR-integrated system exhibits slightly higher overall energy and exergy efficiencies primarily due to reduced CO_2 recycling requirements enabled by higher effective CO_2

conversion. Furthermore, the life cycle assessment results indicate a great reduction in well-to-gate GHG emissions for the PBMR-based SAF pathway by reducing the high-temperature heat demand: about 20 kg of greenhouse gas emission can be avoided per GJ of SAF with renewable heat supplement. These results highlight the potential of RWGS membrane reactor integration for improving both process efficiency and environmental sustainability in SAF production.

Acknowledgments

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ISCRE29 & APCRE11
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PTL0752

Modeling of a rotating packed bed absorber for acrylic acid recovery

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Abstract Category: Process Intensification - Process Intensification / TEA / LCA **Keywords:**

Rotating Packed Bed(RPB), Acrylic Acid Absorption, Process Intensification

Abstract Body.
In industrial processes, acrylic acid (AA) is produced via catalytic oxidation of propylene and must be separated from complex reaction effluents in downstream units. Conventional packed-bed absorbers are commonly used but are limited by low gas–liquid mass transfer efficiency, resulting in large equipment size, high solvent circulation, and significant capital cost. These drawbacks have driven interest in intensified absorber technologies that achieve equal or improved separation within a more compact footprint. Among process-intensification options, rotating packed beds (RPBs) operating under high gravity have emerged as a promising alternative due to their ability to enhance interfacial area and transport rates. In this study, a process-level modeling framework for RPB absorbers is developed as an intensified alternative for AA absorption processes. A rate-based RPB absorber model was constructed using Aspen Custom Modeler (ACM), enabling detailed representation of coupled mass and heat transfer phenomena. The RPB was described as a one-dimensional radial domain with counter-current gas–liquid flow, allowing the characteristic hydrodynamics of high-gravity operation to be captured while maintaining computational tractability.
Gas–liquid phase equilibrium was modeled using an NRTL-HOC-based γ–φ vapor–liquid equilibrium (VLE) formulation, which simultaneously accounts for liquid-phase non-ideality and gas-phase association behavior relevant to AA-containing systems. Interfacial mass and heat transfer were described using the two-film theory, providing a consistent framework for evaluating transport resistances under intensified operating conditions. The governing mass and energy balance equations were formulated as a coupled system of algebraic and partial differential equations. To ensure numerical robustness under convection-dominated transport, the equations were discretized along the radial direction using a first-order backward finite difference scheme.
Model results indicate that absorption performance comparable to that of conventional packed-bed absorbers can be achieved using RPB technology with substantially reduced solvent usage and equipment size. Specifically, the required water flow rate for AA absorption was reduced by approximately 40–60%, while the overall absorber size decreased by about 50–70% relative to conventional packed-bed columns. These improvements clearly demonstrate the impact of enhanced mass transfer induced by highgravity operation on absorber intensification.
Overall, the results suggest that RPB technology offers significant potential for the intensification of AA absorption processes by enabling compact absorber design and reduced solvent circulation. The proposed ACM-based rate-based RPB modeling framework provides a practical and flexible tool for quantitative performance evaluation, preliminary

design, and comparative assessment of intensified AA absorbers, and can serve as a foundation for future process optimization and scale-up studies.

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2026 / SEOUL, KOREA

PTL9700

3D-printed structured adsorbents for CO2 capture - experiments and mathematical modeling

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Capture

Keywords: CO2 capture, Zeolite 13X, monolith structures, reactor study, mathematical model

Abstract Body.

1. Introduction

Global warming caused by CO2 emissions has prompted significant efforts towards carbon capture and storage. Solid adsorbents are alternatives to liquid amines due to their lower regeneration energy requirements. However, the high pressure drops in adsorbent powder and pellets have motivated the development of structured adsorbents like monoliths.[1] In this study, 3D-printed Zeolite 13X monoliths of different geometries are fabricated and tested for their CO2 capture performance.[2]

2. Methods

2.1 Experiments

Monolith structures were 3D-printed using Zeolite 13X powder, binders, and distilled water as the solvent. Structures of diameter 1.7 cm and height 1 cm with single and five channels of diameter 0.3 cm were printed. Moreover, they were scaled up to diameter 4.5 cm and height 3 cm, with five channels of 0.8 cm.

Breakthrough experiments were performed using a 20:80=CO2:N2 gas mixture with the monoliths stacked up to 10 cm. Experiments were conducted in two different column diameters (2 cm and 5 cm) to study scale-up effects. The CO2 concentration at the exit of the bed was measured using a gas analyser, the temperature at the centre of the bed using a K-type thermocouple, and the pressure drop across the bed using a differential pressure transmitter.

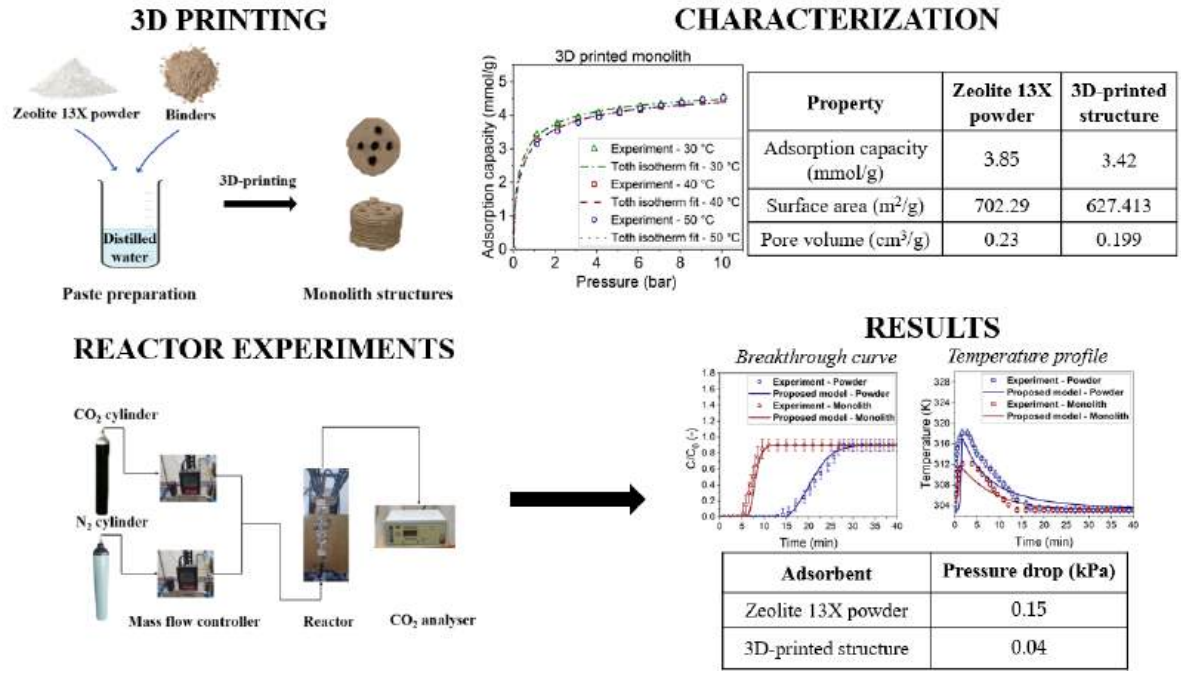
2.2 Mathematical model

A pseudo-2D mathematical model that can predict the effect of monolith channel geometry on CO2 adsorption was developed in MATLAB. The breakthrough curve, temperature profile, and pressure drop across the bed were modeled under experimental conditions, and compared with the experimental results.

3. Results and Discussion

The pressure drop across the structures was approximately 50% lower than that across packed-beds of powder and pellets, although the structures exhibited slightly lower adsorption capacities, due to the presence of binders. Moreover, the structures showed improved thermal management, characterized by lower temperature peaks, due to shorter characteristic heat-transfer lengths. Furthermore, the five-channel structures performed better than the single-channel ones, exhibiting lower pressure drops and temperature peaks. This work also demonstrated the successful fabrication of large-scale monolith structures for CO2 capture. The proposed mathematical model accurately predicted the adsorption performance of structures of various geometries. Figure 1 shows a summary of the

experimental and modeling results of this work.



Property	Zeolite 13X powder	3D-printed structure
Adsorption capacity (mmol/g)	3.85	3.42
Surface area (m^2/g)	702.29	627.413
Pore volume (cm^3/g)	0.23	0.199

Adsorbent	Pressure drop (kPa)
Zeolite 13X powder	0.15
3D-printed structure	0.04

Figure 1: Summary of the experimental and modeling results of this work

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Poster Presentation

Heterogeneous/Homogeneous Catalysis

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

HTT0035

Enhancing Higher Alcohols Selectivity in CO2 Hydrogenation over FeCu Catalysts via Mg Modification

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: CO2 hydrogenation, Higher alcohols, Mg modification

Abstract Body.
CO_2 hydrogenation to higher alcohols (C_2 $^+$ OH) is a promising route for sustainable carbon utilization but remains challenging due to CO_2 stability and difficult C–C coupling. Cu-based catalysts show high CO_2 conversion but mainly produce methanol, while FeCu systems improve CO* and CH_x* formation yet suffer from unstable interfaces. Introducing Mg can tune surface properties, stabilize active sites, and enhance C_2 $^+$ OH selectivity.
In this work, FeCu-based catalysts with different dopants were prepared by co-precipitation. The Mg-modified catalyst 2Na/Fe_1 Cu_2 Mg_1 exhibited the best performance. At 320 °C and 5 MPa, it achieved 25.4% C_2 $^+$ OH selectivity with a space–time yield (STY) of 75.1 mg·g^{-1}·h^{-1}. Raising the temperature to 380 °C increased the STY to 110.1 mg·g^{-1}·h^{-1}, with 55.4% CO_2 conversion and only 6.7% CO selectivity, indicating Mg's key role in regulating catalytic behavior.
Characterization showed that Mg suppressed Fe_2 O_3 and CuO crystallization, reduced particle size, enhanced metal dispersion, and promoted the formation of stable, highly dispersed Cu–χ–Fe_5 C_2 interfaces. CO_2 -TPD, CO-TPD, and in situ DRIFTS confirmed strengthened CO_2 /CO adsorption, stabilized carbonate intermediates, and improved CO insertion while suppressing excessive CH_x formation. These synergistic effects enhanced C–C coupling and boosted C_2 $^+$ OH production.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

HTT0036

Highly Efficient Hydrogenation of CO2 to Heavy Hydrocarbons via NaFeGa Catalysts

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: CO2 hydrogenation, Fischer-Tropsch pathway, Heavy hydrocarbon.

Abstract Body.
Transforming CO2 into heavy hydrocarbons via thermal catalytic hydrogenation has garnered interest for its potential to address resource shortages and reduce atmospheric CO2. In this research, NaFeGa catalysts enriched with Ga additives were synthesized by the coprecipitation method. Various characterization techniques, including Mössbauer spectroscopy, were employed alongside reverse water-gas shift and Fischer-Tropsch synthesis experiments to elucidate the Fe-Ga interaction. This interaction effectively modulated the ratio of active sites Fe5C2 and enhanced CO species adsorption. The Ga additive's anti-hydrogenation effect limited intermediate hydrogenation, leading to increased carbon-hydrogen product yields. The catalyst underwent direct hydrogenation of CO2 under high throughput conditions (space velocity of 50,000 h−1), resulting in efficient CO2 conversion as well as remarkable heavy hydrocarbon selectivity. The catalyst demonstrated a remarkable heavy hydrocarbon space-time yield (STY) of 1460.2 g·kgcat−1·h−1, surpassing the threshold for commercial viability and offering a promising solution for large-scale production of liquid fuels from CO2.

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HTT0057

Investigation of additive-manufactured catalysts in the decomposition of hydrogen peroxide

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Additive-manufacturing, Hydrogen peroxide decomposition, Structured catalyst

Abstract Body.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

HTT0060

Synthesis and Characterization of Additively Manufactured Iron Beta Zeolites for Methane Oxidation

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: methane oxidation, iron zeolites, heterogenous catalysis, exhaust gas treatment, automotive emission control, additive manufacturing

Abstract Body.
Introduction. Within the broader context of climate change mitigation and evolving regulatory landscapes, dual-fuel and gas-powered marine engines offer a potential pathway to reduce emissions. However, CH_4 slip remains a major challenge, highlighting the need for improved aftertreatment technologies. Effective mitigation requires oxidation to CO_2, yet conventional platinum- or palladium-based catalysts are costly and unstable in aqueous or sulfur-rich environments. This drives the search for more economical and robust alternatives. Iron zeolites, already effective in NOx reduction via SCR, have emerged as promising, cost-efficient catalysts for complete CH_4 oxidation and dual-purpose emission control. This study examines the preparation and structural characterization of 3D-printed cordierite bodies coated with iron-containing beta zeolites of various geometries and loadings, along with an evaluation of their catalytic activity.

Methods. The bodies, consisting of cordierite and binder material, were synthesized using a powder-based binder jetting 3D printing process. Linear Cells, honeycomb structures, and Diamond Cells were produced. In parallel, the washcoat containing the catalytically active precursor was prepared by introducing iron nitrate into commercial beta zeolites via liquid ion exchange. The washcoat was applied to the bodies via wetness impregnation. Structural characterization was conducted using methods such as X-ray powder diffraction (XRD), N_2 physisorption analysis, atomic absorption spectroscopy (AAS), pyridine, CO and NO infrared spectroscopy (IR), as well as pressure drop measurements. Catalytic activity was evaluated under defined CH4 and O2 concentrations at temperatures between 300 and 650 °C and pressures up to 6 bar.

Results and discussion. CO IR measurements revealed slight dealumination caused by the liquid ion exchange synthesis, as well as the formation of extra-framework silanol nests. Moreover, an enhanced adsorption capacity was observed due to the formation of Fe–carbonyl groups and the interaction of CO with Lewis framework acid sites upon incorporation of Fe species. Pyridine IR analysis further showed a pronounced increase in acidity with increasing Fe loading, mainly attributed to framework Fe and Al sites. Pressure drop measurements indicated that the lowest pressure drop occurred for geometries with the highest porosity, confirming the strong influence of structural design on flow behavior. Catalytic activity measurements demonstrated that complete CH_4 conversion

leads exclusively to CO_2 formation, while at lower temperatures partial oxidation occurs, resulting in the additional formation of CO with yields of up to 30 %.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

HTT0106

Design and Evaluation of a Molten Metal-Assisted Methane Pyrolysis System with Transition Metal-Based High-Entropy Alloy (HEA) Nanoparticles Dispersed in a Molten Media

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Methane pyrolysis, High-entropy alloy catalyst, Molten metal catalysis, Turquoise hydrogen, Heterogeneous catalysis

Abstract Body.
Introduction. Methane pyrolysis has emerged as a promising route for producing hydrogen without direct CO2 emissions, generating solid carbon as a valuable by-product.[1] However, conventional solid catalysts suffer from rapid deactivation due to carbon deposition, while molten metal systems, despite their operational robustness, exhibit limited intrinsic catalytic activity. To bridge this gap, this study explores a molten metal-assisted methane pyrolysis system incorporating dispersed high-entropy alloy (HEA) nanoparticles as active catalytic centers.[2] By combining the structural stability of molten metals with the multi-metallic synergy of HEAs, the work aims to enhance methane conversion, suppress deactivation, and enable stable hydrogen production for continuous operation.
Methods. Ni–Co–Cu–Fe–Sn high-entropy oxide (HEO) nanoparticles were synthesized via a co-precipitation and calcination route and subsequently dispersed in molten gallium. During reactor operation, the HEO precursor was reduced in-situ to form catalytically active HEA nanoparticles. Methane pyrolysis experiments were conducted in a vertical bubble-column reactor containing a Sn–Ga molten metal bath with 1 wt.% HEA loading. Reactions were performed at 700–1000 oC under CH4/N2 (80%/20%) feeds with methane flow rates ranging from 0.1 to 5.0 L min-1. Gas products were continuously monitored using an NDIR analyzer to quantify methane conversion and CO formation.
Results and discussion. The incorporation of HEA nanoparticles into the Sn–Ga molten metal significantly enhanced methane conversion (56%) compared with the bare Sn–Ga (44%) system across all operating conditions. At 1000 °C and moderate space velocity, the HEA-modified bath exhibited substantially higher and more stable methane conversion, while the unmodified molten metal showed rapid deactivation as flow rate increased. Even at high methane flow up to 0.5 LPM, the HEA-containing system retained appreciable activity, demonstrating strong resistance to kinetic limitations and deactivation.
Temperature-dependent studies revealed a monotonic increase in methane conversion with increasing temperature, and Arrhenius analysis showed a substantially reduced apparent activation energy (Ea= 73 kJ mol-1) relative to non-catalytic molten metal systems,

confirming the true catalytic role of the HEA nanoparticles.

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ISCRE29 & APCRE11
2026 / SEOUL, KOREA

HTT0141

Overcoming Concentration Limits in Continuous HMF Hydrogenation with Long-term Stable THFDM Production in an Aprotic Ether Solvent

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: THFDM, hydrogenation of HMF, aprotic ether solvent

Abstract Body.

The selective hydrogenation of 5-hydroxymethylfurfural (HMF) to 2,5-tetrahydrofurandimethanol (THFDM) represents a vital pathway for producing versatile, bio-based building blocks that can replace petroleum-derived chemicals in various high-value applications. Despite its potential, conventional catalytic processes are often limited by low substrate concentrations (less than 2 wt.%) and rapid catalyst deactivation due to humin formation in typical protic solvents. This study addresses these challenges by developing a scalable, continuous-flow process capable of handling highly concentrated HMF at 25 wt.% while ensuring exceptional long-term catalytic durability.

To achieve this, continuous-flow hydrogenation was conducted in a fixed-bed reactor using a Ru/γ-Al2O3 catalyst at 100 °C and 50 bar. 1,2-dimethoxyethane (DME) was strategically employed as an aprotic ether solvent to enhance HMF solubility and suppress undesirable side reactions. The fundamental role of the solvent in increasing hydrogen solubility was further investigated through COSMO-RS calculations. The robustness of catalytic system was rigorously evaluated through a 200-hour time-on-stream test, followed by comprehensive catalyst characterization using XRD, TEM-EDS, and XPS to monitor structural integrity.

The results demonstrated that DME significantly outperforms conventional protic solvents, achieving nearly 100% HMF conversion and THFDM selectivity even at an industrially relevant concentration of 25 wt.%. COSMO-RS analysis revealed that hydrogen solubility of DME is approximately 1.7 times higher than that of methanol–long recognized as the conventional solvent for hydrogenation–which effectively promotes catalytic turnover. Most notably, the catalytic system maintained its high performance without any sign of deactivation throughout the 200-hour continuous operation. Post-reaction analysis confirmed that Ru nanoparticles remained well-dispersed and that the electronic environment of the active sites was preserved despite minor carbon deposits.

In conclusion, this work establishes a robust and integrated catalytic strategy for the high-concentration production of THFDM enabled by the unique properties of an aprotic ether solvent. By overcoming the critical bottlenecks of low productivity and short catalyst life, this process offers a commercially viable and sustainable route for the mass production of biomass-derived specialty chemicals, paving the way for the broader replacement of petrochemicals.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

HTT0143

Limiting Dispersion of Pt Supported on Alumina with Different Crystal Phases during Oxychlorination Treatment

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: propane dehydrogenation, highly dispersed platinum-based catalyst, oxychlorination regeneration, carrier properties, sintering

Abstract Body.
The structural stability of propane dehydrogenation catalyst in reaction-regeneration cycle is the key to its industrial application. A series of Al2O3 supports with different crystalline phases (γ-/θ-Al2O3) and pore structures were prepared by controlling the calcination temperature of pseudo-boehmite (600, 800, and 1000 °C). Platinum was then loaded onto these supports at two different loadings (0.3 and 0.5 wt%) using the incipient wetness impregnation method. For the sintered catalysts, two regeneration strategies were systematically investigated: prolonged oxychlorination treatment and multiple cycles of oxychlorination-decoking. The influence of support properties on the regeneration behavior and performance of highly dispersed Pt catalysts was thoroughly examined using characterization techniques such as HAADF-STEM, CO-DRIFTS, XPS, H2-TPR, TGA, and performance testing. The results show that the regeneration path and limiting dispersion of Pt are dominated by the intrinsic properties of the support. γ-Al2O3 (especially 800 °C) with high specific surface area is more conducive to Pt redispersion and smaller limit particle size, while θ-Al2O3 (1000 °C) shows better coking resistance due to stronger metal-support interaction. At high loading, the ability of the catalyst supported on a low specific surface area support to recover activity through regeneration is reduced.

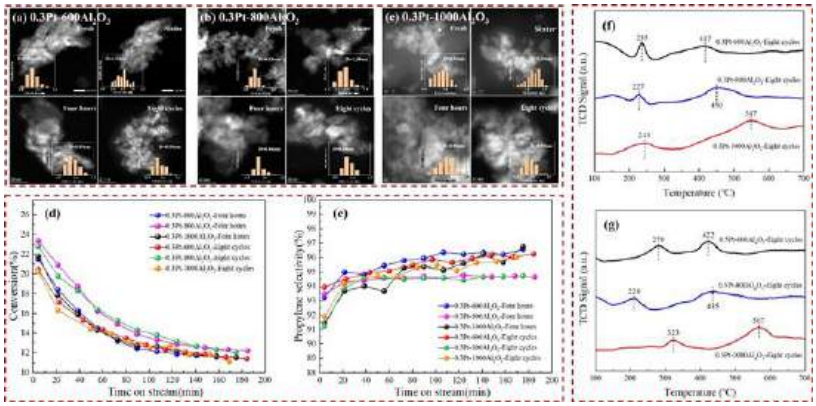

Fig. 1 Structural properties and catalytic performance of Pt/Al2O3 catalysts; a)-c) HAADF-STEM images, d)-e) catalytic performance, f)-g) H2-TPR results.

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HTT0152

DME conversion to gasoline-range hydrocarbon fuels on hybridized FER@ZSM-5 zeolite

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: DME conversion to gasoline, Hybridized zeolite, FER and ZSM-5

Abstract Body.

Introduction

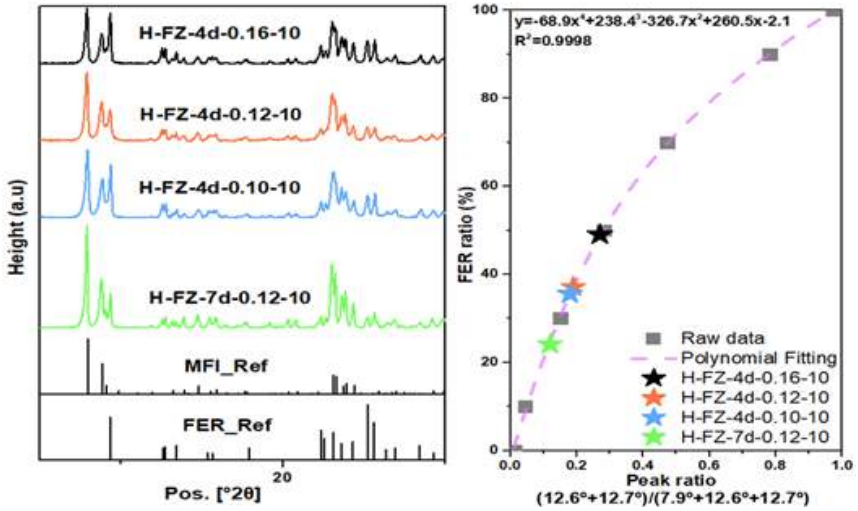
Solid acid ZSM-5 zeolite is well known for DME conversion to gasoline-range hydrocarbons (fuels) production, which shows a higher C2-C4 olefin selectivity due to the presence of strong acidic sites. To further enhance gasoline-range fuels through oligomerization of olefins, FER zeolite can be hybridized with FER zeolite through one pot synthesis. Gasoline-range hydrocarbons, as alternative fuels from CO2, can be synthesized from dimethyl ether (DME) conversion by using sloid acid zeolites, where DME can be produced by a gas-phase CO2 hydrogenation. Various solid acid zeolites, especially ZSM-5, have been widely studied for DME conversion to gasoline-range fuels in commercial scale, and catalyst stability is still under investigation to develop stable processes by using various zeolite composites. In the present study, the hybridized FER@ZSM-5 was introduced by one-pot synthesis to verify the enhanced catalytic stability and selectivity to gasoline-range hydrocarbons.

Methods

The ratio of FER/ZSM-5 on the hybridized zeolites was tuned by changing Na/Si ratio of synthetic gel, and the effects of FER/ZSM-5 ratio were verified by using FER@ZSM-5 with reference zeolites such as physically mixed zeolites. The FER@ZSM-5 was synthesized by using two structure directing agent (SDA) such as CTAB and pyrrolidine. Synthetic gel was transferred to autoclave for hydrothermal synthesis at 160 ºC for 96 h in a tumbling agitation vessel. After an ion-exchange by using NH4NO3, catalytic activity of the synthesized H-form FER@ZSM-5 zeolites were tested in a fixed-bed tubular reactor at the reaction condition of DME/N2 = 5/95 (molar ratio) at GHSV = 3600 L/(kgcat·h), T = 300 ºC and P = 0.1 MPa.

Results and discussion

As shown in Figure 1, the FER/ZSM-5 weight ratios were calculated by using XRD peak area, and the closely connected composite structures according to the FER/ZSM-5 ratios on the FER@ZSM-5 zeolites were largely altered by Na/Si ratio and aging time. Compared to the reference pristine ZSM-5, showing 50.9% gasoline-range hydrocarbons selectivity, the optimized FER@ZSM-5 (Na/Si ratio = 0.10 and Si/Al ratio = 10) revealed a higher selectivity to 68.0% due to the adjusted acidic sites and suppressed coke depositions.


H-FZ-4d-0.16-10
H-FZ-4d-0.12-10
H-FZ-4d-0.10-10
H-FZ-7d-0.12-10
MFI_Ref
FER_Ref
Height (a.u)
Pos. [°2θ]
20
y=-68.9x⁴+238.4³-326.7x²+260.5x-2.1
R²=0.9998
FER ratio (%)
Peak ratio
(12.6°+12.7°)/(7.9°+12.6°+12.7°)
Raw data
Polynomial Fitting
H-FZ-4d-0.16-10
H-FZ-4d-0.12-10
H-FZ-4d-0.10-10
H-FZ-7d-0.12-10

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HTT0154

Hydroxyalkylation of Phenol with Formaldehyde over 2D MWW-Type Zeolite Catalysts: The Effect on Performance and Isomer Distribution of Bisphenol F Synthesis

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Bisphenol F, 2D MWW zeolites, hydroxyalkylation

Abstract Body.

Purpose

Bisphenol F (BPF) is a significant intermediate for the production of epoxy and polycarbonate resins due to its thermal resistance and electrical insulation properties. With increasing demand, the development of efficient BPF synthesis routes has attracted attention. Conventional BPF synthesis using liquid protonic acids suffers from hazardous waste generation, corrosion, operational risks, and poor recyclability. In this study, zeolite-based solid acids have emerged as a promising alternative owing to their porous structures, adjustable acidity, and hydrothermal stability. Specifically, this study aims to construct two-dimensional (2D) MWW-type zeolites with open-layered architectures to improve active-site accessibility and transport of bulky BPF intermediates.

Method

The MWW precursors, B-, Al-, and Si-MWW(P) were prepared through the reported literature. The 2D B-, Al-, and Si-MWW catalysts were synthesized by treating MWW(P) with cetyltrimethylammonium bromide and tetrapropylammonium hydroxide at 80 °C for 16 h, followed by sonication and acidification (pH < 2). The 2D Ni-MWW catalyst was prepared by hydrothermal treatment of B-MWW(P) in 1.0 M Ni(NO3)2·6H2O solution at 160 °C for 4 d. All samples were calcined at 550 °C for 8 h. Structural and acidic properties were characterized by PXRD, N2 sorption, FT-IR, and pyridine-IR spectroscopy. The BPF reaction was carried out at 90 °C and the products were analyzed by HPLC.

Results

PXRD patterns and N2 sorption analyses confirmed the successful transformation of 3D MWW into 2D structure with enhanced external surface area and accessibility. Pyridine-IR revealed a systematic increase in Brønsted acid concentration with heteroatom incorporation by order Si-MWW < B-MWW < Ni-MWW < Al-MWW, while Lewis acid densities were relatively similar. Catalytic evaluation in the BPF reaction showed a strong correlation between Brønsted acidity and catalytic performance, confirming its dominant role in conversion and yield, whereas Lewis acid sites mainly influenced isomer distribution. Consequently, the catalytic activity followed the order Al-MWW > Ni-MWW > B-MWW > Si-MWW.

Conclusions

2D MWW-type zeolitic materials were successfully synthesized via hydrothermal treatment at 160 °C and/or by delamination of 3D MWW zeolite precursors at 80 °C. Catalytic

evaluation in BPF synthesis revealed that the catalytic performance followed the order Al-MWW > Ni-MWW > B-MWW > Si-MWW. This trend is strongly correlated with the nature of the heteroatoms incorporated into 2D MWW framework, which governs the density and strength of Brønsted acid. Notably, Brønsted acidity plays a dominant role in determining the overall reaction efficiency, whereas Lewis acid primarily effect on distribution of BPF isomers.

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HTT0196

Flash Joule Heating Enabled α-MoC Synthesis Route and Phase Fraction Dependent Performance in H2 Free Acetylene Hydrogenation

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Hydrogen free, Acetylene conversion, α-MoC, Flash joule heating

Abstract Body.
Molybdenum carbide has attracted attention as a robust catalyst for selective hydrocarbon transformations, yet the role of phase composition in acetylene conversion remains insufficiently quantified. Here, we evaluate phase fraction dependent performance of α-MoC prepared by two synthesis routes, flash joule heating (FJH) and fixed bed carburization, for H2 free selective acetylene hydrogenation in a batch reactor. The carbide phase fractions were quantified by X ray diffraction combined with Rietveld refinement, enabling a comparative assessment of α-MoC rich and mixed phase samples. Catalytic tests were conducted under hydrogen free conditions, and acetylene conversion and ethylene selectivity were used as key performance metrics. Across catalysts synthesized by both routes, increasing α-MoC phase fraction was correlated with improved acetylene conversion and enhanced ethylene selectivity, indicating that phase composition provides an effective lever for tuning catalytic behavior. In addition, the two synthesis routes offered distinct handles to modulate phase fraction, highlighting FJH as a rapid alternative to conventional carburization while maintaining comparable structure performance trends. These results demonstrate that controlling α-MoC phase fraction is a practical strategy to optimize catalytic performance for hydrogen free selective acetylene hydrogenation and motivate further studies on synthesis–structure–reactivity relationships for carbide catalysts.

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HTT0219

Inverse design of ORR catalyst active sites using an HPC-based topological deep generative model

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Inverse design, Catalysis, Deep generative model

Abstract Body.
This study designs topological structure representations and features, and integrates them with deep generative models (e.g., Multi-VAE, Transformer, and GNN-based generators) to build a framework that automatically generates interpretable catalyst structures. Using an iterative design–validation loop, the framework maximizes computational efficiency and enables high-throughput screening. It also quantitatively analyzes structure–performance relationships and applies real-time feedback to guide subsequent designs. Finally, the study proposes strategies to enhance applicability, scalability, and model sophistication across diverse catalyst systems, presenting a new paradigm for accelerating the development of eco-friendly energy materials.

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HTT0244

Enhanced Oxidative Performance of Pt–Transition Metal Catalysts Supported on Activated Carbon for the Selective Oxidation of Glucose to Glucaric Acid

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Glucose oxidation, Glucaric acid, Pt bimetallic catalysts, Biomass valorization, C–C bond cleavage

Abstract Body.

Enhanced Oxidative Performance of Pt–Transition Metal Catalysts Supported on Activated Carbon for the Selective Oxidation of Glucose to Glucaric Acid

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Abstract
Glucose valorization offers a sustainable pathway for the production of high-value platform chemicals from renewable biomass resources. In this work, the selective oxidation of glucose to glucaric acid was systematically investigated over Pt-based bimetallic catalysts supported on activated carbon (AC). The catalysts were composed of 5 wt.% Pt combined with varying loadings (0.5–5%) of a transition metal (TM). Among the investigated catalysts, the 5Pt–1.5TM/AC exhibited the highest glucaric acid yield of up to 65%. The oxidation of glucose to glucaric acid proceeds through three consecutive steps: (i) glucose to gluconic acid, (ii) gluconic acid to glucuronic acid, and (iii) glucuronic acid to glucaric acid, with the second step identified as the rate-determining step. Achieving high selectivity toward glucaric acid is intrinsically challenging due to the energy-intensive oxidation of both terminal functional groups and the tendency of strongly adsorbed intermediates to undergo C–C bond cleavage, leading to undesired low-carbon products, such as C2–C3 acids and CO2. Parametric studies revealed that an optimal temperature lies in the range of 60–80 °C, while the reaction is highly sensitive to pH, with the maximum glucaric acid yield obtained at pH 8-9. Lower pH-reaction suffered from low activity, whereas strongly alkaline conditions (pH > 13) favored excessive C-C bond scission. These results indicate that mild reaction conditions are essential for suppressing over-oxidation and maximizing C6 product selectivity. Comprehensive physicochemical characterization demonstrated that the superior performance of the 5Pt1.5TM/AC catalyst compared to monometallic 5Pt/AC originates from the promotional role of the TM, which induces electronic and geometric modifications of Pt. These effects enhance oxygen activation for secondary oxidation step. Catalyst recyclability tests showed a slight decrease in activity over three consecutive runs, which is attributed to

the strong adsorption of reactants and intermediates on the catalyst surface.

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HTT0246

Effects of Sr-substituted La0.8-xSrxMnNiO3 perovskite structures for dry reforming of methane with CO2

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Dry reforming of methane (DRM), Sr-dopped LaMnNiO3 catalyst, Perovskite structures, Exsolution

Abstract Body.

Introduction

Dry reforming of methane with carbon dioxide reaction has been investigated to produce syngas by using Ni-based heterogeneous catalysts because product gases can be utilized through subsequent conversions to petrochemicals and liquid fuels [1]. Although Ni-based catalysts are attractive for syngas production, they suffered from a fast deactivation due to carbon depositions and aggregations of active metals. In the present study, Ni exsolution method was applied to generate anchored Ni nanoparticles with their higher sintering resistant natures by generating active oxygen vacant sites with an enhanced oxygen mobility to suppress coke depositions through their surface gasification [2], which improved the catalytic activity and stability under the DRM conditions.

Methods

The mixed metal oxides of Sr-substituted LaMnNiOx catalysts, abbreviated with La0.8-xSrxMn0.8Ni0.2O3-δ (x = 0-0.4, LSMNOx(La/Sr) with different La/Sr ratio), were prepared by using a Pechini method with chelating agents. The prepared LSMNOx gel was calcined at 800 °C for 6 h, and DRM reaction was carried out with CH4/CO2/N2 (molar ratio) of 1/1/2 at a gas hourly space velocity (SV) = 30,000 mL/(gcat·h), T = 800 oC and P = 0.1 MPa.

Results and discussion

The catalytic activity of the LSMNOx catalysts measured at 800 °C revealed volcano pattern according to Sr content with the highest CH4 and CO2 conversion (72% and 80%) on the LSMNOx(6/2) (x = 0.2) catalysts as shown in Figure 1(A) due to the abundant oxygen vacant sites. TEM images also confirmed the exsolved and anchored Ni nanoparticles on the perovskite structures as shown in Figure 1(B), which was found to be effective to suppress the aggregations of Ni nanoparticles even under DRM reaction condition by forming stable exsoluted Ni nanoparticles with ~25 nm in size. Figure 1(C) summarizes XPS results on the reduced LSMNOx catalysts, where the surface oxygen ratios were related with oxygen vacant sites and the surface metallic Ni^0 fraction was increased with the maximum value on the optimized LSMNOx(6/2) catalyst. We believe that the higher catalytic activity was mainly attributed to the stabilized Ni nanoparticles with abundant oxygen vacant sites on the thermally stable LSMNOx(6/2) catalyst.

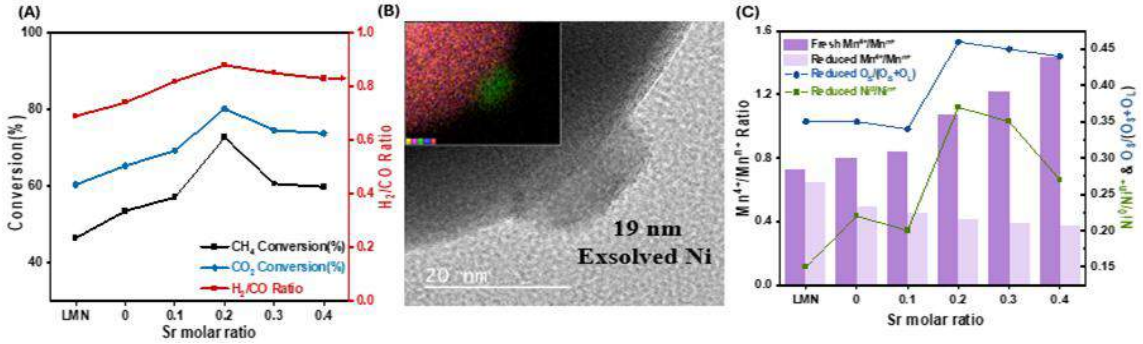

Figure 1. (A)Trends of catalytic performance at 800 °C on the LSMNOx catalysts (B)TEM images and EDS mapping of LSMNOx(6/2) with the exsoluted Ni nanoparticles (19 nm) on the LSMNOx surfaces (C)Summary of XPS results on the reduced LSMNOx catalysts.

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HTT0254

CO2 hydrogenation to dimethyl ether on Cu nanoparticles-supported mesoporous SiO2-incorporated Al2O3

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: CO2 hydrogenation to methanol; SiO2-incorporated mesoporous Al2O3; Evaporation Induced Self-assembly; Cu nanoparticles; acidic sites

Abstract Body.
Introduction. CO2 hydrogenation is one of the most interesting approaches for CO2 utilization for the production of value-added chemical intermediates. The highly ordered mesoporous Cu-Al2O3-based catalysts revealed one of the most promising candidates for direct CO2 hydrogenation to oxygenates including methanol and dimethyl ether (DME). Furthermore, the ordered mesoporous Al2O3 can induce a higher dispersion of active metals, resulting in high conversion of CO2. However, a higher CO selectivity and faster catalyst deactivation are reported as main disadvantages to be commercialized. In the present study, the silica-incorporated mesoporous alumina with various silicon to aluminum ratios (Si/Al) were prepared to be used as supporting material, which can suppress a reverse water-gas shift (RWGS) reaction and provide the active acidic sites for methanol dehydration to form DME.
Methods. Silica-incorporated mesoporous alumina was prepared by using an evaporation induced self-assembly (EISA) method, while tetraethyl orthosilicate (TEOS) precursor was used as a silica source. Copper nanoparticles were added on the SiO2-modifed Al2O3 support by using an incipient wetness impregnation (IWI) method with the fixed amount of 10 wt%Cu, which was calcined at 350 oC for 2 h and denoted as Cu/AlSi catalysts.
Results and discussion. With increasing Si/Al ratio of the Cu/AlSi catalysts, DME selectivity was increased up to 50%, suggesting that the methanol dehydration to DME was promoted due to the synergistic contributions of the increased acidic sites as shown in Figure 1(a). The CO selectivity was also decreased and CO2 conversion rapidly decreased with an increase of silica contents due to the structural instability. This was also attributed to the difficult reduction behaviors of the catalysts as shown in Figure 1(b). The Cu nanoparticles on the silica-incorporated alumina were found to be difficult to be reduced, suggesting a relatively smaller active metallic Cu nanoparticles, which further promoted RWGS reaction activity.

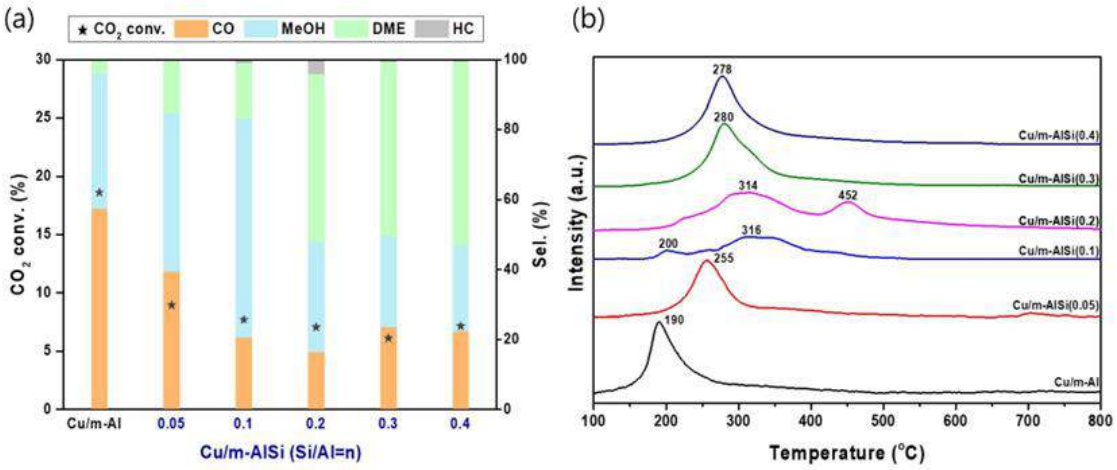

Figure 1. (a) Catalytic performance of Cu/AlSi catalysts with various silicon-to-aluminum ratio (Si/Al) (b) H2-TPR patterns of Cu/AlSi catalysts.

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HTT0322

Effect of alumina supports on non-oxidative direct conversion of methane over Fe catalysts

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Methane conversion, Fe/Al2O3 catalyst, Hydrocarbon yield, Long-term stability

Abstract Body.
Introduction. Direct methane conversion remains fundamentally challenging due to the high C-H bond dissociation energy of methane (439.3 kJ mol^{-1}) [1]. Although metal cations can lower the apparent reaction temperature compared to conventional methane pyrolysis, suppressing coke formation remains a major challenge. In this study, non-oxidative methane conversion (NMC) over Al2O3 supported Fe catalysts was systematically investigated to elucidate the role of Fe cations and Al2O3 supports for producing hydrocarbons.
Methods. A series of Fe/Al2O3 catalysts were prepared by incipient wetness impregnation using commercial a-Al2O3 supports with different particle sizes. Highly crystalline a-Al2O3 exhibited weak metal-support interactions with Fe species, which limited the formation of additional surface sites responsible for radical termination reactions. NMC was conducted at 900 °C under a WHSV of 2000 mL gcat-1 h-1. A post catalytic zone was positioned downstream of the catalyst bed to allow sufficient gas-phase reactions for hydrocarbon formation. Long-term stability was evaluated by reaction-regeneration cycle for up to 1000 h. Several characterizations were also performed to understand the physicochemical properties of catalytic surfaces.
Results and discussion. The C2-C5 hydrocarbon yield exhibited a volcano-type dependence on the particle size of Al2O3, with a maximum at 90–100 nm. Further optimization of Fe loading revealed that 0.1 wt% Fe supported on optimally sized Al2O3 achieved the highest selectivity (62.5 %) toward C2-C5 hydrocarbons and aromatics at 2.7 % methane conversion. The optimized catalyst maintained stable activity over 1000 h without noticeable deactivation during repeated 100 h reaction - 1 h O2 regeneration cycles. These results demonstrate that Al2O3 supported Fe catalysts provide a robust platform for initial C–H activation and stable non-oxidative methane conversion to value-added hydrocarbons.

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HTT0325

Ag nanoparticles synthesis: Population balance investigation

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: population balance equation, silver nanoparticles, CFD modelling, particle size distribution

Abstract Body.

Introduction.

The synthesis of nanoparticles (NPs) is a vital process in industry with a wide range of applications (catalytic reactions, medicine, material science etc.). Computational fluid dynamics (CFD) simulations coupled with population balance equation (PBE) provide a platform to calculate, control and optimise the particle size distribution (PSD) of metal NPs. In this work, we aimed to develop a CFD model to determine the PSD of synthesised Ag NPs in a perfectly mixed batch reactor and continuous flow reactor. Experimental data regarding the Ag NPs synthesis were obtained from literature [1].

Modelling Methodology.

The model was developed using COMSOL Multiphysics software version 6.2 where PBE, kinetic rates of the synthesis and boundary conditions were utilised to solve the problem, assuming the formation of Ag NPs via reduction of the AgNO3 precursor and NaBH4 reducing agent where only nucleation and growth is taking place. The same concentration of 0.25 mM was utilised for both solutions of AgNO3 and NaBH4 in order to produce a final Ag concentration of about 26 mg L−1. The Ag formation was conducted under boiling temperature and around 100 min. The PBE used can be described as:

$$\partial n/\partial t+\nabla \cdot(un)+\partial(G(S,L)n(L))/\partial L=v/Sc\ \nabla\ ^2\ n+B\_nuc\ \delta(L-L\_0) \quad (1)$$

(Selected) Results and discussion.

Figure 1 presents the comparison of PSD between the results in the perfectly mixed batch reactor. Experimentally, it was found that the particles had size of 13.7±6.2 nm, while simulations showed the mean particle size to be around 12 nm indicating the very good validation between the experimental and simulated results. Additional investigations include the effect of reaction temperature and residence time and initial concentration

of AgNO3 precursor.

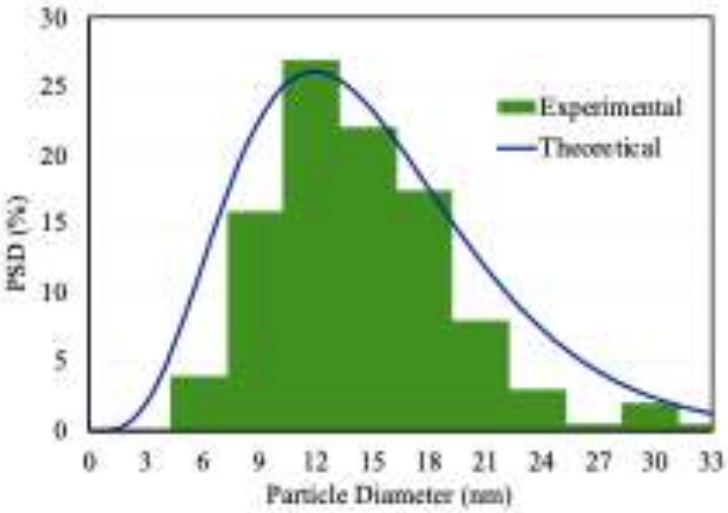

Figure 1. Comparison of Ag NPs PSD between the experimental and CFD modelling results.

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HTT0333

Ga-modified $ZnZrO_2$ metal oxides for chemical looping-based oxidative dehydrogenation of propane

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Chemical looping-based oxidative dehydrogenation, Propane dehydrogenation, Ga–Zn bimetal oxides, CO_2 utilization.

Abstract Body.
Chemical looping–based oxidative dehydrogenation (ODH) of propane using CO_2 as an oxidant is a promising strategy to enhance olefin selectivity while suppressing excessive combustion and coke formation. Zn-based catalysts provide active sites favorable for selective propane dehydrogenation, leading to high propylene selectivity, whereas Ga species exhibit a superior redox property and oxygen mobility, which promote oxygen transfer and suppress coke formation. Therefore, the rational combination of Zn and Ga metal oxide is expected to synergistically improve both hydrocarbon activation and catalyst regeneration in chemical looping-based ODH reaction. In this study, Ga-modified $ZnZrO_2$ bimetal oxides were designed to verify the synergy effects of Zn and Ga metal oxides within zirconia matrix to achieve enhanced activity, selectivity, and stability under cyclic ODH reaction. Chemical looping–based oxidative dehydrogenation (ODH) of propane using CO_2 as an oxidant is a promising strategy to enhance olefin selectivity while suppressing excessive combustion and coke formation. Zn-based catalysts provide active sites favorable for selective propane dehydrogenation, leading to high propylene selectivity, whereas Ga species exhibit a superior redox property and oxygen mobility, which promote oxygen transfer and suppress coke formation. Therefore, the rational combination of Zn and Ga metal oxide is expected to synergistically improve both hydrocarbon activation and catalyst regeneration in chemical looping-based ODH reaction. In this study, Ga-modified $ZnZrO_2$ bimetal oxides were designed to verify the synergy effects of Zn and Ga metal oxides within zirconia matrix to achieve enhanced activity, selectivity, and stability under cyclic ODH reaction. As shown in Figure 1, $ZnZrO_2$ exhibited moderate propane conversion with a high propylene selectivity, confirming the intrinsic roles of Zn in selective C–H bond activation. Upon Ga incorporation, the $GaZnZrO_2$ catalyst showed increased propane conversion while maintaining high selectivity, indicating beneficial effects of Ga metal oxide on redox behaviors and catalyst regeneration. The presence of Ga facilitated the regeneration of surface oxygen vacancies during CO_2 activation step, leading to suppressed coke formation and improved stability during cyclic ODH reaction. The synergistic interactions between Ga and Zn metal oxides were resulted in a superior catalytic performance compared to Ga-free $ZnZrO_2$. Among the tested catalysts, the $GaZnZrO_2$ catalyst with an intermediate Ga loading exhibited the highest activity and stable performance over successive cycles. In conclusion, the rational incorporation of Ga metal oxide into $ZnZrO_2$ provides an effective strategy for designing efficient and durable bimetallic catalysts for CO_2 -assisted chemical looping-based ODH reaction of propane.

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HTT0335

Carbon-coated zeolite tandem catalysts for SAF-range product distribution control in CO2-derived Fischer–Tropsch synthesis

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Fischer-tropsch synthesis, CO2 hydrogenation, tandem catalyst, zeolite

Abstract Body.
Producing sustainable aviation fuel (SAF) via CO2-derived Fischer–Tropsch (FT) synthesis is an attractive pathway under increasingly stringent carbon constraints. However, conventional iron-based FT catalysts follow the Anderson–Schulz–Flory (ASF) distribution, producing a broad hydrocarbon spectrum and inherently limiting selectivity toward the SAF range (C8–C16). Catalyst and process strategies that enable SAF-oriented product control are therefore required.

Fe–zeolite tandem catalysts have been explored to reshape FT product distributions, yet they often suffer from two critical issues: (i) excessive cracking driven by strong zeolitic acidity, which shifts products toward lighter fractions and reduces SAF selectivity, and (ii) catalyst deactivation accelerated by water generated during FT synthesis. Here, we propose a carbon-coating strategy for zeolites to shield external acid sites responsible for unselective cracking and to increase surface hydrophobicity, thereby improving both selectivity and stability in tandem catalysis. Zeolite surfaces were carbon-coated using PVDF (poly(vinylidene fluoride)), glucose, and sucrose as carbon precursors to tune coating coverage and surface properties without compromising micropore accessibility.

Carbon-coated tandem catalysts enhance oligomerization of FT-derived light olefins while substantially suppressing excessive cracking of heavier hydrocarbons. In particular, C8+ hydrocarbons often face diffusion limitations in zeolite micropores and therefore tend to react at acid sites on the external surface and near pore mouths, where excessive cracking is more likely. By selectively masking these external acid sites, the carbon coating minimizes the breakdown of C8+ products into light gases and gasoline-range fragments, shifting the product slate toward heavier, SAF-relevant fractions and enabling more controlled upgrading behavior. Under wet conditions representative of the FT environment, coated catalysts also exhibit improved resistance to deactivation and maintain more stable activity than uncoated counterparts, consistent with reduced water uptake.

In conclusion, Fe–zeolite tandem catalysts incorporating carbon-coated zeolites suppress excessive cracking driven by external acid sites while mitigating deactivation under wet conditions relevant to CO2-based FT synthesis, thereby maintaining more stable catalytic performance. These combined effects go beyond conventional post-FT upgrading and demonstrate a practical catalyst design strategy to reshape the ASF-limited product distribution toward SAF-range fractions. Moreover, because the coating precursor and

coverage can be tuned to control acid-site accessibility and surface wettability, this approach provides a scalable platform for simultaneously improving selectivity and stability in CO2-to-SAF tandem FT upgrading.

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HTT0373

Effect of Transition Metal Oxide Structures on Selective Ammonia Oxidation to NO

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: ammonia oxidation, nitric oxide, transition metal oxides

Abstract Body.
Selective oxidation of ammonia to nitric oxide (NO) is a key step in industrial nitric acid production. However, conventional Pt-Rh catalysts suffer from high cost, metal volatilization at high temperatures, and the formation of the undesired N2O, motivating the search for cost-effective non-noble metal alternatives. In this study, transition metal oxide catalysts are investigated for their ability to selectively oxidize ammonia to NO. By varying calcination temperature and synthesis method, catalysts with different oxide structures including spinel and perovskite phases are systematically prepared. The influence of metal identity and oxide structure on ammonia conversion and NO selectivity is examined to establish clear structure-performance relationships. This study focuses on identifying catalyst compositions and structural features that promote NO formation while minimizing undesired byproducts. The findings provide fundamental insights into the role of transition metal oxides in ammonia oxidation and offer design principles for thermally stable and economically practical non-noble metal catalysts suitable for nitric acid production.

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HTT0374

Hydrogenation and rearrangement of furfural towards the production of furfuryl alcohol and cyclopentanone over Ni-doped Cu/SiO2 catalysts in batch and continuous systems

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Furfural; Furfuryl alcohol; Hydrogenation; Rearrangement

Abstract Body.
Introduction. Furfural (FUR), a significant platform chemical derived from biomass, can be selectively converted into furfuryl alcohol (FOL) and cyclopentanone (CPONE) through hydrogenation and rearrangement pathways. This study investigates the hydrogenation of furfural using a Ni-doped Cu/SiO2 catalyst using both high pressure batch and fixed bed reactors. This research aims to explore the role of different active sites within the catalyst surface, establish a robust catalyst design that could withstand catalyst deactivation, and to set up a steady-state operation with increasing furfural concentrations in the feedstock.
Methods. Various material characterizations (BET, XRD, XPS, in-situ DRIFTS) were done to elucidate the physical and chemical characteristics of the Ni-Cu/SiO2 catalysts. Reaction screening was conducted over a range of temperatures, H2 pressures, reaction times, and furfural concentrations to establish the optimum conditions. Liquid samples were collected via manual filtration to separate the used catalysts.
Results and discussion. Under optimized reaction conditions of 120oC, 30 bar H2 pressure, and reaction time of 6 hours, the catalyst favored the production of FOL. Material characterization confirmed that the nature of the Cu species present in the catalyst surface significantly influenced the selectivity of the products. After confirming under feed concentration screening, an optimal FOL yield was achieved at 10 wt% FUR concentration in isopropanol (IPA) solvent. Adjusting the IPA-to-water ratio showed preference towards CPONE under lower values. Furthermore, the catalyst exhibited high tolerance to common impurities, achieving an 84.31% FOL yield even at low purity levels of FUR. Furthermore, the catalyst exhibited high tolerance to common impurities, achieving an 84.31% FOL yield even at low purity levels of FUR.
Conclusion. In conclusion, the Ni-doped Cu/SiO2-XE catalyst was proven effective towards the selective hydrogenation and rearrangement of furfural, with feed concentration and catalyst characteristics playing significant roles in influencing the product distribution.
Acknowledgments
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HTT0377

PdM bimetallic catalyst for propylene acetoxylation: Insight into the alloy effect and support effect

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: propylene acetoxylation, bimetallic catalyst, alloy effect, support effect, kinetic model

Abstract Body.

Introduction. The acetoxylation of propylene to allyl acetate is a fascinating route for catalytic conversion of propylene to high value-added chemicals and could be another paradigm for bimetallic catalysis of palladium following the success of vinyl acetate [1].

Methods. Systematical characterizations (HRTEM, XPS, in-situ DRIFTS, etc), DFT calculations and kinetic modelling have been performed to elucidate the geometric and electronic effects of the second metal and support on the Pd catalysts.

Results and discussion. Electron transfer from Sb to Pd occurs in the bimetallic Pd-Sb alloy, which could efficiently promote the reduction of Pd species and maintain the stability of Pd0. The theoretical simulations also show that the addition of Sb can lower the d-band center of Pd and weaken the strong adsorption of propylene and acetic acid, which inhibits the over-oxidation. Furthermore, the coupling reaction between the dissociatively adsorbed C3H5* and OAc* species was determined to be the rate-determining step at low and high coverages of acetate, and it can be efficiently promoted at the Pd7Sb1 bimetallic sites. Furthermore, DFT calculation demonstrated that, the PdSb-TiO2 interface sites displayed a higher catalytic activity for activation of O2 and acetic acid, and also a higher acetoxylation activity compared with the PdSb surface active sites. The kinetic model based on the surface mechanism showed relatively poor fitting effect. In constrast, the surface-interfacial coupling kinetic model displayed a good fitting effect, which confirms the important catalytic effect of interfacial sites, and provides not only a theoretical basis for the reactor design, but also a new perspective for further design of kinetic models and the acetoxylation catalyst.

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HTT0383

Effect of CeO_2 Precipitation Digestion Temperature on the Pt/CeO_2 Catalyst for Sulfur Tolerant Water-Gas Shift Reaction

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Keywords: Water–gas shift reaction; Sulfur tolerance; Pt/CeO_2 catalyst; CeO_2 Precipitation digestion temperature

Introduction.

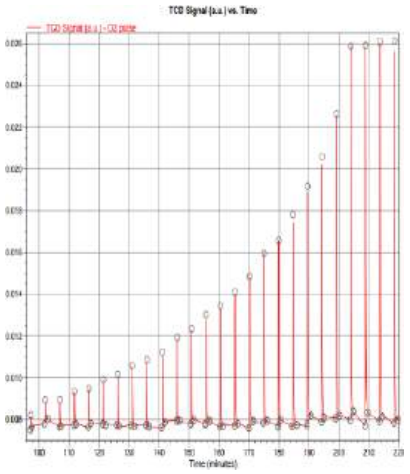
The water-gas shift (WGS) reaction is a key process that converts CO in reformate gas while producing additional H_2. However, syngas generated from waste and biomass contains sulfur compounds, which rapidly deactivate the catalyst [1]. Existing studies have highlighted the necessity of developing sulfur-tolerant catalysts [2, 3]. In this study, we investigate the effect of controlling the digestion temperature during CeO_2 precipitation for the sulfur tolerance of Pt/CeO_2 catalysts in the sulfur-containing WGS reaction.

Methods.

CeO_2 was synthesized by the precipitation method while varying the aging temperature (RT, 40, 60, and 80 °C), and Pt was subsequently deposited by the incipient wetness impregnation. In all catalysts, the Pt content was fixed as 2 wt%, and the CeO_2 support content was kept constant at 98 wt%. The catalysts were characterized using various physicochemical techniques to investigate their structural and surface properties. Catalytic performance and stability were evaluated during the WGS reaction under sulfur-injection conditions by monitoring CO conversion.

Results and discussion.

Physicochemical characteristic reveals a strong dependence of Pt dispersion and oxygen storage capacity (OSC) on the CeO_2 aging temperature. Among the samples, the 80 °C aged catalyst showed the highest Pt dispersion (45.16%) and OSC (0.64 mmol/g). In contrast, the catalysts aged RT, 40, 60 °C exhibited Pt dispersions (23.76-34.34%), whereas OSC remained comparably low (0.18-0.21 mmol/g).



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2026 / SEOUL, KOREA

HTT0386

Effect of Catalyst Synthesis Method on the Sulfur Tolerance of Pt/CeO2 Catalyst for Water-Gas Shift Reaction

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Water-gas shift, Sulfur tolerance, Pt/CeO2 catalyst, CeO2 synthesis methods

Abstract Body.

Effect of Catalyst Synthesis Method on the Sulfur Tolerance of Pt/CeO2 Catalyst for Water-Gas Shift Reaction
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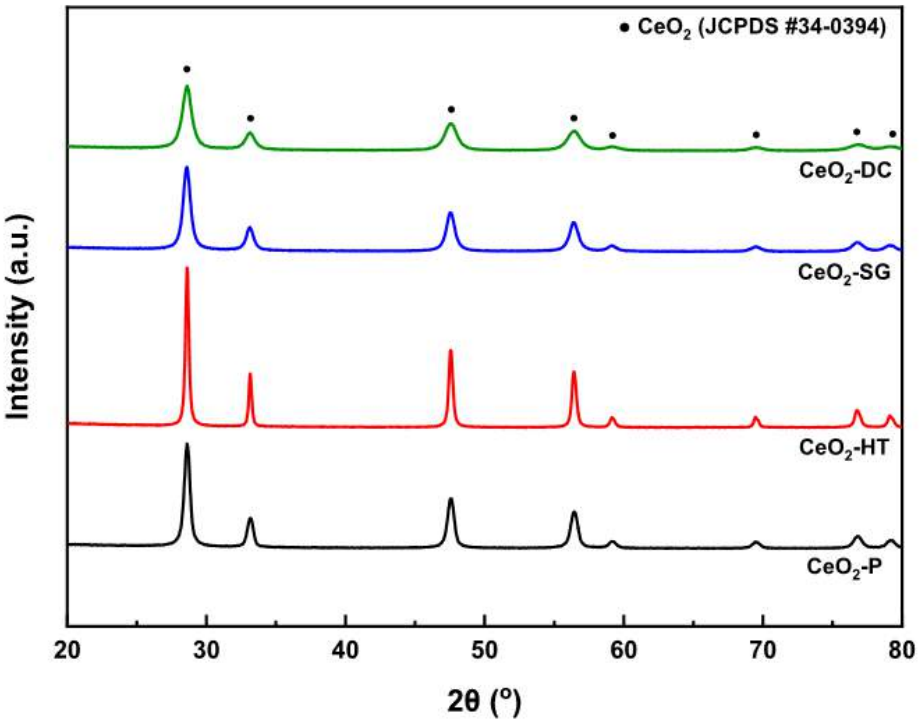
Keywords: Water-gas shift; Sulfur tolerance; Pt/CeO2 catalyst; CeO2 synthesis methods

Introduction.
Sulfur species are inevitably present in syngas derived from waste and biomass, and they severely deteriorate the performance of water-gas shift (WGS) catalysts. Previous studies have emphasized that the development of sulfur-tolerant WGS catalysts is essential for the direct utilization of waste-derived syngas without requiring upstream desulfurization processes [1, 2, 3]. In this context, this study aims to investigate how CeO2 synthesis methods influence the sulfur tolerance and stability of Pt/CeO2 catalysts under sulfur-injected WGS reaction conditions.

Methods.
CeO2 supports were synthesized by precipitation, hydrothermal, sol-gel, and direct calcination methods, followed by 2 wt% of Pt deposition via incipient wetness impregnation. The catalysts were characterized using various physicochemical techniques to investigate their structural and surface properties. Catalytic performance and stability were evaluated during the WGS reaction under sulfur-injection conditions by monitoring CO conversion.

Results and discussion.



CeO2 supports were synthesized via precipitation, hydrothermal, sol-gel, and direct calcination methods, and their crystalline structures were compared as a function of the synthesis route. All samples exhibited diffraction features characteristic of fluorite-type cubic CeO2, consistent with the reference pattern (JCPDS #34-0394), confirming the formation of a single CeO2 phase. Differences in peak broadening and relative intensity were observed among the supports, suggesting synthesis-dependent variations in crystallinity and crystallite size. The specific surface area also showed a difference from 44.3 to 89.7 m2/g. These results reveal that the preparation method directly affects the physicochemical properties of the CeO2.

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HTT0389

Achieving Industrial-Scale Longevity in CO2-to-C5+ Conversion using Na-Modified FeAlOx Catalysts

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: CO2 conversion, Alkali metal, Deactivation

Abstract Body.
Converting CO2 into long-chain hydrocarbons (C5+) via Fischer-Tropsch Synthesis (CO2-FTS) offers a promising path to carbon neutrality. However, two bottlenecks remain. The first is insufficient C5+ selectivity. The second is rapid catalyst deactivation caused by reoxidation. While alkali promoters are standard for electronic enhancement, a clear rationale for their role in ensuring long-term structural stability has yet to be established.
We developed Fe–Al oxide catalysts with high sodium loadings (up to 20 wt%), designated as Nay–FeAlOx. In a continuous fixed-bed reactor (330 °C, 3.5 MPa), the Na20–FeAlOx catalyst achieved a C5+ yield of 22% after 500 hours. More importantly, it demonstrated exceptional durability over 2,000 hours of operation, maintaining a decay rate of only 0.005% h-1.
Our analysis reveals that sodium performs a dual role, functioning not only as an electronic promoter but also as a critical structural architect. During catalyst preparation, excess Na forms NaFeO2, which further transforms into Na2O/Na2O2. This phase shift effectively blocks the interaction between Fe and Al, preventing the formation of the inactive Fe–Al spinel phase. Thus, the catalyst develops a stable core–shell architecture: a χ-Fe5C2 (and eventually Fe7C3) core protected by a Fe3O4/AlOx shell. This specific configuration shields the active iron carbides from H2O reoxidation and prevents particle pulverization.
This study redefines the role of alkali promoters in CO2-FTS. By strategically utilizing Na to inhibit spinel formation and stabilize core-shell domains, we provide a design template for catalysts that combine high productivity with industrial-scale longevity.

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HTT0402

Effect of citric acid treatment with adjusted acidic sites of Ferrierite zeolite for gas-phase DME carbonylation activity

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: DME carbonylation, Ferrierite, Citric acid, Acidic treatment, 8 membered-ring (8-MR) channels.

Abstract Body.
Introduction. Due to significantly increasing syngas production from industrial society, many researchers have focused on utilization of syngas. Indirect change of syngas to ethanol is also get focused by thermo-catalysis researchers. Indirect change of syngas through multi-step syngas conversion like COx hydrogenation, dimethyl ether (DME) carbonylation and methyl acetate (MA) hydrogenation are focused with their chemical stability in procecss and economic characteristics of applied catalysts. For the indirect conversion of syngas to ethanol, dimethyl ether DME carbonylation is an important intermediate step to achieve higher yield of ethanol.
For a gas-phase DME carbonylation reaction, Modernite (MOR) or Ferrierite (FER) zeolite, which has active Bronsted acid sites in 8 membered-ring (8-MR) channels, are well known to be effective for enhancing catalytic activity and stability for DME carbonylation. However, the acidic sites in 10-membered ring channels (10-MR) in those zeolites mostly cause severe coke depositions related to catalyst deactivations.
Methods. To improve catalytic activity, for weak acid treratment, citric acid was applied for modulating surface acid sites and structures of FER zeolite. Impregnation method was applied for weak acid treatment, and FER zeolite was treated with the citric acid solution at 80 °C for 5 h. According to different concentrations of the citric acid solution, catalytic performances of each citric acid treatment catalyst were compared.
Results and discussion. After citric acid treatment, the change in structures and acid sites of FER zeolite were found to have proper physical and chemical characteristics with an improved catalytic activity and stability due to the adjusted acidic sites. There were no significant changes in structure, surface area, and pore volume distribution by weak acidic treatment. Through specific chemical analysises, decreased deactive 10-MR were measured in FER zeolite, catalytic behavior of FER zeolite was improved in both DME conversion and MA selectivity. More stable and enhanced catalytic activity was observed after citric acid treatment. Enough amount and acidic characteristics could improve through specific treatments and continued to be imroved catalytic performance. In the future study, more relation between citric acid treatment and zeolite will be analyzed and observed.

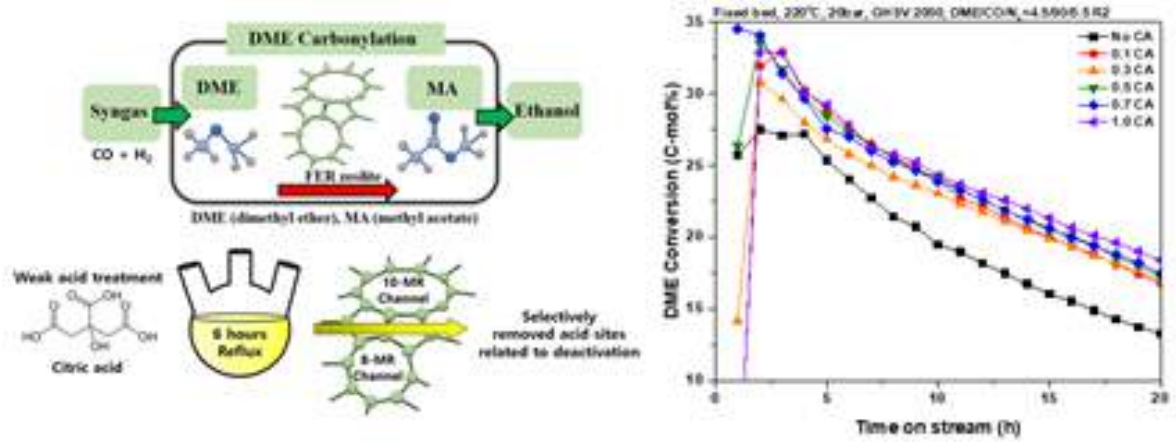

Figure 1. Illustration of citric acid treatment on FER zeolite and DME Conversion of catalysts

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HTT0405

Exsolved nickel nanoparticle-based Ce/Ni@SiO2 catalysts for dry reforming of methane

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Dry reforming of methane (DRM), Nickel nanoparticle, Exsolution, Ceria promoter, Oxygen vacancy

Abstract Body.

Introduction. Dry reforming of methane reaction with carbon dioxide (CH4 + CO2 = 2H2 + 2CO, DRM) has been largely investigated to produce syngas using Ni-based heterogeneous catalysts and produced C1 gases can be recycled with subsequent conversions to liquid fuels and chemicals [1]. In general, Ni nanoparticles having comparable activity can be easily sintered to form less active and larger agglomerates with facile coke deposition natures for dry reforming of methane [2]. Exsolved catalysts have advantages in maintaining small nanoparticles not to aggregate with their strong metal-support interaction. Moreover, cerium oxide can be used to enhance oxidizing coke species with its oxygen vacancies [3]. In the present study, Ni@SiO2 core-shell structure was synthesized to prepare uniformly sized nanoparticles and spheric silica support, and cerium oxide promoter was impregnated on the shell. Stability of exsolution of nickel nanoparticles was investigated, which was induced to form new interactions between nickel and outer ceria particles during DRM reaction.

Methods. Ni@SiO2 core-shell catalyst was prepared by the previously reported reverse microemulsion method [4]. Nickel nitrate, NH3OH, and TEOS were sequentially injected into the micellar solution. The precipitates were centrifuged, dried, and calcined at 800 °C to earn Ni@SiO2 catalyst. Cerium nitrate precursor was dry impregnated on the Ni@SiO2 with the cerium loading of 2, 5, 10 wt%, then the dried powder was calcined again at 550 °C. The powder catalysts were evaluated in a 3/8-inch tubular reactor after reduction. Characterizations of the catalysts were conducted by N2-sorption, H2-TPR, XRD, and XPS.

Results and discussion. The morphologies of the catalysts were analyzed by transmittance electron microscopy (TEM), and the images of the Ce(5)/Ni@SiO2 catalyst were presented in Figure 1(A). Before reduction, nickel nanoparticles and ceria particles were dispersed separately by the shell. During the reaction, the nickel nanoparticles were exsolved and formed an interaction with the ceria particles, which improved reduction properties of nickel species and DRM reaction stability as shown in Figure 1(B).

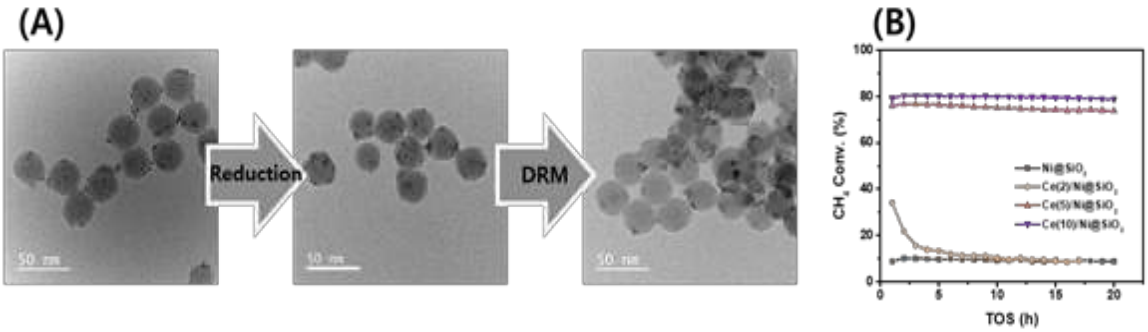

Figure 1. (A) TEM images of the Ce/Ni@SiO2 catalyst after calcination, reduction, and reaction; (B) CH4 conversion for the DRM reaction at 800 °C

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HTT0411

Synergistic Ir-Co Bimetallic Effects in Fischer-Tropsch Catalysts Modulate Catalytic Performance under CO-Dominant Surface Coverage

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Iridium, Bimetallic effect, CO coverage, hydrogenation, Fischer-Tropsch Synthesis

Abstract Body.
Despite decades of research in Fischer–Tropsch synthesis (FTS), optimizing activity and selectivity remains a key goal. Here in, we demonstrate that Ir promotion modifies the CO-dominated surface state of Ir-Co/SiO_2 catalysts and thereby affects activity and selectivity. In particular, the effective CO coverage and adsorption type can influence catalytic performance and product distribution. In this regime, Ir promotion can tune the electronic structure of Co and the surface adsorption environment, thereby modulating CO binding strength and effective coverage. Such promotion may also influence the hydrogenation propensity of hydrocarbon intermediates, as reflected in shifts in olefin/parrafin (O/P) selectivity under CO-rich conditions. Moreover, Ir promotion can be accompanied by reorganization of the active structure, including refinement of Co domains, changes in the crystal phase (hcp/fcc) fraction, and Ir-Co proximity interactions. However, studies that clarify how changes in CO adsorption behavior (coverage, adsorption modes, and binding strength) correlate with catalytic activity and selectivity remain limited. Across Co/SiO2 and Ir(x)Co/SiO2catalysts (x = 0.3-1.3) were evaluated under high-pressure FTS conditions (20 bar, 230 oC), CO adsorption behavior strengthens and correlates with activity and selectivity trends. CO-DRIFTS under FTS-relevant conditions reveals intensified linear and bridged Co-CO bands with a blue shift of the linear CO band, indicative of enhanced CO-CO dipole coupling at higher effective CO coverage. CO-TPD corroborates strengthened CO adsorption, with CO uptake increasing from 335 to 382 $\mu mol \cdot gcat^{-1}$ (Co/SiO2→Ir(1.3)Co/SiO2) and the main desorption feature shifting from 550 to 650 oC, indicative of stronger CO binding on catalysts. In parallel with these adsorption changes, catalytic performance increases systematically: TOF and CTY increase by factors of 2.2 and 1.8, respectively, and overall product distributions (CH4, C2–4, and C5+) changed only

slightly, whereas the C2–4 O/P ratio decreased from 64% to 52%, indicating a shift toward more saturated products via enhanced olefins hydrogenation. Liquid-phase product distributions exhibited increases in both the long-chain (C20–28) and light–middle (C7–13) ranges, suggesting the coexistence of chain-growth and hydrogenation-driven chain stabilization/earlier termination pathways. Moreover, XPS, lattice d-spacing analysis, and TEM-EDS elemental mapping indicate close Ir-Co association, while XRD/TEM reveal smaller Co domains (14.8 → 9.6 nm), suggesting that Ir incorporation increases the density of interfacial ensembles and modulates FTS reactivity and selectivity. Overall, strengthened CO adsorption is associated with increased intrinsic activity and a lower O/P ratio, alongside Ir-induced structural and electronic restructuring. These results suggest that Ir-Co interactions may modulate the CO-dominated surface state and thereby influence high-pressure FTS performance.

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HTT0422

Improving metals recovery in catalysts: Advanced modelling of leaching in porous structures

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Circular Economy; Metals Recycling; Hydroprocessing Catalysts; Hydrometallurgical Leaching; Porous Networks; Diffusion-Reaction Modelling

Abstract Body.

Introduction

Stricter regulations on sulfur content in fuels have increased the use of hydrotreating catalysts, leading to higher quantities of spent catalysts [1]. Hydrometallurgy offers a promising route for managing this waste by recovering valuable metals from spent catalysts, often regarded as secondary ores [2]. This work addresses the environmental and economic challenges of catalyst recycling, focusing on critical metal extraction via hydrometallurgical leaching while minimizing support degradation. This enables the reuse of both the leachate and the catalyst support.

Catalysts are complex materials that facilitate interactions between species through weak electrostatic forces, strong ion-covalent bonds, or crystalline interactions on the surface of its mesoporous matrix. Leaching therefore depends on the nature of species and these often-overlooked interaction mechanisms. This study aims at developing a multi-scale grain model that incorporates interactions between crystalline species and the support as well as the support's pore network structure, thereby allowing optimization of leaching processes for closed-loop recycling. This approach aligns with the EU's targets to increase recycling rates of critical metals such as cobalt and nickel by 2030, which are essential for catalytic and energy-storage applications.

Results

The research combines experimental and modeling approaches to refine leaching processes. Experimental methods include solubility tests, desorption kinetic measurements, and support characterization. The effects of variables such as acid concentration, pH, particle size, and temperature on leaching are studied, employing a fresh, calcined catalyst as a model for spent catalysts to study diffusion and desorption. A 1D grain model is developed to simulate leaching kinetics and pore network tortuosity, integrating Fick's law to capture the interplay between diffusion and chemical reaction. This model simulates desorption kinetics for refractory species, incorporating a tortuosity parameter to represent the pore networks. A 3D pore network model is also constructed to provide insights into the pore size distribution and connectivity effects on leaching efficiency. The research anticipates delivering a methodology to identify limiting factors and maximize leaching yields while minimizing support degradation.

Conclusions

The models are intended to guide the design of efficient leaching processes, adopting closed-loop recycling and reducing environmental impact. Broader applications include battery recycling and noble metals recovery, contributing to sustainable technologies. This work represents a significant contribution to the circular economy, addressing critical challenges in recycling and supporting global sustainability objectives.

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HTT0424

Enhancing zeolite stability in DME conversion: the role of passivation, hierarchization and etching

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Hierarchical zeolites, DTO, Light olefins, Deactivation, Kinetics

Abstract Body.
Introduction. The sustainable production of light olefins via dimethyl ether (DME) dehydration relies on acid catalysts like MFI-type zeolites. However, deactivation due to coke formation limits their efficiency. This study investigates how passivation, hierarchization and etching influence zeolite stability and catalytic performance, enhancing catalyst lifetime.
Methods. MFI-type zeolites with two different Si/Al ratios (25 and 50) were synthesized using literature methods [1-4]. Hierarchical structures were obtained via hydrothermal synthesis, etching of parent zeolite was done treating it with NH4+/HF solution at 25 °C, while passivation was achieved through silicalite-1 deposition [3]. The catalysts were characterized for textural and acidic properties and tested in a fixed-bed reactor under relevant operating conditions (400 NL/g/h, 3 vol.% DME/N2, 2 bar, 300-375 °C) to evaluate their performance. The acidity of samples was measured using NH3-TPD and FT-IR spectroscopy using d3-acetonitrile as probe. Lastly, the deposited coke was quantified with TGA, while the soluble part was analyzed with GC-MS. Lastly, kinetic parameters for deactivation were derived from the tests.
Results and discussion. All hierarchical (HZ) and passivated (PAS) samples exhibited improved stability compared to conventional MFI-type zeolites (MFI) as shown in Figure 1. N2 physisorption confirmed a bimodal pore size distribution in hierarchical samples, which facilitated coke diffusion and reduced pore blockage. The passivated samples, featuring a silicalite-1 shell, displayed lower acidity and slower deactivation rates. Hydrothermal synthesis proved more effective than etching (ETC) in preserving catalyst activity over prolonged time-on-stream (TOS). Among the tested samples, HZ-25 maintained higher stability than ETC-25, while PAS-25 exhibited the slowest deactivation rate, highlighting the beneficial effect of surface passivation. Light olefins selectivity ranged from 40% to 60%, with propylene as the dominant product. A milder acidity correlated with enhanced stability, as coke formation was mitigated. These findings demonstrate that tailored structural modifications effectively enhance zeolite lifetime, enabling more sustainable olefin production.

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Low-Temperature Oxidation of Indoor VOCs with Pt Catalysts: The Role of Zeolite Architecture

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Metal-support interactions, indoor air quality, novel zeolites, low temperature oxidation, platinum nanoparticles, VOC oxidation

Abstract Body.
Introduction. Indoor volatile organic compounds (VOCs) are major pollutants affecting air quality and health, whose abatement requires efficient low-temperature catalytic oxidation. Platinum catalysts efficiently promote oxygen and VOC activation under mild conditions; however, economically viable systems require low metal loadings and optimized metal-support interplay. Acid supports, such as ZSM-5, can promote VOC adsorption and activation. This work investigates low-temperature VOC oxidation, focusing on support acidity and pore architecture in microporous and hierarchical ZSM-5 hosting size-controlled Pt nanoparticles.
Methods. Platinum (Pt) nanoparticles were synthesized via a polyol reduction method1, designed to achieve controlled particle size and morphology, and subsequently deposited at 0.5 wt% on different supports to ensure a homogeneous active phase while isolating support effects. The supports included commercial ZSM-5 (SiO2/Al2O3=50, 80, 117), SBA-15 mesoporous silica as a non-acid reference, and hierarchical ZSM-5 (Si/Al=25, 50, 100) hydrothermally synthesized in a single step using CTAOH2 as mesoporogen. All zeolites were pre-calcined to the proton form. Catalysts were calcined, reduced in H2, and pre-treated at 110 °C in air. Catalytic oxidation was conducted in a fixed-bed quartz U-tube reactor with 100 ppm VOCs in air (GHSV 12,000-24,000 h-1). Characterization included N2 physisorption, NH3-TPD, 27Al and 1H-NMR, TEM, CO chemisorption, and DRIFTS during VOC adsorption.
Results and discussion. TEM analysis showed spherical, uniformly dispersed Pt nanoparticles smaller than 3 nm for all catalysts, with similar size and morphology regardless of the support. CO chemisorption confirmed 60-80% accessible metal sites, indicating that differences in catalytic performance are not governed by the Pt phase itself. Pt/ZSM-5 achieved complete conversion below 100 °C for ethylene and 150 °C for toluene (Fig.1). While all Pt/ZSM-5 catalysts outperformed Pt/SBA-15, which lacks acidity, the zeolite-supported catalysts exhibited very similar performance among themselves. This suggests that, in purely microporous ZSM-5, Brønsted acid sites, predominantly inside micropores3, have limited accessibility and restricted interaction with Pt nanoparticles, hindering a synergistic metal-acid mechanism. Hierarchical ZSM-5 materials were designed to increase mesoporosity while preserving zeolite nature. 1H-NMR spectra revealed dominant signals from Brønsted protons and silanols, confirming high crystallinity, uniform Al distribution and

minimal defects. Mesoporosity was introduced to enhance low-temperature VOC oxidation by improving accessibility of Brønsted acid sites involved in VOC adsorption and their proximity to Pt nanoparticles, facilitating VOC activation and oxidation at the metal–acid interface.

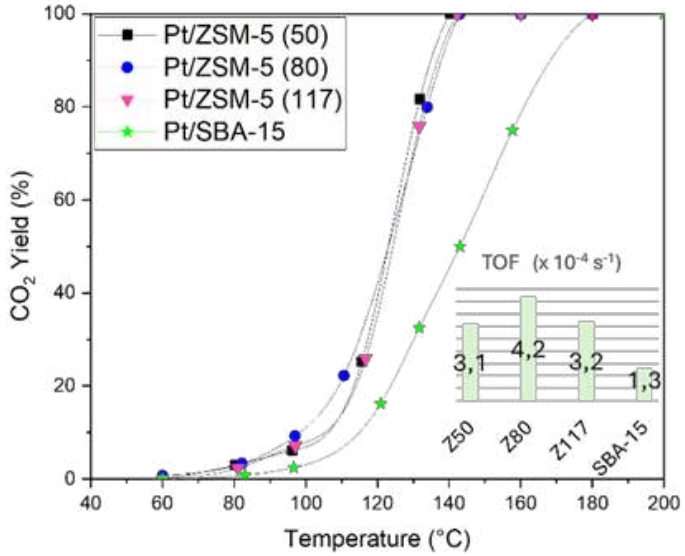

Figure 1. Catalytic oxidation of toluene (50 mL min-1). TOF is evaluated at 100 °C.

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HTT0434

Tailoring $MgO–Al_2O_3$ Interactions in Ni-Based Catalysts for Enhanced Reverse Water–Gas Shift Performance

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: RWGS, MgO-Al2O3 mixed oxide supports, Metal-Support interaction, Basicity

Abstract Body.

This work systematically investigates the role of $MgO–Al_2O_3$ interactions and calcination temperature on the physicochemical properties and RWGS performance of Ni-based catalysts. A series of 5 wt% Ni catalysts supported on MgO, Al_2O_3, $MgAl_2O_4$ spinel, and a physical mixture-derived $MgO–Al_2O_3$ (30:70) were synthesized via wet impregnation and calcined at 500 and 850 °C to tune metal–support interactions and mixed-oxide formation. The catalysts were evaluated in a fixed-bed reactor for the reverse water–gas shift reaction ($CO_2 + H_2 \rightarrow CO + H_2O$) in the temperature range 350–550 °C at atmospheric pressure with equimolar CO_2/H_2 feed, and the structure–activity relationships were established through comprehensive characterization (BET, XRD, H_2-TPR, CO_2-TPD, TEM, and UV–vis). Catalysts calcined at 500 °C (NiMgAl500, NiMg500, NiAl500, PM500) exhibit higher specific surface areas, finer Ni dispersion, and weaker sintering propensity than their 850 °C counterparts, resulting in improved reducibility and higher RWGS activity. Mixed-oxide supports containing both MgO and Al_2O_3 (NiMgAl, NiMg, PM) generate a larger density of basic surface sites, as confirmed by CO_2-TPD, which promotes CO_2 adsorption/activation and translates into higher CO_2 conversion compared with Ni/Al_2O_3. Under identical conditions (600 °C, 1 bar, $H_2:CO_2$ = 1:1), NiMg500 > NiMgAl500 > PM500 > NiAl500 is observed for the 500 °C series, while PM850 > NiMgAl850 > NiMg850 > NiAl850 is obtained for the 850 °C series, with PM850 achieving CO_2 conversion up to 30.8% and NiAl500 only 16.6%.

XRD, H_2-TPR, and TEM analyses reveal that $MgO–Al_2O_3$ cooperation in spinel or mixed matrices stabilizes Ni species, enhances metal–support interaction, and suppresses Ni sintering, whereas strong $Ni–Al_2O_3$ interaction at high temperature favors $NiAl_2O_4$ formation, which is largely inactive for RWGS and diminishes the number of accessible Ni^0 sites. Catalysts supported on $MgO–Al_2O_3$ also show a clear preference toward the RWGS pathway with higher CO selectivity relative to Ni/Al_2O_3, which tends to favor methanation at comparable conditions. Overall, the results demonstrate that rational control of MgO/Al_2O_3

composition and calcination temperature is a powerful strategy to tune basicity, metal–support interaction, and phase evolution in Ni-based catalysts, thereby achieving improved CO_2 conversion and CO selectivity in the RWGS reaction.

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HTT0442

Enhancing Light Olefin Selectivity in CO2-Modified Fischer-Tropsch Synthesis Using Mesoporous MFI Zeolites in a Tandem Dual-Bed System

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: MFI zeolite, mesoporosity, light olefins, hydrocarbon pool, CO2 hydrogenation, tandem reaction

Abstract Body.
Introduction. CO2-modified Fischer–Tropsch synthesis (CO2-FTS) is a promising route for direct CO2 hydrogenation, but the Anderson–Schulz–Flory (ASF) chain-growth mechanism inherently produces a broad hydrocarbon distribution. Although Fe-based CO2-FTS catalysts generate olefin-rich primary products, selective formation of light olefins (C2=–C4=) remains limited by wide carbon-number distribution and diffusion constraints. To address these challenges, a tandem dual-bed reactor combining CO2-FTS with downstream upgrading over mesoporosity-controlled MFI zeolites was employed to tailor the final product distribution.
Methods. CO2-FTS was performed over a stable Fe-based catalyst in the first bed, followed by secondary conversion over MFI zeolites in the second bed under fixed reaction conditions to isolate the zeolite effect. Mesoporous MFI zeolites were synthesized via a bottom-up approach by varying the content of the amphiphilic organosilane TPHAC, thereby tuning mesopore volume and distribution. The catalysts were characterized by XRD, N2 sorption, FE-SEM, NH3-TPD, and Py- and DTBPy-IR spectroscopy, and their catalytic performance was evaluated at 0.1 MPa and 300–600 °C using a commercial ZSM-5 as a reference.
Results and discussion. In the tandem configuration using unmodified CO2-FTS effluent as feed, increasing mesoporosity led to a monotonic increase in light olefin selectivity with a concomitant decrease in BTEX aromatics, indicating a clear selectivity trade-off. The MFI zeolite with a TPHAC/(TEOS+TPHAC) ratio of 4% achieved a stable light olefin selectivity of 56.8% (hydrocarbon basis) at 500 °C.
Model reactions using 1-octene confirmed that the enhanced olefin selectivity did not originate from nonselective overcracking on external strong acid sites, as no significant increase in CH4 or C2H6 was observed despite higher external acidity. Instead, the selectivity trends are attributed to intrinsic mesoporosity, which alleviates diffusion limitations and redistributes effective acid sites. This structural modification enhances the olefin-based cycle while suppressing the aromatic-based cycle in the hydrocarbon pool, simultaneously improving selectivity and resistance to aromatic accumulation.

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Microwave Synthesis for Enhancing the Selectivity of HEA Catalysts in Acetylene Hydrogenation

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Acetylene hydrogenation, High-entropy alloy catalyst, Non-precious metals, Microwave-assisted synthesis

Abstract Body.
Selective hydrogenation of acetylene is a critical step in producing polymer-grade ethylene. Although conventional Pd-based catalysts exhibit high activity, their widespread application is limited by the high cost of precious metals and the tendency toward excessive ethylene hydrogenation. Therefore, developing cost-effective, non-precious metal catalysts with high activity and selectivity is highly desirable. This study presents a novel synthesis strategy for high-entropy alloy (HEA) catalysts composed exclusively of non-precious metals and supported on carbon nanotubes (CNTs). These HEA catalysts were rapidly synthesized via microwave heating, enabling ultrafast alloy formation. To suppress nanoparticle agglomeration, key synthesis parameters—including sample loading, dispersion state, and microwave irradiation time—were systematically optimized. The resulting HEA catalysts demonstrated significantly enhanced ethylene selectivity in the selective hydrogenation of acetylene compared to catalysts prepared by conventional wet impregnation methods. This enhancement is attributed to synergistic effects from the multicomponent metal composition and superior nanoparticle dispersion achieved through microwave-assisted synthesis. The proposed microwave-based approach enables rapid catalyst fabrication with precise control over metal composition, offering strong potential for cost reduction and performance improvement in acetylene hydrogenation processes.

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HTT0469

Effect of Precipitation Route on the Physicochemical properties of Multi-Component Ni-Co-Mg-Al-Ce Catalysts for Dry Reforming of Methane

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Dry Reforming of Methane (DRM), Co-precipitation, Precipitation sequence, Ni-Co catalyst

Abstract Body.
Introduction. Methane Dry Reforming (DRM) is an ideal 'Carbon Loop' technology as it simultaneously converts two major greenhouse gases (CH4 and CO2) into industrially valuable syngas . However, carbon deposition remains a critical barrier for conventional Ni catalysts, leading to structural degradation and chemical deactivation[1]. To overcome carbon deposition and thermal sintering inherent in Ni-based catalysts, multi-component systems incorporating promoters such as Co, Mg, Al, and Ce are extensively studied. However, the structural homogeneity of these complex catalysts is heavily dependent on the synthesis protocol. This study investigates the critical influence of the precipitation route on the physicochemical properties of catalysts.
Methods. A catalyst with a specific mass composition of 25Ni-15Co-40Mg-15Al-5Ce (wt%) was synthesized via co-precipitation using metal nitrates and NaHCO3 as a precipitant. Two distinct pH control routes were employed at 60°C: the Acid-to-Base (AB) route, where the mixed metal solution was added dropwise into an excess precipitant solution (constant high pH), and the Base-to-Acid (BA) route, where the precipitant was added to the metal solution (gradual pH increase). The resulting precipitates were calcined at 750°C. Characterization including BET, TPD, XRD, TEM, TGA, Catalytic performance were analyzed to evaluate the textural properties and phase homogeneity of the synthesized catalysts.
Results and discussion. The precipitation route induced drastic differences in catalyst morphology and structure. The AB sample was obtained as a dense, deep black powder, indicating the successful formation of a homogeneous solid solution (e.g., Ni-Co spinel) due to simultaneous co-precipitation. Conversely, the BA sample appeared as a fluffy, light brown powder, suggesting severe phase segregation where the abundant Mg species (40 wt%) precipitated later, encapsulating the active Ni/Co species. the catalytic performance in DRM. The reaction conversion rate was approximately 1.7 times higher than that of the conventional 5Ni-95Al catalyst. This enhanced performance is attributed to the formation of a homogeneous solid solution (spinel), which stabilized highly dispersed Ni-Co active sites against thermal sintering and carbon deposition.

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Aromatic hydrogenation under CO-contaminated hydrogen over Pd: mechanistic insights and structure sensitivity

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Hydrogenation, structure sensitivity, crude hydrogen, LOHC

Abstract Body.

Introduction

Aromatic hydrogenation is a fundamental reaction, involved in the production of bulk and fine chemicals and enabling hydrogen storage in liquid organic hydrogen carriers. Economically, using impure H2 for hydrogenation reactions is attractive, as industrial or biogenic crude H2 is about half the price of high-purity H2 [1]. However, common hydrogenation catalysts are susceptible to CO poisoning, with crude H2 after water-gas shift containing up to 2 % CO [2]. While research on aromatic hydrogenation with crude H2 is limited, studies show that Pd-based catalysts have significantly higher activities compared to other metals [3]. Here, we combine kinetic studies, structure sensitivity analysis and in situ spectroscopy to identify the most active Pd sites in aromatic hydrogenation under CO-contaminated H2.

Our results show that the presence of CO induces a shift in both the rate-determining step (RDS) and structure sensitivity in aromatic hydrogenation and allow the design of more active and CO-tolerant hydrogenation catalysts.

Experimental

Pd/Al2O3 catalysts with varied precursors and particle size were synthesized by wet impregnation. Hydrogenation of benzyltoluene (BT) was performed in a batch autoclave with pure H2 and with 1.6 vol% CO in H2 at 240 °C and 30 bar H2 pressure.

Results & discussion

Under pure H2, BT hydrogenation over Pd is structure insensitive across 1 to 10 nm particle size. Kinetic parameters also align well with reported literature values of various aromatic substrates and underline that the H-addition to the activated aromatic ring is the RDS [4-6]. Adding CO fundamentally changes this behaviour: apparent activation energy and BT reaction order increase sharply (Figure 1a), while the H2 reaction order remains unchanged. This indicates that BT adsorption is inhibited by competitive adsorption with CO and that BT adsorption becomes the new RDS.

This mechanistic shift also induces structure sensitivity: productivity (normalized to surface Pd) reaches a maximum over Pd nanoparticles at ~2 nm (Figure 1b). CO-DRIFTS in the presence of toluene, complemented by HAADF-STEM and XANES, shows that toluene preferentially adsorbs at Pd edge sites in the presence of CO. We conclude that under CO-contaminated H2, BT is predominantly hydrogenated on Pd edges. These insights enable rational catalyst design of more CO-tolerant hydrogenation catalysts by maximizing Pd edge site density.

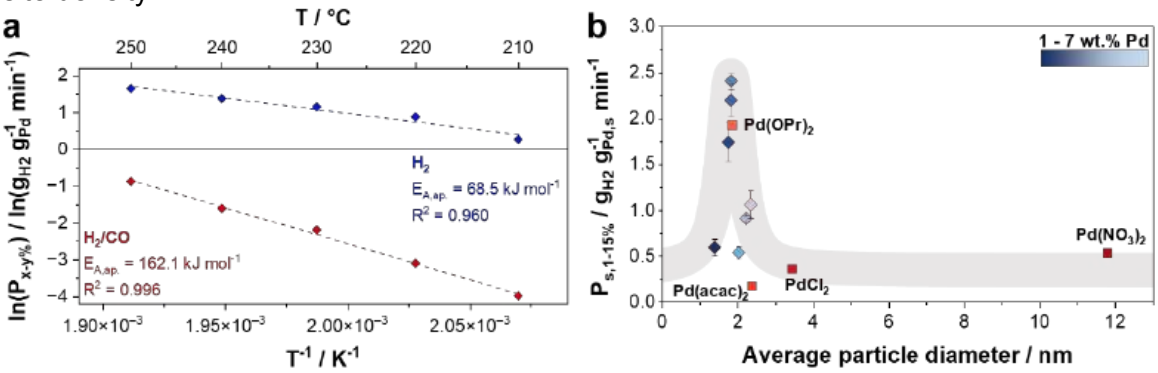

Figure 1: (a) Arrhenius plot under pure H2 and 1.6 vol.% CO in H2. (b) Productivity (normalized to surface Pd) over Pd particle diameter for 4 wt.% Pd/Al2O3 (different precursors) and 1–7 wt.% Pd/Al2O3 (Pd-acetate precursor) under 1.6 vol.% CO in H2.

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HTT0488

Porous Organic Polymer Catalyst for the Efficient Glycolysis of Post-Consumer PET

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Polyethylene terephthalate (PET), Glycolysis of PET, Porous Organic Polymer (POP), Catalyst recyclability, Circular economy

Abstract Body.
Introduction. Glycolysis is an effective chemical recycling route that depolymerizes polyethylene terephthalate (PET) into bis(2-hydroxyethyl) terephthalate (BHET), enabling closed-loop production of high-quality recycled PET [1]. However, efficient BHET recovery requires catalysts that remain active and stable under high-temperature, strongly polar ethylene glycol conditions. Conventional homogeneous catalysts often suffer from leaching and limited recyclability, while many heterogeneous systems still require harsh reaction conditions to achieve sufficient activity [2, 3]. Porous organic polymers (POPs) offer a promising platform due to their tunable porosity, robust stability, and strong metal–ligand interactions, making them suitable candidates for developing durable and recyclable PET glycolysis catalysts [4].
Methods. A catechol-based porous organic polymer (POP) was synthesized via Friedel–Crafts alkylation and subsequently functionalized through Fe loading, chemical reduction, and carbonization to obtain a magnetically separable Fe@C-POP_red catalyst. The materials were characterized by XRD, Raman, XPS, BET, TGA, FT-IR, TEM/EDS, SEM, and ICP-OES to elucidate structural evolution, metal dispersion, and Fe speciation. PET glycolysis was carried out in ethylene glycol under varied temperatures, reaction times, catalyst loadings, and EG/PET ratios, and the reaction mixtures were analyzed using HPLC to quantify BHET and oligomer distributions.
Results and discussion. The Fe@C-POP_red catalyst exhibited uniform dispersion of Fe nanoparticles within a carbonized POP matrix, providing strong magnetic response, enhanced structural stability, and suppressed metal leaching. Under optimized reaction conditions, the catalyst achieved complete PET conversion with BHET yields exceeding 90%, while maintaining performance over repeated cycles. These findings demonstrate the effectiveness of POP-derived carbon–metal hybrid catalysts for PET glycolysis and highlight their potential for enabling sustainable plastic circularity.
Acknowledgments
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HTT0494

Simultaneous Achievement of High Activity and Reproducibility in Large-Scale Synthesis of Zn-P-ZSM-5 for Methanol-to-Aromatics

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Methanol-to-aromatics, ZSM-5, Zn-P modification, large-scale, reproducibility

Abstract Body.
Introduction. The methanol-to-aromatics (MTA) reaction over ZSM-5 zeolites is a key pathway for carbon-neutral chemical production. The modification of ZSM-5 with Zn and P is widely used, because Zn promotes dehydrogenation and phosphorus can tune acidity and improve stability. [1,2] However, inconsistent optimal loadings and preparation sequences reported in the literature hinder rational design. While determining the optimal procedure for loading, a critical challenge lies in the scale-up of powder catalysts; the conventional incipient wetness impregnation method, while effective for activity, often lacks uniformity and reproducibility when scaled up. In this study, we investigated optimal loading procedures and amounts of Zn and P to resolve these issues, confirming that the optimization strategy highly depends on the SiO2/Al2O3 ratio (SAR) of ZSM-5.
Methods. ZSM-5 zeolites with different SARs were employed to evaluate the impact of acidity on metal modification. Zn and P were introduced using various methods including incipient wetness, sequential wet impregnation, co-impregnation, and repeated impregnation with diluted solutions. All catalysts in this work were synthesized at a scale of over 50 g to rigorously evaluate scale-up feasibility and reproducibility. The catalytic activity was evaluated in a fixed-bed reactor at 430 °C, and catalyst lifetime was determined based on a conversion threshold of 90%.
Results and discussion. Catalytic trends were strongly governed by the SAR of ZSM-5 and the preparation method. High-SAR ZSM-5 showed modest dependence on the introduction sequence, while low-SAR ZSM-5 exhibited pronounced sensitivity to the loading amount of P and introduction sequence of Zn and P. The sequential incipient wetness impregnation provides high activity, but it showed limitations in maintaining uniformity at the large scale. In contrast, sequential wet impregnation was advantageous for reproducibility at the 50 g scale, but it resulted in relatively lower catalytic activity compared to the incipient wetness method. Among the tested procedures, we established that co-impregnation of Zn and P simultaneously provides the highest aromatics yield and improved lifetime while ensuring reproducibility. This method facilitates the intimate interaction between precursors, promoting the incorporation of Zn into the zeolite framework and preventing the formation of unfavorable zinc oxide species. This study provides the correlation between the preparation method and MTA performance, and the practical routes for synthesizing large-scale Zn-P/ZSM-5 with reproducible manner.

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HTT0503

Carbon Suppression Mechanisms in Ethanol Steam Reforming over Silicalite-1–Encapsulated Ni Nanoparticle Catalysts

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Ni catalyst,zeolite-encapsulated structure,bio-oil,steam reforming

Abstract Body.
Introduction.
Ethanol steam reforming, a model compound for bio-oil, has been widely studied for syngas production. On Ni-based catalysts, ethanol is dehydrogenated to acetaldehyde, which then decomposes to CO and CH4. The CO is subsequently converted to CO2 and H2 via the water–gas shift reaction. Although Ni-based catalysts show high activity, they suffer deactivation from sintering, carbon deposition, and hydrothermal degradation. To address these issues, Silicalite-1-encapsulated Ni nanoparticle catalysts (Ni@S-1) were developed and showed excellent carbon suppression at 600-800 oC [1]. However, the reaction pathway most strongly influenced by Ni@S-1 to suppress carbon deposition remains unclear. This study investigates ethanol steam reforming by focusing on acetaldehyde formed via ethanol dehydrogenation as a key intermediate, elucidating the Ni@S-1–affected reaction pathways responsible for carbon deposition.
Methods.
Ni@S-1 was prepared by introducing nickel phyllosilicate into zeolite mother liquor followed by hydrothermal treatment. For comparison, Ni/S-1 was prepared by a conventional impregnation method. The morphology of Ni was confirmed by TEM. The reaction was carried out in a fixed-bed reactor at 650 oC under a continuous flow of reactant gases (steam/carbon = 1.5). The carbon deposition was analyzed by TG-DTA and SEM.
Results and discussion.
TEM observation confirmed that the average particle size of Ni in Ni@S-1 was approximately 4 nm before and after the reaction, in agreement with previous studies [1]. The steam reforming of ethanol and acetaldehyde produced H2, CO2, CH4, and CO as products (Fig.1). Notably, Ni@S-1 produced a negligible amount of CH4, which is a carbon-forming species. This can be attributed to the encapsulation structure of Ni@S-1, which preserves Ni nanoparticles below 5 nm. These sub-5 nm Ni particles effectively suppress the methanation reaction while maintaining high steam-reforming activity [2]. In ethanol steam reforming, carbon decreased from 11.4 wt% on Ni/S-1 to 1.3 wt% on Ni@S-1. In acetaldehyde reforming, it declined from 18.5 wt% on Ni/S-1 to 8.3 wt% on Ni@S-1. Acetaldehyde undergoes C-C cleavage and carbon deposition more readily than ethanol, but Ni@S-1 exhibited carbon suppression activity in both reactions due to its Ni nanoparticles. In conclusion, Ni@S-1 suppresses carbon deposition by maintaining 5 nm Ni nanoparticles that

inhibit CH4 formation, a key carbon precursor.

Acknowledgments
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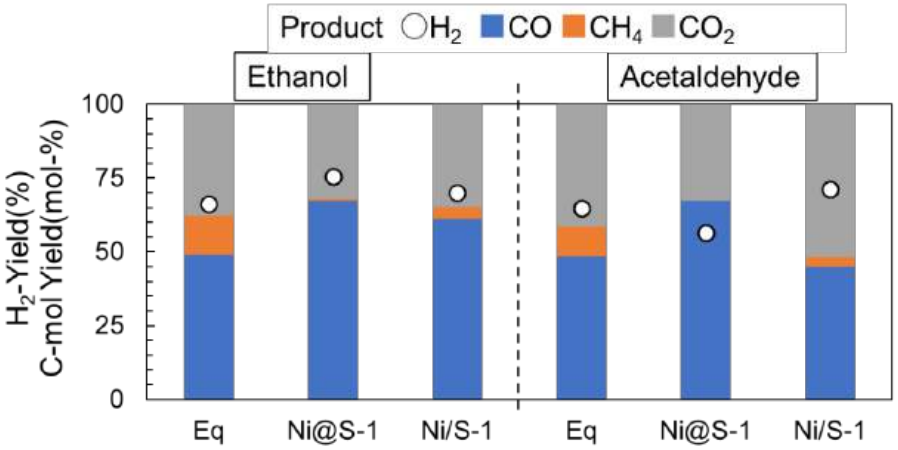

Fig.1. Ethanol and acetaldehyde catalyst activity at 650 ° C for 4 hours.

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HTT0514

Accelerating catalyst discovery through machine learning–based screening and deactivation analysis

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Machine learning; Catalyst screening; Deactivation rate modeling; Dehydrogenation catalysis; Time-on-stream; Structure–performance relationships

Abstract Body.
Introduction. Propane dehydrogenation and dry reforming of methane represent two pivotal heterogeneously catalyzed reactions; however, both are significantly hindered by catalyst deactivation resulting from carbon deposition (coking). Experimental evaluation of catalyst performance and stability over time-on-stream is resource-intensive, limiting the efficient exploration of catalyst compositions and operating conditions. Data-driven approaches offer a promising alternative for accelerating catalyst screening while enabling quantitative analysis of deactivation behavior.

Methods. A generalized machine-learning framework is developed for catalyst screening and deactivation-rate modeling, with propane dehydrogenation and dry reforming of methane serving as a representative case study. A literature-derived dataset spanning 2000–2025 was compiled, integrating catalyst physicochemical descriptors (surface area, pore characteristics, active metal loading, promoter identity, and pretreatment conditions) and operating variables (reaction temperature, feed composition, and time-on-stream) with performance metrics including conversion, selectivity, product yield, and activity decay. Following systematic preprocessing and feature engineering, ensemble and gradient-boosting ML models were trained to predict both steady-state performance and time-dependent deactivation indicators, such as conversion decay and selectivity loss rates.

Results and discussion. The ML models accurately captured nonlinear structure–performance–stability relationships across a wide range of catalyst formulations and operating conditions. Model comparison revealed that gradient-boosting approaches showed superior predictive capability for selectivity and product yield, while ensemble-based methods more effectively captured conversion and deactivation trends. Feature-importance analysis highlighted the dominant influence of reaction temperature, active metal loading, promoter identity, and textural properties on both catalytic activity and deactivation rate. The results demonstrate that no single ML model is sufficient to describe all aspects of catalytic behavior, emphasizing the value of multi-model analysis for robust catalyst screening and stability assessment. By explicitly incorporating time-on-stream and deactivation metrics, the proposed framework enables quantitative evaluation of performance–stability trade-offs that are critical for industrial catalyst design. More broadly, this ML-assisted methodology provides a transferable strategy for accelerating catalyst discovery and understanding

deactivation phenomena in dehydrogenation and related heterogeneous catalytic systems.

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HTT0515

Dynamic nature of catalyst surface during CO oxidation on Cu(111) surface

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Dynamic nature of active sites, CO oxidation, adsorbate-induced surface reconstruction

Abstract Body.
In computational catalysis, it is often assumed that the catalyst surface remains static and independent of adsorbate coverage. However, advances in in situ characterization techniques with high spatial and temporal resolution, together with the increasing availability of high-performance computing, have revealed that strongly bound adsorbates can induce surface reconstruction. As a result, the catalyst surface can evolve dynamically in response to the local chemical environment and operating conditions. This dynamic behavior implies a continual change in the registry of active sites, which may deviate substantially from ideal lattice descriptions.
The O/Cu(111) system provides a prototypical example of this behavior. At high oxygen coverages, oxygen atoms are capable of abstracting terrace Cu atoms from their lattice positions. We observe that oxygen atoms preferentially form specific cluster motifs on the pristine Cu surface, giving rise to dynamically evolving structures. These structures exhibit chemical reactivities distinct from those of the pristine surface, thereby reducing the reliability of predictions based on static catalyst models. In this work, we investigate the prototypical CO oxidation reaction on a pre-oxygen-adsorbed Cu(111) surface. Using ab-initio density functional theory (DFT) calculations, we sample a diverse set of configurations that include these dynamic surface structures. We find that motifs involving O–Cu–O linkages are significantly more reactive than static surface Cu atoms. Energy barriers computed using the nudged elastic band (NEB) method reveal a substantial reduction compared to the idealized static case involving an isolated O atom and a CO molecule on an unreconstructed surface.

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HTT0573

Mesoporous Beta Zeolite Nanosponge Supporting Ni Nanocatalysts for Oligomerization of Light Olefins to SAF-Range Hydrocarbons

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Olefin Oligomerization, Beta Zeolite Nanosponge, Sustainable Aviation Fuel (SAF)

Abstract Body.

Introduction

The oligomerization of light olefins (C2–C4) represents a promising route for the production of Sustainable Aviation Fuel (SAF) precursors, particularly when utilizing mixed olefin streams derived from the Methanol-to-Olefins process. Although Ni-based zeolite catalysts have been extensively investigated for olefin oligomerization, most previous studies have focused on single-component feeds, thereby overlooking competitive adsorption and reaction pathways intrinsic to multicomponent mixtures. In addition, conventional bulk zeolites often suffer from severe mass transfer limitations, whereas amorphous supports lack the shape selectivity required for controlled hydrocarbon growth. To overcome these challenges, this study explores the oligomerization of a model mixed light olefin feed over Ni nanocatalysts supported on hierarchical nanosponge Beta zeolite (NS-Beta), emphasizing the combined roles of enhanced diffusion and zeolitic confinement.

Methods

The NS-Beta was synthesized using a hexa-quaternary ammonium surfactant, denoted as N6-diphe, as previously reported [1]. Zeolite supports were loaded with 5 wt% Ni via incipient wetness impregnation using an aqueous nickel nitrate solution, followed by drying and calcination. Light olefin oligomerization was conducted in a stainless-steel fixed-bed reactor over the Ni-supported catalysts under the following conditions: reaction temperature of 393 K, total pressure of 30 bar, and a feed molar composition of C2:C3:C4 = 40:40:20.

Results and discussion

The catalytic performance of Ni-supported zeolite catalysts was systematically evaluated for the oligomerization of light olefins using Ni/NS-Beta, Ni/bulk Beta, and Ni/Siralox catalysts. Among the catalysts, Ni/NS-Beta exhibited markedly superior activity and selectivity toward SAF-range hydrocarbons (C8–C16). In the case of Ni/bulk Beta, poor dispersion of Ni species led to the formation of large Ni particles, resulting in ineffective activation and conversion of light olefins. Consequently, oligomerization proceeded only to a limited extent over this catalyst. In contrast, Ni/Siralox exhibited well-dispersed Ni species; however, the weak acidity of the amorphous support restricted chain growth, allowing the conversion of light olefins primarily to middle-distillate-range hydrocarbons without further transformation into SAF-range products. Notably, the Ni/NS-Beta catalyst combined highly dispersed Ni nanocatalysts with strong zeolitic acid sites, enabling efficient sequential conversion from light olefins to middle distillates and ultimately to SAF-range hydrocarbons. This synergy between metal dispersion and acidity is critical for promoting both oligomerization and

subsequent chain growth reactions. Furthermore, comprehensive parametric studies examining the effects of Ni loading, zeolite framework topology (e.g., MFI), and acidity provided deeper insights into the structure–function relationships governing oligomerization performance and catalyst durability.

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HTT0574

Production of Monolaurin from Glycerol via Esterification of Lauric Acid over a ZnO/γ-Al2O3 Catalyst

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Monolaurin, Lauric acid, ZnO/γ- Al2O3 catalyst, Esterification

Abstract Body.
Monolaurin (ML) is a high-value monoacylglycerol with antimicrobial and food-grade emulsifying properties, widely used in food, pharmaceutical, and cosmetic industries. However, selective ML synthesis from glycerol and lauric acid is challenging because consecutive acylation can produce dilaurin (DL) and trilaurin (TL), reducing ML selectivity. In this study, ML production via esterification of lauric acid with glycerol was evaluated using a ZnO/γ-Al2O3 heterogeneous catalyst (20 wt.% ZnO/g-Al2O3), which exhibits bifunctional acid–base properties favoring ML formation. The physicochemical properties of the catalyst were characterized using X-ray diffraction (XRD), Brunauer–Emmett–Teller (BET) surface area analysis, NH3 temperature-programmed desorption (NH3-TPD), CO2 temperature-programmed desorption (CO2-TPD), and scanning electron microscopy coupled with energy-dispersive X-ray spectroscopy (SEM–EDS).The effects of catalyst loading, lauric acid-to-glycerol molar ratio (LA:GLY), and reaction time were investigated. The results showed that lauric acid conversion exceeded 85% with ML selectivity exceeding 90%, while the formation of DL and TL was very low. Under optimized conditions, 15 wt.% catalyst loading relative to lauric acid, LA: GLY of 1:4, a reaction temperature of 160 °C and a reaction time of 180 min, a lauric acid conversion of 94.5%, corresponding to a ML yield of 84.74% were achieved. These results demonstrated the potential of ZnO/γ-Al2O3 as an efficient and sustainable heterogeneous catalyst for ML production.

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HTT0576

Catalytic depolymerization of waste PET into BHET using Mn-supported g-C3N4

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: PET glycolysis, heterogeneous catalyst, sustainable energy, chemical recycling

Abstract Body.
Catalytic glycolysis of polyethylene terephthalate (PET) into bis(2-hydroxyethyl) terephthalate (BHET) is an emerging chemical recycling strategy that offers lower energy consumption and reduced greenhouse gas emissions compared to incineration, pyrolysis, and other recycling routes. The produced BHET can be directly reused for the synthesis of virgin-grade PET, enabling a closed-loop recycling process [1]. However, conventional PET glycolysis generally requires high reaction temperatures and prolonged reaction times, highlighting the need for efficient catalytic systems to enhance reaction kinetics and overall process efficiency [2]. Graphitic carbon nitride (g-C3N4) is a promising green catalyst support owing to its high thermal and chemical stability, low cost, and nitrogen-rich framework. Its heptazine-based structure contains abundant pyridinic nitrogen sites that enable strong coordination with metal ions, facilitating uniform metal dispersion and enhanced metal-support interactions. These properties facilitate enhanced PET glycolysis through synergistic metal-support interactions and efficient reactant activation. In this study, g-C3N4 nanosheets were prepared via a combined ultrasonication-thermal exfoliation strategy. Bulk g-C3N4 was first ultrasonicated in ethanol, during which solvent intercalation and swelling were indicated by a slight shift of the (002) diffraction peak toward lower angles. Subsequent thermal treatment induced effective exfoliation, evidenced by a shift of the (002) peak to higher angles and a significant increase in specific surface area. Mn species were then introduced via impregnation, yielding Mn loaded g-C3N4 catalysts with Mn contents of 0.5 wt%. Structural integrity and uniform Mn dispersion were confirmed by XRD and TEM analyses. The Mn/g-C3N4 catalyst exhibited excellent catalytic performance, achieving complete PET conversion and a BHET yield of up to 95% under optimized conditions. The high activity is attributed to the synergistic interaction between Mn ions and the g-C3N4 support. Specifically, nitrogen sites in the g-C3N4 framework promote the deprotonation of ethylene glycol to generate nucleophilic species, while Mn ions act as Lewis acid centers that activate the carbonyl groups of PET, thereby facilitating ester bond cleavage. Owing to this cooperative catalytic mechanism, the Mn/g-C3N4 system demonstrates superior efficiency compared with conventional metal oxide catalysts.

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HTT0582

Mechanistic insights into deactivation of commercial and lab-scale three-way catalysts for natural gas vehicles

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Keywords: Natural gas vehicles; Three-way catalyst; Catalyst deactivation; compressed natural gas (CNG).

Introduction

Natural gas vehicles (NGVs) are promising alternatives to diesel and gasoline vehicles due to abundant natural gas reserves, lower cost, and reduced emissions. However, three-way catalysts (TWCs) used in NGVs experience high-temperature exposure, leading to catalyst deactivation. Increasingly stringent emission regulations worldwide demand catalysts with high hydrothermal stability under the operating conditions. Hence, understanding deactivation mechanisms is essential for accurate lifetime prediction and the development of durable catalysts.

Methods

Fresh and thermally aged commercial Pd/Rh-Al_2O_3 three-way catalysts (TWCs) were characterized using in-situ DRIFTS, ICP-MS, N_2 physisorption, XRD, HRTEM, CO chemisorption, XPS, and H_2-TPR to elucidate structural and morphological changes. Catalytic light-off activity was evaluated in a lab-scale reactor under stoichiometric conditions. The influence of pretreatment atmospheres (N_2, O_2/N_2, H_2/N_2) on the catalytic activity was assessed. Subsequently, Pd/Rh catalysts supported on SSZ-13, ZSM-5, MOR, and Beta zeolites were synthesized, and their structure-activity relationships were investigated. Thermal stability of the catalysts was examined by aging at 700 °C for 16 h and 900 °C for 50 h.

Results and discussion

Thermal aging led to a significant increase in the light-off temperatures of CH_4, CO, and NO, with maximum CH_4 conversion decreasing from 78% over the fresh catalyst to 58% at 550 °C over the aged catalyst. O_2 pretreatment of the aged catalyst lowered the light-off temperatures of all three species (Fig. 1). Similar DRIFTS spectra for fresh and aged samples indicates partial surface restoration after O_2 pretreatment. H_2 pretreatment enhanced CO and NO activity for both fresh and aged catalysts, likely due to an increased fraction of metallic Pd. Structural characterization confirmed the stability of the support upon aging. However, sintering of active metals and support particles weakened metal-support interactions. Zeolite-supported catalysts remained structurally stable under the aging conditions, except SSZ-13, which exhibited significant framework degradation after aging at 900 °C. Activity results for the zeolite-supported catalysts will be discussed in the full paper.

Conclusions

Thermal aging leads to activity loss in commercial TWCs, primarily due to active metal sintering and weakened metal-support interactions. O_2 pretreatment serves as an

effective strategy for partial activity recovery of the thermally aged catalysts. Overall, the zeolite-supported catalysts exhibit high structural stability under the aging conditions.

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HTT0586

Pt supported on Sn incorporated CoAl2O4 spinel as a heterogeneous catalyst for the hydrogenolysis of post-consumer PET to BTX

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Polyethylene terephthalate (PET), Hydrogenolysis, BTX

Abstract Body.
The continuous increase in polyethylene terephthalate (PET) consumption has resulted in large amounts of post-consumer waste, making the development of efficient chemical recycling technologies essential. Hydrogenolysis of PET has recently been reported as a promising route for the direct production of benzene, toluene, and xylene (BTX). In particular, selective formation of p-xylene is advantageous, as it can significantly reduce the energy cost associated with the separation of mixed xylenes in conventional petrochemical processes. However, most of the reported catalysts suffer from limited stability in addition to restricted activity, highlighting the need for highly active and durable catalysts that can selectively produce p-xylene. Spinel oxides feature a stable structure where divalent cations occupy tetrahedral sites and trivalent cations occupy octahedral sites. Their excellent thermal stability, tunable composition make them ideal catalyst supports for harsh reaction environments.
In this study, Pt catalysts supported on Sn-substituted CoAl2O4 spinel oxides were prepared by a co-precipitation method. A-site doped with Sn as Co1-xSnxAl2O4 (x = 0, 0.01, 0.03, 0.04, and 0.06), catalytic activity and stability were examined in PET hydrogenolysis together with kinetic studies and structural analyses. Notably, Sn substitution into CoAl2O4 exhibit uniform dispersion of Pt particles and enhanced Lewis acidic sites to adsorb and activate C=O bonds. Meanwhile Pt promotes H2 dissociation. These properties enable the catalyst to achieved complete PET conversion within 12 h with a p-xylene selectivity of 94%. Furthermore, Sn doping in the spinel framework promoted strong metal-support interactions and facilitated electron transfer from Sn to Pt, effectively suppressing Pt sintering and catalyst deactivation. As a result, the catalyst demonstrated excellent durability, maintaining stable performance over eight consecutive reaction cycles. This study highlights the critical role of Sn-modified spinel supports in enhancing both selectivity and stability for PET hydrogenolysis to BTX aromatics, offering a promising route for sustainable plastic upcycling.

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HTT0590

Syngas Production by Mixed Reforming of n-Hexadecane over Exsolution-Derived Nanosized LaNiO3 Catalysts: A Strategy for Plastic Pyrolysis Oil Utilization

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Mixed reforming, Waste plastic pyrosis oil, Exsolution, Perovskite, LaNiO3

Abstract Body.
Driven by global efforts to mitigate plastic pollution, pyrolysis of waste plastics has gained considerable attention as a sustainable pathway for chemical recycling and syngas generation. In this study, mixed reforming of n-hexadecane, a model compound for crude waste plastic pyrolysis oil (WPPO), was investigated over a perovskite-type LaNiO3 catalyst at 700 °C with a WHSVoil = 0.05 g min-1. Under identical reaction conditions, mixed reforming significantly outperformed dry and steam reforming, indicating a synergistic enhancement in syngas yield. Moreover, LaNiO3exhibited markedly higher activity and stability than a conventional alumina-supported Ni catalyst. The superior performance of LaNiO3 originates from the intrinsic advantages of exsolution-derived catalysts, which provide strongly anchored Ni nanoparticles with high resistance to coking and sintering, making them particularly well suited for reforming environments prone to severe deactivation. LaNiO3 catalysts were synthesized via a solvothermal route, in which a basic gel environment was deliberately established to obtain nanosized perovskite particles. The reduced particle size increased Ni dispersion and, in conjunction with exsolution-enabled stabilization, led to enhanced H_2 selectivity and prolonged catalyst lifetime under highly deactivating conditions.

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HTT0591

Templated synthesis of nitrogen-doped carbon as a platform for highly active cobalt single-atom catalysts

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Layered silicate, N-doped carbon, oxidative dehydrogenation, SAC

Abstract Body.

Introduction.

Nitrogen-doped graphene and nano-graphene have been attracting considerable attention as next-generation materials owing to their potential metal-coordination ability and unique electronic structures, which provide unique thermal and electro catalytic properties[1].
In this study, we demonstrated the synthesis N-doped nano-graphene (NNG) via a unique post-synthetic thermal carbonization of bipyridine trapped in the interlayer space of a layered silicate. Furthermore, cobalt was introduced to fabricate a Co-based single atom catalyst (Co-NNG). The synthesized Co-NNG exhibited high catalytic activity in the oxidative dehydrogenation of benzyl alcohol.

Methods.

NNG-silica composite was synthesized via post-synthetic thermal carbonization of layered silicate at 723-1273 K under N2 flow. The silica template was removed using aqueous NaOH solution, and solid product was collected by centrifugation. Co-NNG catalysts were prepared by dispersing NNG in an aqueous cobalt solution (1 g/L), followed by centrifugation. Oxidative dehydrogenation of benzyl alcohol was carried out at 353 K under O2 atmosphere (0.4 MPa).

Results and discussion.

The obtained N-doped carbon exhibited a tunable nitrogen content with C/N ratios ranging from 4.5 to 20, depending on the carbonization temperature. A C/N ratio of around 5 (corresponding to an N content of ca. 17 at%) is generally high among reported N-doped carbon materials, and such high nitrogen loading is expected to provide a large number of N4 (or N3) coordination sites. These structural features highlight strong potential as a platform for various applications, such as single-atom catalysis and electrochemical catalysis. After Co loading, elemental analysis revealed a cobalt content of 0.5 wt% for the Co-NNG material.
Oxidative dehydrogenation of benzyl alcohol was conducted as a model reaction to compare the catalytic performance with previous reports. The Co-NNG catalyst exhibited a markedly higher reaction rate, comparable to that of a benchmark Pt/C catalyst under identical reaction conditions. These results demonstrate the potential of the N-doped carbon catalysts as viable alternatives to precious metal catalysts.

Table 1 – Oxidative Dehydrogenation of Benzyl Alcohol over Co-NNG catalysts

catalyst	conversion [%]	metal loading [wt %]	rate [mol s^{-1} mol_{Co}^{-1}]	report
Co/C	-	5	4.7×10^{-5}	[2]
Co/N-C	-	1.5	3.3×10^{-4}	[2]
Pt/C	-	3	0.20	[2]
Co-N-NG 773K	67.4	0.501	0.22	this work
Co-N-NG 973K	48.5	0.500	0.16	this work

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HTT0597

Engineering Electron-enriched Sites for Alkane Dehydrogenation

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Heterogeneous catalysis, Alkane dehydrogenation, Zeolite

Abstract Body.
Alkane dehydrogenation represents a route for producing important light olefins, and the exploration of efficiently alternative oxide catalysts for this reaction is both significant and challenging. Our previous studies revealed the first C–H cleavage as rate-determining step in alkane dehydrogenation process.[1-5] This step follows an oxidative additive pathway via metal sites insertion into C–H bond and proceeds with a three-center (CxHy*–M–H*) transition state (Left panel, depicts a typical case on single-atom Co).[1] Consequently, an electron-enriched active site can facilitate this step via enhanced electron transfer from metal sites to antibonding C–H orbitals.[1,3,4] Guided by this insight, we developed tailored pretreatment[1,3,4] and ligand-assisted hydrothermal strategies[2,5-7] to modulate electron-enriched active centers, thereby improving alkane activation capacity (Right panel, show typical cases). As a result, the optimized (CO)Co-ZSM-5 and IrGe@S-1 catalysts exhibit promising catalytic performance compared to most frontier Pt-based catalysts.

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HTT0631

Effect of Kneading Conditions on the Textural Properties of Heterogeneous Catalyst Supports

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Kneading; Boehmite pastes; Gamma-alumina supports; Textural properties

Abstract Body.

Introduction

Controlling the mechanical and textural properties of heterogeneous catalyst supports is a key challenge in the design and manufacture of high-performance catalytic materials. In particular, the microstructure of γ-alumina supports strongly influences both mass transport within the porous network and mechanical resistance. Industrially, γ-alumina supports are commonly produced from boehmite pastes through a kneading–extrusion process, in which the operating conditions of each unit operation play a critical role in determining the final properties of the solid [1, 2]. This experimental study focuses on the kneading step and aims to quantify the effects of kneading conditions and paste composition on the properties of boehmite pastes.

Materials and methods

Boehmite pastes were prepared from Pural SB3 powder, consisting of micrometer-sized grains ranging from 1 to 100 µm, with a BET surface area of 260 m²/g and significant meso- and macroporosity. Dense pastes containing 40 wt% boehmite were processed in a laboratory-scale pilot kneader equipped with torque and temperature sensors. The effects of kneading duration (3 min to 4 h), blade rotation speed (10–100 rpm), and paste composition were investigated. Paste composition was adjusted by varying the pH during the neutralization step, leading to final paste pH values between 5.2 and 8.7. After kneading, the pastes were dried and characterized by nitrogen adsorption and mercury intrusion porosimetry.

Results and discussion

In-situ measurements revealed distinct torque and temperature evolutions associated with peptization, neutralization, and paste homogenization. While kneading speed and duration significantly affected the temporal evolution of torque and temperature, the torque curves obtained under different operating conditions collapsed onto a single master curve when plotted as a function of the accumulated deformation, defined as the product of kneading speed and duration. This result highlights the mechanical nature of the kneading process. In contrast, paste composition, and particularly pH, had a strong influence on both torque evolution and the textural properties of the dried pastes. Increasing pH led to substantial increases in pore volume, exceeding the effects induced by extended kneading duration

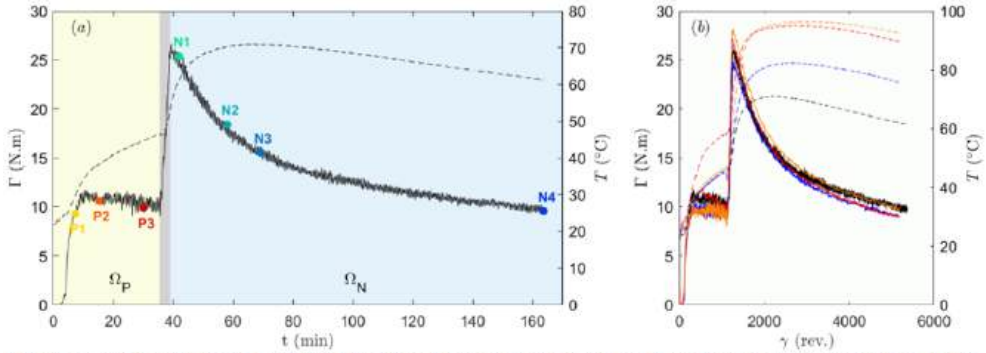

Figure 1. (a) Time-evolution of torque Γ (continuous line) and temperature T (dashed line) as measured in-situ in the kneader during a typical kneading experiment performed on a 40% neutralized paste (peptization – neutralization) (b) Torque Γ and temperature T evolution vs. accumulated deformation γ (line colors refer to various pairs of rotation speeds)

alone.

Conclusions

An empirical control parameter combining mechanical (accumulated deformation) and physicochemical (pH) effects was defined, allowing all experimental data to be collapsed onto master curves. Although phenomenological, this descriptor captures the coupled influence of kneading conditions and paste chemistry and provides a practical guideline for tuning the textural properties of γ-alumina supports in industrial applications. Future work will assess the generality of this approach for other paste formulations and synthesis routes.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

HTT0658

Nanosponge MFI Zeolites Zeolite Catalysts for Methanol Conversion to Valuable Hydrocarbons

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - 선택 없음

Keywords: Nanosponge, MFI, Aromatics

Abstract Body.
Introduction. Methanol-to-Aromatics (MTA) conversion has gained increasing attention as a key route to produce valuable aromatic hydrocarbons from non-petroleum sources. Among various catalysts, zeolites with shape-selective microporous frameworks play a crucial role in tuning product selectivity and enhancing catalytic stability. Particularly, MFI-type zeolites have been widely studied due to their well-defined pore channels that enable the selective formation of valuable hydrocarbons. However, conventional bulk MFI catalysts often suffer from rapid deactivation due to coke formation and limited diffusion of bulky intermediates through the narrow micropores. To address these challenges, recent studies have focused on the design of hierarchical or nanoscale MFI structures that provide improved accessibility to active sites and enhanced mass transport. Among them, Nanosponge (NS) MFI zeolites, which feature a 3D network of interconnected nanosheets with both microporous and mesoporous domains [1], have demonstrated promising performance in hydrocarbon conversion reactions. Nevertheless, their application to the MTA process remains underexplored. In this study, we investigate the catalytic performance of NS MFI zeolites in the MTA reaction, focusing on their influence on methanol conversion and light olefin selectivity compared to conventional MFI structures.
Methods. Nanosponge MFI zeolite was synthesized by adapting Kim's method with modification, employing C18-6-4 as a structure-directing agent (SDA) [1]. For the catalytic reaction, methanol was introduced into a fixed-bed reactor system by bubbling it into a carrier gas stream and feeding the vaporized methanol into the catalyst bed at 450 °C under atmospheric pressure..
Results and discussion. Catalytic evaluation revealed that the NS MFI zeolite achieved the highest methanol conversion among the tested catalysts, maintaining stable performance over the reaction period. In particular, the NS MFI exhibited significantly improved light olefin selectivity, likely due to its enhanced diffusion pathways and reduced secondary reactions within the interconnected nanosheet network. The hierarchical structure appears to facilitate the rapid desorption of intermediates, thereby suppressing coke deposition and enhancing

overall selectivity toward desired products such as ethylene, propylene, and butenes. Furthermore, the unique textural properties of the NS MFI, including increased external surface area and mesoporosity, contributed to its superior catalytic behavior compared to conventional MFI zeolites. These results suggest that nanosponge-type zeolites are promising candidates for selective hydrocarbon upgrading processes.

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HTT0665

Scalable Co-production of MWCNTs and H2 from HDPE: Process Optimization and Reaction Mechanism Analysis

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Carbon nanotube, HDPE, Catalytic chemical vapor deposition, Fixed-bed reactor, Reaction mechanism

Abstract Body.
Introduction. Plastic waste, such as high-density polyethylene (HDPE), presents a significant environmental challenge. To convert them via catalytic chemical vapor deposition (CCVD) to co-produce value-added carbon materials as multi-walled carbon nanotubes (MWCNTs) and high heating valued fuels like hydrogen (H2) offers a potential upcycling strategy.
Methods. This study investigates the effects of pyrolysis temperature (400–600 °C), HDPE-to-catalyst weight ratio (0.5:1, 1:1, 1.5:1, 2:1, and 3:1), and catalyst stability (1–5 cycles) on the yield and properties of MWCNTs. A 2.5-cm tubular two-stage batch reactor was used, where HDPE underwent a flash pyrolysis in the 1st-stage reactor, followed by CCVD in the 2nd-stage reactor at 800 °C under N2 flow using the as-prepared NiMo/MgO catalyst (30 wt% metal loading with Ni:Mo is 2:1, w/w) without H2 pre-reduction.
Results and discussion. The results revealed that the maximum yields of MWCNTs (14 nm in average diameter of MWCNTs) at 68 wt% and H2 (~81% purity in exhaust gas) at 71 wt%, could be achieved at a relatively lower pyrolysis temperature of 450 °C using a fixed HDPE-to-catalyst ratio of 2:1 (w/w). It was observed that pyrolysis temperatures above this threshold (500–600 °C) resulted in too rapid HDPE decomposition, leading to lower product yields. The optimal HDPE-to-catalyst ratio was found to be at 1.5:1 (w/w) with the highest carbon yield of 74% by keeping its H2 yield as high as 87% with 85% H2 purity. For catalyst recyclability test to simulate a continuous feed system, the H2 yields gradually decreased from 87 to 77 wt%, while the MWCNT yield remained constant in a range of 74–77 wt% at each cycle with a total accumulated yield of 5.3 gCNT/gCatalyst after five cycles. This led to a potential scalable co-production of MWCNT and H2 from HDPE. In brief, it requires precise adjustment of pyrolysis temperature to control the feedstock decomposition rate and the inlet concentration of hydrocarbon vapors due to limited surfaces of metal catalyst precursors. The optimum HDPE-to-catalyst ratio is also necessary to establish an appropriate balance of competitive reactions to maximize product yields for larger-scale production.

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HTT0672

Ni NPs decorated ZrO2 Phase-dependent activity for Furfural hydrogenation to yield THFA and CPO selectively

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Furfural, Tetrahydrofurfuryl alcohol, Cyclopentanone, Hydrogenation, Ring Rearrangment

Abstract Body.
Biomass is an inexhaustible, renewable carbon source that can be converted into chemicals and fuels currently derived from fossil resources. In this context, biomass is first transformed into highly reactive intermediate compounds known as platform chemicals, which are subsequently converted into target products through various processes such as hydrogenation and hydrodeoxygenation.
In this work, we prepared a series of Ni-loaded ZrO2 catalysts with three different crystalline phases: tetragonal (t), monoclinic (m), and a mixed phase (mix). These phases were synthesized with Ni loadings ranging from 5–15 wt%, and the catalysts were designated as 5Ni/t-ZrO2, 10Ni/t-ZrO2, 15Ni/t-ZrO2, 5Ni/m-ZrO2, 10Ni/m-ZrO2, 15Ni/m-ZrO2, and 15Ni/mix-ZrO2.
The catalysts exhibited distinct activities in the hydrogenation of furfural (FFR), leading to the formation of tetrahydrofurfuryl alcohol (THFA) and cyclopentanone (CPO) via furfuryl alcohol (FAL) as an intermediate. Among them, 10Ni/t-ZrO2 demonstrated excellent performance, achieving complete conversion with 92% selectivity toward THFA at 130 °C and 20 bar H2 pressure, using water as the solvent, within 6 h. In contrast, 10Ni/m-ZrO2 also achieved complete conversion but with 80% selectivity toward CPO under the same reaction conditions, with a reaction time of 4 h. Recyclability studies revealed that the catalyst maintained 100% furfural conversion and approximately 90% selectivity toward THFA over 4 consecutive cycles.
The structure–activity relationship was established through detailed physicochemical characterization using XRD, BET, HR-TEM, XPS, NH3-TPD, pyridine FT-IR, H2-TPR, Raman spectroscopy, and EPR analysis. Finally, based on the catalytic activity data, literature reports, and physicochemical properties, a reaction mechanism has been proposed for product formation under identical reaction conditions with Ni loaded on different crystalline phases of ZrO2.

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HTT0689

Effect of Acid Treatments on Zirconia in Ni/Zirconia using Palmitic Acid at Different Operating Conditions for BioJet Fuel Production Yield

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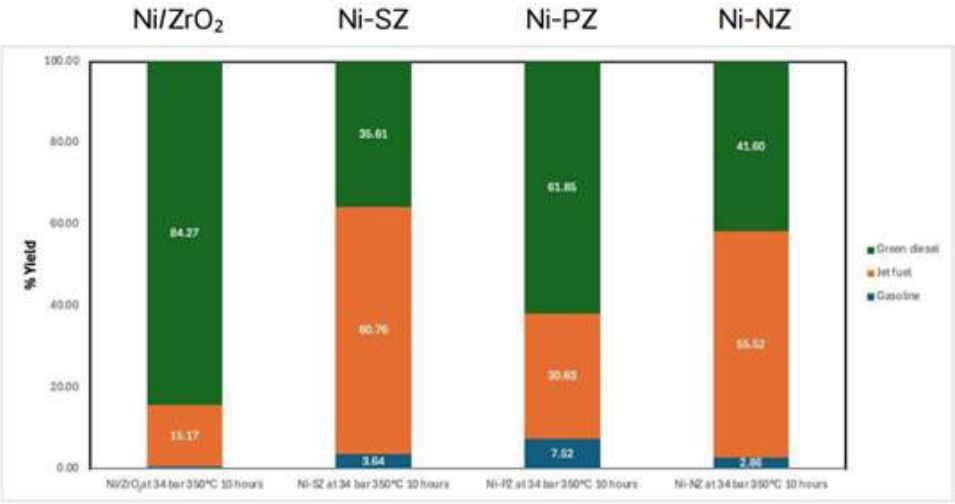
Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Jet fuel, Palmitic acid, Ni-based catalysts, Zirconia, Surface treatment

Abstract Body.
Introduction. Bio-jet fuel can be produced by using many types of catalysts. Nickel (Ni) is commonly used because it is inexpensive, resistant to corrosion and temperature variations, and has been widely studied for the synthesis of bio-jet fuel. Zirconium dioxide (ZrO2) is a promising choice as a support material due to its properties, including low thermal conductivity and high thermal stability. The effects of Ni/ZrO2 catalysts with surfaces modified by H2SO4, HNO3, and H3PO4 were investigated, along with the impact of temperature and pressure. Palmitic acid was used as the feedstock to evaluate the yield of bio-jet fuel produced.
Methods. Acid modification for the zirconia surface was modified from the previous study using H2SO4, HNO3, and H3PO4 [1,2]. Production of biofuel from palmitic acid was conducted with hydrogen gas in a semi-batch reactor. The amount of catalyst used was 0.1 g and 10 g of palmitic acid. The hydrogen gas flow rate was maintained at 20 mL/min. Pressures were set at 1, 17, and 34 bar, and temperatures were 300, 350, 400, and 450 °C. Reaction times were set at 2, 6, and 10 hours.
Results and discussion. The results showed that Nickle was well dispersed in all treated and untreated zirconia. All acid treatments were successfully treated on zirconia surface. The results showed that Ni/ZrO2 with all acid treatments can produce higher yield of bio-jet than that without the acid treatment at 10 hours, 34 bar, and 35O°C condition, as Figure below.



Acknowledgments
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HTT0696

Effect of Zeolite Hydrophilicity on Water-Assisted Polyethylene Hydrocracking

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Polyethylene, Upcycling, Plastic waste, Zeolite, Hydrophilicity

Abstract Body.
The extensive use of polyethylene (PE) poses a significant environmental challenge. While pyrolysis is widely studied, catalytic hydrocracking (200–300 °C) offers a more sustainable route with superior liquid fuel yields. Recently, we reported that water enhances Ru/HY-catalyzed PE hydrocracking [1]. However, this effect is not universal across all zeolites, and the water–catalyst–PE interactions remain unclear. Given the intrinsic hydrophobicity of polyolefins, understanding the interaction between water and catalytic sites is critical. Here, we investigate zeolite hydrophilicity as a key design parameter for water-mediated PE upcycling. Reactions utilized a 50 mL high-pressure batch reactor loaded with 0.5 g catalyst, 1.7 g LDPE, and 0.5 g water (if required). The system was pressurized to 30 bar with H2 and heated to 250 °C. Products were analyzed via gas chromatography (Agilent 8890) equipped with FID and TCD detectors. Water addition resulted in strongly zeolite-dependent performance divergence based on zeolite wettability. Strongly hydrophilic catalysts showed significant enhancement. The conversion increased from 80.6% (dry) to 96.1% (wet) for Ru/HY(30), and from 46.5% to 64.0% for Ru/HMOR(20). Conversely, hydrophobic catalysts such as Ru/HZSM-5(30) and Ru/HBEA(25) showed negligible or negative effects, with conversions decreasing from 34.5% to 31.2% and 63.3% to 46.9%, respectively. These results suggest that water-induced promotion is governed by surface wettability. To elucidate the mechanism, we varied component-addition sequences to manipulate interfacial contact. While standard direct water-catalyst contact yielded 96.1% conversion, spatially separating water from the catalyst by adding it atop the PE layer drastically reduced conversion to 33.5%. This suppression indicates that the hydrophobic PE melt acts as a barrier, preventing water from accessing the catalyst surface. Consequently, the promotional effect stems principally from favorable water-catalyst interactions rather than water-polymer interactions, demonstrating that direct interfacial access enabled by hydrophilic frameworks is essential for efficient water-mediated upcycling.

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HTT0697

Engineering Oxygen Vacancies with Atomically Dispersed WOx: A Strategy for Superior CO2 Hydrogenation Performance and Stability on Pd/CeO2

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: CO2 Hydrogenation, Oxygen vacancy, Atomically dispersed catalyst

Abstract Body.
Introduction. Despite extensive efforts, achieving efficient and stable heterogeneous catalysts for the hydrogenation of CO2 to value-added fuels and chemicals remains challenging [1]. Although structurally sophisticated heterogeneous catalysts have been reported [2], the functional roles of this complexity—particularly in regulating oxygen vacancies and metal–support interactions—are still insufficiently understood, hindering rational catalyst design. Moreover, limited CO2 activation and catalyst deactivation under water-producing conditions restrict long-term operation [3]. Here, we show that atomically dispersed WOx species modulate oxygen vacancy formation and Pd–CeO2 interfacial interactions, thereby enhancing catalytic activity and stability. These results demonstrate oxygen-vacancy engineering as an effective strategy for advancing CO2 hydrogenation catalysts.

Methods. Catalytic activity tests were performed between 250 ℃ and 400 ℃ at atmospheric pressure and 30 bar using a fixed-bed quartz reactor and a stainless-steel reactor, respectively. An ultra-high-purity gas mixture of CO2, H2, and N2 (1:3:6) was supplied at a gas hourly space velocity of 60,000 mL·h–1·gcat–1. The catalysts were pretreated under 10% CO/Ar prior to reaction. Products were analyzed online using gas chromatograph equipped with FID and TCD.
Results and discussion. The catalyst containing atomically dispersed WOx showed the highest CO2 activation, whereas activity decreased with increasing WOx loading (Fig. 1a), indicating that CO2 activation is maximized only at atomic WOx dispersion. O 1s XPS analysis revealed an increase in surface oxygen vacancies from ~21% for Pd/CeO2 to ~39% for the atomically dispersed WOx catalyst (Fig. 1b), followed by a decrease at higher WOx loadings due to WOx aggregation. Consistently, Raman spectroscopy showed increasing W–O–W features with increasing WOx loading (Fig. 1c). In situ DRIFTS further indicated the formation of formate and methoxy species without bicarbonate accumulation on the atomically dispersed WOx catalyst (Fig. 1d), highlighting the role of atomic WOx dispersion in vacancy-mediated CO2 activation.

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HTT0701

Boron nitride-modified SiO2 supports for enantioselective hydrogenation over Pt catalysts

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: h-BN-modified SiO2, Pt catalyst, Enantioselective hydrogenation

Abstract Body.
In heterogeneous catalysis, catalytic performance is fundamentally governed by the adsorption of reactants on the catalyst surface. In particular, for Pt-catalyzed enantioselective hydrogenation, the stable adsorption of chiral modifiers plays a decisive role in determining enantioselectivity. Chiral modifiers, such as cinchona alkaloids, adsorb on the Pt surface to form chiral active sites, where subsequent adsorption and complexation of substrates enable selective formation of the desired enantiomer. In this study, we introduce hexagonal boron nitride (h-BN) as a key component to enhance the stable adsorption of chiral modifiers at the Pt surface, thereby enabling improved catalytic performance.
The SiO2 was dispersed in deionized water, and h-BN was added at a ratio of x (x = 0, 1, 2, 3, 4). After stirring at 298 K for 5 h, the resulting suspension was dried at 373 K for 12 h. The dried powder was then calcined at 623 K for 1 h. Pt was subsequently loaded onto the calcined supports by wet impregnation.
The structural and chemical integrity of h-BN on the SiO2 was verified by FT-IR transmittance, Raman, XRD, XPS, confirming that the h-BN was preserved after catalyst preparation. In the enantioselective hydrogenation of α-keto esters, the BN-modified Pt catalyst exhibited a pronounced enhancement in performance, increasing from 77.8% (unmodified Pt catalyst) to 97.6% enantiomeric excess (ee), corresponding to an ~20% improvement. To identify the origin of this enhancement, the adsorption behavior of the chiral modifiers was quantitatively evaluated by UV-vis. This analysis revealed that increasing the h-BN content led to more stable and enhanced adsorption of the chiral modifier on the catalyst surface. Consistently, ATR-IR and CO chemisorption further supported the improved chiral modifier adsorption on the h-BN-modified Pt catalysts. This enhancement was also observed for other α-keto esters and chiral modifiers, and 97.6% ee was maintained over 10 recycling tests, demonstrating robust performance.
The h-BN modification of SiO-2 significantly enhances and stabilizes chiral modifiers adsorption at the Pt surface without altering the intrinsic electronic structure of Pt, thereby boosting enantioselective hydrogenation performance.

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HTT0712

Metal Promoter Effects on Pd/CNT Catalysts for Selective Hydrogenation of High-Concentration Acetylene

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Selective acetylene hydrogenation, high-concentration acetylene, Pd/CNT catalyst, metal promoter, non-petroleum-based C2 streams

Abstract Body.

Selective hydrogenation of acetylene is a critical step in C2 stream upgrading, particularly for non-petroleum-based routes that generate ethylene-containing feeds with relatively high acetylene concentrations. The objective of this study is to investigate how metal promoters influence the catalytic behavior of Pd/CNT-based catalysts for selective hydrogenation under high-acetylene feed conditions.

Pd/CNT-based catalysts modified with metal promoters were prepared and evaluated under identical reaction conditions to minimize the influence of process variables. Catalytic behavior was examined using ethylene-containing feeds with elevated acetylene fractions, representative of C2 streams derived from non-petroleum-based processes. Experimental observations were interpreted in conjunction with density functional theory (DFT) calculations to examine promoter-dependent modifications of Pd surface characteristics and adsorption–activation behavior.

The introduction of metal promoters resulted in condition-dependent changes in acetylene hydrogenation behavior and time-on-stream performance characteristics of Pd/CNT catalysts under high-acetylene conditions. Ethylene selectivity also showed measurable variations depending on the metal promoter employed. These observations indicate that promoter-induced modification of Pd surface properties can influence reaction pathways and deactivation tendencies in high-acetylene feeds.

This study provides a systematic comparison of metal-promoted Pd/CNT catalysts for selective hydrogenation of high-concentration acetylene in ethylene-containing C2 streams. The findings offer insight into promoter effects relevant to catalyst design for emerging non-petroleum-based C2 processing routes.

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HTT0716

Engineering High Surface Area CeO2 with Abundant Oxygen Vacancies to Boost Low-Temperature CO2 Methanation over CeO2-Supported Ni Catalysts

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: CO2 methanation, Ni/CeO2, Oxygen vacancy, in-situ analysis

Abstract Body.
CO2 methanation is a promising Power-to-Gas route to mitigate anthropogenic CO2 emissions while enabling chemical energy storage that buffers the intermittency of renewable power. Supporting grid stability and sector coupling, the process of converting collected CO2 into synthetic methane using green H2 allows for the storage and transportation of excess power through the existing natural-gas infrastructure. Among various catalysts, Ni supported on CeO2 has attracted significant attention due to the unique redox property of ceria and the presence of abundant oxygen vacancies (Ov), which can facilitate CO2 activation. However, conventional CeO2 supports typically exhibit low specific surface area, limiting Ni dispersion and making it difficult to achieve high catalytic activity, particularly at low temperatures. In this study, a two-step hydrothermal synthesis strategy was introduced to fabricate a enriched oxygen-vacancy sites CeO2 support with high surface area. Ni was subsequently impregnated on the synthesized CeO2 to prepare a Ni/CeO2 catalyst, which was evaluated for CO2 methanation performance. The catalyst derived from the two-step CeO2 support was systematically compared with a reference catalyst prepared using a conventional one-step CeO2 synthesis. To clarify the origin of activity enhancement, ex situ characterization was combined with in situ analyses under reaction-relevant conditions to investigate Ni dispersion, interfacial structure, and Ov-related properties. The Ni catalyst supported on the two-step synthesized CeO2 exhibited markedly improved CO2 methanation activity at low temperatures relative to the reference catalyst. Structural and spectroscopic analyses revealed that the two-step route enabled a higher density of Ov sites and a larger surface area, leading to ultra-highly dispersed, cluster-sized Ni species. In addition, the formation of an Ov-rich Ni/CeO2-x interfacial region was maximized, which correlated strongly with enhanced CO2 activation and hydrogenation performance. The superior low-temperature CO2 methanation performance is attributed to the synergistic effect of increased oxygen-vacancy concentration and improved Ni dispersion, resulting in a maximized Ni/CeO2-x interface. This work demonstrates that rational support engineering via a two-step hydrothermal synthesis is an effective strategy to overcome the surface-area limitation of conventional CeO2 and to design highly active Ni/CeO2 catalysts for CO2 methanation.

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HTT0721

Engineering Oxygen-Vacancy-Derived Strong Basic Sites through Macropore Design for Coke-Resistant Ni/γ-Al_2O_3 Catalysts in Methane Bi-Reforming

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Ni/Al_2O_3, macropore, coke resistance, oxygen vacancy, basic site, bi-reforming

Abstract Body.

This work assesses how γ-Al_2O_3 macropore size (90–350 nm) modulates the surface acid–base site distribution of 15 wt% Ni/Al_2O_3 catalysts, and impacts on Ni phase evolution, catalytic performance, and coke resistance during bi-reforming of methane (BRM). Macropore architecture directly regulates Ni precursor diffusion, metal dispersion, and metal–support interaction strength, thereby rebalancing the population and nature of surface acid and basic sites. Catalysts with small macropores (≈90 nm) impose severe diffusion constraints on Ni precursors, resulting in preferential Ni deposition near the external surface and limited interfacial contact with the alumina framework. This configuration stabilizes surface NiO species while preserving a high density of exposed Lewis acid sites associated with coordinatively unsaturated Al^{3+} centers. The acid-dominant surface chemistry disfavors H_2O activation, suppresses oxygen mobility, and accelerates carbon nucleation and coke growth, leading to rapid catalyst deactivation under BRM conditions. By contrast, catalysts with intermediate macropores (~250 nm) achieve optimal Ni penetration and maximized Ni–Al_2O_3 interfacial contact, promoting partial solid-state interaction between NiO and the alumina lattice and driving the formation of $NiAl_2O_4$-like spinel domains. Critically, this strong metal–support interaction induces a high concentration of interfacial oxygen vacancies, generated via lattice distortion and charge compensation mechanisms. These oxygen vacancies function as intrinsic basic sites with enhanced electron density, serving as preferential adsorption and activation centers for CO_2 and H_2O molecules. The resulting acid–base equilibrium—characterized by moderated Lewis acidity and vacancy-derived basicity—facilitates sustained reforming activity, enhanced syngas productivity, and superior coke resistance. Further enlargement of macropores (350 nm) weakens metal–support interactions, reducing both spinel formation and oxygen vacancy density. The consequent decline in basic site availability limits oxidant activation and redox efficiency, partially compromising long-term stability despite improved mass transport. Overall, this study demonstrates that macropore size is a decisive structural lever for engineering oxygen-vacancy-driven basicity in Ni/Al_2O_3 catalysts. An optimized macropore diameter of ~250 nm strategically maximizes vacancy-mediated oxidant activation, delivering sustained BRM

performance and intrinsic resistance to carbon accumulation.

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HTT0722

Active-Site Structural Evolution in Ni–W/Al_2O_3 during Methane Dry Reforming: Tungsten Phase Transformations and Long-Term Stability

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Phase transformation, Defective WC, Ni-WC interface

Abstract Body.

Introduction. Ni-based dry reforming of methane (DRM) catalysts deactivate at high temperatures due to coking and sintering; mesoporous Al_2O_3 and promoters improve dispersion, stability, and carbon resistance [1]. Tungsten (W) is a particularly effective modifier for Ni/Al_2O_3 because Ni-W interactions tune Ni ensembles and in situ WC/W_2C formation enhances CO_2 adsorption/activation, supporting coke removal and stability [2]. However, the distinct contributions of Ni-W alloys versus W carbides are often assumed rather than proven with phase-resolved evidence, and the formation/evolution of WC defects under DRM and their impact on CO_2 activation and durability remain unclear.

Method: xW_9Ni@Al_2O_3 catalysts (x = 9, 17, 20, 31 wt% W; Ni:Al_2O_3 = 9:91 w/w) were prepared by a one-pot solvothermal method using ASB in 2-butanol with $Ni(NO_3)_2 \cdot 6H_2O$ and $(NH_4)H_2(W_2O_7)_6$ (ethanol/ultrasonication), followed by autoclaving at 120 °C for 6 h, drying (70 °C, 24 h), and calcination (600 °C, 6 h). 0W_9Ni@Al and 17W0Ni@Al were synthesized similarly, without W or Ni precursors.

Results and discussion: The durability of Ni-based DRM catalysts is governed by reaction-driven evolution of W phases. We tracked tungsten carbide formation in xWNi@Al to clarify how Ni–WC interfacial coupling and WC/W_2C defect chemistry sustain activity. Stability depends strongly on W loading and time on stream: 0W_9Ni@Al rapidly deactivates from severe coking, whereas W-modified catalysts progressively stabilize. Under DRM, $Ni_{17}W_3$ decomposes into metallic Ni and W carbides, and W carburizes to form Ni-WC interfacial domains. WC is the primary CO_2-activation site, while defective WC_{1-x} and W_2C provide oxygen-vacancy sites that promote O* formation. The evolving WC/W_2C balance suggests a defect healing–regeneration cycle that removes carbon on adjacent Ni, enabling sustained CO_2 activation and long-term stability.

ISCRE29 & APCRE11
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HTT0724

Role of Phosphorus Doping in Tuning Surface Properties, Ni–Support Interaction, and Coke Resistance of Macroporous Ni/Al2O3 Catalysts for Dry Reforming of Methane

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Dry Reforming of Methane, phosphorus doping, macroporous Ni/Al2O3, coke resistance, acidity reduction

Abstract Body.
This work examines how phosphorus (P) incorporation influences the surface characteristics and coke tolerance of nickel catalysts supported on macroporous alumina for the dry reforming of methane (DRM). Three catalyst formulations were synthesized: pristine Ni/MaAl, a sample with phosphorus introduced prior to nickel impregnation (Ni/P–MaAl), and a catalyst in which phosphorus was added after nickel loading (P–Ni/MaAl). Comprehensive characterization using N2 physisorption, NH3-TPD, H2-TPR, XRD, XPS, and TEM was conducted to establish correlations between physicochemical properties and catalytic behavior. The findings demonstrate that phosphorus modification significantly lowers the surface acidity of the alumina support and effectively inhibits carbon accumulation. In particular, strong interactions between phosphorus species and the alumina matrix in P–Ni/MaAl lead to a pronounced reduction in acid sites while preserving a higher extent of NiAl2O4 formation compared with Ni/P–MaAl, which promotes the generation of highly dispersed metallic Ni active sites upon reduction. As a result, the modified catalysts display improved DRM performance, evidenced by elevated CH4 and CO2 conversions, enhanced H2 yield, and improved operational stability. Among the investigated catalysts, P–Ni/MaAl achieves the optimal balance between structural robustness, resistance to coking, and active phase dispersion, underscoring the critical importance of phosphorus addition sequence in tuning catalyst properties for DRM.

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HTT0732

Polystyrene Hydrocracking over Ni/Zeolite Catalysts: The Role of Brønsted Acidity and Polymer Accessibility

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Polystyrene, Chemical recycling, Ni catalyst, Zeolite

Abstract Body.
Introduction. Polystyrene (PS) is widely used alongside polyolefins; however, its chemical recycling remains below 1% [1]. Most chemical recycling research has focused on polyolefins, such as PE and PP, resulting in limited systematic understanding of the factors that govern PS depolymerization [2,3]. In this study, we investigate PS hydrocracking using supported Ni catalysts. To link catalytic properties with reaction behavior, we establish a correlation between PS hydrocracking activity and Brønsted acidity together with polymer accessibility. These results provide catalyst design guidelines for upcycling plastics such as PS, where aromatic intermediates and secondary acid reactions strongly shape the reaction network, and they offer a basis for extending catalytic recycling to more complex polymers.
Methods. The reaction was conducted in a batch reactor. The reactor was charged with 0.1 g of catalyst and 1.0 g of PS, pressurized to 3 MPa with H2. After the reaction, gas and liquid products were analyzed by gas chromatography equipped with TCD and FID detectors.
Results and discussion. To elucidate the role of acidity, we compared PS reactivity over non-acidic Ni catalysts and a zeolitic Ni/HY catalyst (Figure. 1a). In the absence of solid acid, all catalysts gave <10% PS conversion, whereas Ni/HY(30) achieved 47% conversion. This contrast indicates that productive PS depolymerization cannot proceed with the metallic function alone and requires an acid function. To quantitatively rationalize these differences, we characterized acidity. NH3-TPD revealed that the most active catalyst is Ni/HY(30), with a total acidity of 1.147 mmol·g-1, followed by Ni/SiO2, Ni/Al2O3, and Ni/TiO2 with total acidities of 0.583, 0.446, and 0.145 mmol·g-1 respectively (Figure. 1b). However, despite possessing ~50% of the total acidity of Ni/HY(30), Ni/SiO2 exhibited negligible conversion, demonstrating that total acidity alone cannot account for the observed activity gap. We therefore conducted pyridine-FTIR to resolve acid-site identity. Pyridine-FTIR revealed clear Brønsted acid sites (BASs) on HY, whereas BAS signals are largely absent on the oxide-supported catalysts (Figure. 1c). Overall, the activity contrast in PS hydrocracking is governed not by total acidity, but by the presence of accessible BAS.

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HTT0736

In situ ATR-IR study of product poisoning phenomena in heterogeneous C=C enantioselective hydrogenation

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Enantioselective hydrogenation, In situ ATR-IR, Mechanism study

Abstract Body.
Introduction. Heterogeneous enantioselective catalysis is a promising strategy for synthesizing optically pure compounds, which are crucial intermediates for pharmaceuticals and fine chemicals. However, enantioselective hydrogenation of C=C bonds over chirally modified Pd catalysts has been less intensively investigated, which is a model reaction for synthesizing chiral carboxylic acids. It is hypothetically suggested that products poison the chiral site during the reaction and decreasing the enantioselectivity. [1] However, there was little evidence to elucidate this phenomenon. Therefore, in situ ATR-IR is adopted to monitor the behavior of product under reaction condition. It is discovered that adsorbed products were interacting with chiral modifiers, while poisoning the chiral sites. This study suggests the key challenges in heterogeneous C=C enantioselective hydrogenation for enhancing enantioselectivity with in situ ATR-IR studies.
Methods. A 3 wt% Pd/Al2O3 for enantioselective hydrogenation of α-phenylcinnamic acid and in situ ATR-IR studies was synthesized using chemical reduction. In situ ATR-IR studies were conducted using a homemade flow system for supplying the H2 and 1 mM solution to simulate the reaction condition.
Results and discussion. Enantioselective hydrogenation of were performed to investigate the poisoning effect of chiral sites by introducing the product after adsorbing a chiral modifier onto a 3 wt% Pd/Al2O3 catalyst. It was observed that the poisoning of chiral active sites led to a decrease in enantioselectivity. Analysis of the product adsorption behavior on a bare Pd surface using in situ ATR-IR revealed the disappearance of the carboxylic acid peak and the formation of carboxylate species, confirming that the product chemisorbs onto Pd in the form of a carboxylate. Next, the adsorption peaks of the product were compared in the presence and absence of the chiral modifier. In the presence of the modifier, a new carboxylate adsorption peak appeared at 1558 cm^{-1}, distinct from the peaks common to both cases. Previous studies have reported that carboxylate adsorption peaks shift depending on amine modification. [2] Therefore, this new peak can be attributed to the product interacting with the chiral modifier, confirming that the product does not merely occupy the catalyst surface but also interacts with the chiral modifier. Furthermore, upon purging with the solvent, the peak at 1558 cm^{-1} persisted, while the intensity was gradually decreased. Consequently, it was observed that the product species interacting with the modifier remained even after purging, which is the key evidence of product poisoning phenomena.

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HTT0740

Catalytic Methane Decomposition over Ni-CeO2 Catalysts for CO2-Free Hydrogen Production

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Catalytic methane decomposition, Ni-CeO2 composite, Oxygen vacancies, Filamentous carbon

Abstract Body.

Purpose. Catalytic Methane decomposition ($CH4 \rightarrow C + 2H_2$) has emerged as a promising pathway to produce hydrogen without CO_2 emissions, with CH_4 being converted into H2 and solid carbon. Compared to thermal routes, the use of catalysts achieves superior methane conversion at reduced temperatures. In this study, we investigate a Ni–CeO2 bulk catalyst to elucidate how its unique interfacial structures dictate catalytic activity and stability in methane decomposition.
Methods. A Ni-CeO2 bulk catalyst series was synthesized by co-precipitation with the Ni content varied from 20 to 80 wt.%. In contrast, the reference Ni/CeO2 catalyst was prepared via a conventional wet-impregnation method.
Results and discussion. The structural characteristics of the Ni-CeO2 bulk catalysts and the Ni/CeO2 catalyst were investigated using high-resolution transmission electron microscopy (HRTEM) and X-ray diffraction (XRD). The Ni-CeO2 bulk catalyst exhibited superior methane conversion and hydrogen yield compared to Ni/CeO2 catalysts. H2-TPR analysis reveals a higher density of Ni-O-Ce interfacial sites compared to conventional Ni/CeO2, attributed to a tailored population of Ce^{3+} states and oxygen-vacancy sites. Furthermore, initial-rate kinetic comparisons imply a lower apparent barrier and improved low-temperature performance. Post-reaction carbon analysis was conducted to characterize the carbonaceous deposits. TEM imaging confirmed the presence of filamentous carbon structures on the Ni-CeO2 surface. Raman spectroscopy revealed that the Ni-CeO2 catalyst promotes the formation of more graphitic carbon compared to Ni/CeO2. This trend is consistent with a higher oxygen-vacancy density and strengthened Ni-CeO2 interfacial interactions, which stabilize metallic Ni sites and favor diffusion-precipitation driven filamentous carbon growth rather than amorphous encapsulation.
Conclusion. Ni-CeO2 bulk catalyst synthesized via co-precipitation exhibits enhanced density of Ni-O-Ce interfacial sites and increased formation of oxygen vacancies, which facilitate efficient methane activation and hydrogen production. Overall, these findings highlight the critical role of interfacial engineering in designing robust catalysts for CO2-free hydrogen production and the synthesis of valuable carbon nanomaterials.

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HTT0749

Investigation of mechanical stability of CuO/ZnO-based catalyst pellets

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: catalyst pellet, mechanical stability, particle attrition

Abstract Body.

Introduction.
Tableted catalyst pellets are widely employed in large-scale industrial heterogeneous chemical processes, particularly in fixed-bed and trickle-bed reactors, due to their mechanical robustness, simple and controlled manufacturing process, and favorable fluid dynamic properties in a packed-bed setting.
Mechanical stresses resulting from thermal treatments and chemical transformations of the catalyst tablets result in particle attrition over time, ultimately leading to an increased pressure drop and negatively impacting reactor performance and operating costs. Minimizing particle attrition remains one of the main challenges for reactor systems that utilize catalyst pellets. [1] This study investigates the influences of reduction process and feed water content on the crush strength of cylindrical CuO/ZnO-based catalyst pellets.

Methods.
Tableted commercial CuO/ZnO-based catalysts were used. The mechanical stability of catalyst tablets was measured using a Side-Crush-Strength (SCS) testing device. The collected SCS data was evaluated using Weibull statistics. The SCS stability of catalyst pellets were tested in oxidic fresh state, after treatment with water vapor or liquid water and after reduction treatment. Fresh, water treated and reduced pellets were characterized using Temperature-Programmed reduction (TPR), X-Ray Diffraction (XRD) and N2 physisorption.

Results and discussion.
Fresh CuO/ZnO-based catalyst pellets exhibited higher mechanical stability compared to reduced catalyst pellets as expected. Water vapor treatment of fresh catalyst pellets resulted in different mechanical stability when compared to fresh catalyst pellets. Water vapor treatment had no beneficial impact on mechanical stability of reduced catalyst pellets. Treatment of fresh catalyst pellets with liquid water had a different influence on the mechanical stability when compared to treatment with water vapor. N2 physisorption experiments of reduced pellets showed differences in BET surface area when compared to fresh pellets.

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HTT0759

Exploring the effect of local temperature gradients on Fe-based catalysts during inductively heated reverse water gas shift

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: CO2 utilization, magnetic heating, supported metal catalysts, Reverse water-gas shift

Abstract Body.
Purpose
Catalytic reactors for CO2 utilization via reverse water gas shift (RWGS) can benefit from the localized heating, precise temperature control and fast heating rates of magnetic induction. Fe nanoparticles can be inductively heated to RWGS reaction temperatures by an alternating magnetic field in the order of 40 mT. This work studies the magnetic and catalytic properties of Fe-based catalysts containing ferromagnetic nanoparticles and catalytic sites to efficiently catalyze an endothermic reaction such as RWGS. The stability of Fe phases under RWGS reaction conditions is improved by different pretreatments and promoters Combining operando XRD-XAS with the characterization of spent catalysts after induction shows the unique effects of induction heating of the catalyst in contrast to conventional external heating.
Methods
Supported monometallic Fe and bimetallic Fe-Cu and Fe-Co catalysts were prepared by wet impregnation on different mesoporous supports. The catalysts were characterized by in-situ XRD, temperature-programmed reduction and operando XAS. The catalysts were tested in a lab scale 9 mm ID fixed bed reactor equipped with a copper coil generating an alternating magnetic field. Temperature under induction was measured with an infra-red sensor focused on the upper layer of the bed.
Results
Catalysts containing ca. 20 wt.% metal loading inductively self-heat up to 600°C under inert. Operando XAS and XRD revealed that, under RWGS, catalytic activity and inductive heating are maintained as long as the carbidation of Fe can be avoided. Strategies effective are the formation of a Fe3O4 precursor and the formation of FeCo alloys [1]. Here we show that, by adding 2-4% Cu loadings, these catalyst achieves high RWGS activity (0.256 mol CO gcat-1 h-1 at WHSV=25 LCO2 gcat-1 h-1) while keeping the magnetic properties of Fe nanoparticles. Interestingly, different Fe phases are formed under RWGS when the catalysts are inductively heated from inside the material in comparison to reaction at similar conditions in an externally heated oven.
Conclusions
Role of support and a second metal in redox properties of Fe nanoparticles is highly relevant for their stable performance as inductive heaters under RWGS catalytic conditions. We

found that the differences are more pronounced when supports with poor thermal conductivities are used, pointing to the existence of temperature nanogradients in the catalytic bed. We are currently studying the effects of temperature local gradients and controlled temperature oscillations on the activity and stability of these Fe-based inductively heated RWGS catalysts.

[1] S. Spyroglou et al. ACS Catal. 16 (2026) 344-355.

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HTT0764

SiO_2 -Modified Pt–M/Al_2O_3 Catalysts for Coke-Resistant Propane Dehydrogenation: Machine Learning Guided Catalyst Deactivation Study

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Keywords: Propane dehydrogenation; Bimetallic catalysts; Mesoporous SiO_2 –Al_2O_3 ; CO_2 -assisted PDH; Catalyst stability; Coke suppression

Introduction. The growing global demand for propylene, driven by its extensive use in polypropylene, oxo-alcohols, and acrylic derivatives, has increased interest in on-purpose propylene production technologies. Propane dehydrogenation (PDH) offers a direct and selective route; however, its commercial application is limited by rapid catalyst deactivation caused by metal sintering and coke formation. These issues lead to frequent regeneration cycles and increased energy consumption and CO_2 emissions. Recent studies have shown that bimetallic catalyst systems and tailored support architectures can effectively improve metal dispersion, tune surface acidity, and suppress side reactions. In this work, mesoporous SiO_2 –Al_2O_3 supported bimetallic Pt–M (M = Cu, Zn) catalysts are developed to enhance activity, selectivity, and stability for non-oxidative PDH.

Methods. Bimetallic Pt–M catalysts supported on mesoporous SiO_2 –Al_2O_3 were synthesized using a neutral templating method followed by controlled calcination in air. Catalyst formulations included 0.3Pt–0.5(Cu/Zn)/m-SiO_2 –Al_2O_3 . Physicochemical characterization was performed using BET surface area analysis, chemisorption studies, TPDRO, XRD, FTIR, XPS and TGA. Catalytic evaluation was carried out in a fixed-bed reactor at atmospheric pressure in the temperature range of 550–650 °C using C_3H_8/N_2 feed mixtures. Product analysis was conducted by online gas chromatography. Aspen Plus simulations employing R-Gibbs and R-Plug reactor models were used to study thermodynamic equilibrium and reaction kinetics, and a power-law kinetic model was fitted to the experimental data. Machine Learning Models are also applied to understand the coke deposition on the catalysts.

Results and discussion: The synthesized catalysts exhibited high specific surface areas and well- defined, uniform mesoporous structures, which facilitated effective dispersion of Pt and secondary metal species on the SiO_2 –Al_2O_3 support. The introduction of a second metal in bimetallic Pt–M catalysts led to a notable enhancement in catalytic performance, reflected in higher propane conversion and propylene selectivity compared to their monometallic counterparts. In addition, bimetallic systems demonstrated substantially suppressed coke formation, indicating improved resistance to deactivation under reaction conditions. Among the catalysts investigated, the Pt–Cu catalyst supported on 10 wt% SiO_2 -modified Al_2O_3 exhibited superior performance, achieving approximately 35% propane conversion with 98% propylene selectivity at 600 °C. Importantly, this catalyst maintained stable activity and selectivity over 20 h of continuous operation. Post-reaction analysis revealed significantly lower coke deposition (<2 wt%) on the SiO_2 -modified support compared to the unmodified Al_2O_3 support (~8 wt%), highlighting the role of SiO_2 incorporation in mitigating carbon accumulation. Furthermore, catalyst deactivation trends

were systematically analyzed using a machine-learning-based model, which identified key physicochemical properties governing deactivation behavior, thereby providing mechanistic insights to guide rational catalyst design.

Acknowledgments

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HTT0772

Positive CO Conversion–Selectivity Relationship in Tandem Catalysis of Fischer–Tropsch Synthesis and Catalytic Cracking

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Fischer–Tropsch synthesis; precipitated iron-based catalysts; ZSM-5; Tandem catalysts; CO conversion–selectivity relationship

Abstract Body.

Fischer–Tropsch synthesis (FTS) is a suitable process for converting syngas (CO+H2) into synthetic liquid fuels, and the tandem process, which involves both hydrocarbon growth and hydrocracking, can improve selectivity to liquid-range hydrocarbons. For industrial processes, high CO conversion and high selectivity for liquid-range hydrocarbons (C5–C20) are simultaneously required to ensure process efficiency and performance. However, FTS often exhibits a trade-off relationship between CO conversion and selectivity for desirable products, with selectivity decreasing as CO conversion increases [1]. Previous studies on tandem catalysts have mainly focused on improving liquid-range hydrocarbon selectivity by adjusting catalyst properties and operating conditions [2]. Despite its importance, systematic investigations of the relationship between CO conversion and product selectivity in tandem catalysts remain limited, particularly at high CO conversion levels [3]. In this study, we examined product distributions at different CO conversion levels to explore the conversion–selectivity relationship in tandem catalysis.

We prepared precipitated iron-based catalysts (P-Fe) for FTS and tandem catalysts by physically mixing P-Fe with ZSM-5. Physical mixing has been reported to limit undesirable chemical interactions between the two catalysts [4]. The catalytic performance was evaluated under different gas hourly space velocity (GHSV) conditions, which can influence both CO conversion and hydrocracking, and the CO conversion–selectivity relationship was independently assessed under conditions where hydrocracking was controlled.

For P-Fe, C2–C4 selectivity increased and C5+ selectivity decreased as CO conversion increased, indicating a conversion–selectivity trade-off. In contrast, the tandem catalysts showed a consistent trend in which C2–C4 selectivity decreased and C5–C20 selectivity increased as CO conversion increased. As CO conversion increased from 37.8% to 87.3%, the selectivity for C5–C20 hydrocarbons consistently increased from 59.4 wt% to 79.4 wt%. When the selectivity for C5–C20 hydrocarbons reached its highest value (79.4 wt%), the selectivity of gasoline-range (C5–C11) hydrocarbons was as high as 68.5 wt%.

This study reports the CO conversion–selectivity relationship of P-Fe and tandem catalysts, composed of P-Fe and ZSM-5, for FTS. While P-Fe exhibited a conversion–selectivity trade-off, the tandem catalysts showed a positive relationship between the CO conversion level and the selectivity of liquid-range hydrocarbons. These results indicate that tandem catalysts are worth investigating further for efficient liquid-fuel production under industrial processes

that require both high CO conversion and high selectivity.

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HTT5688

Screening of Transition-Metal Catalysts for NH3 Decomposition

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: ammonia decomposition, catalyst screening, transition metal

Abstract Body.
As concerns over climate change continue to grow, hydrogen has gained attention as a clean energy carrier. However, its low volumetric energy density and the need for cryogenic conditions during liquefaction present challenges for storage and transportation. In contrast, ammonia (NH_3), with its high hydrogen content and established infrastructure, is considered a promising alternative hydrogen carrier. Efficient hydrogen production from ammonia therefore requires the development of active and economically viable decomposition catalysts. In this study, a screening was conducted to identify transition-metal catalysts suitable for ammonia decomposition. Catalyst performance was assessed using NH_3 dissociation energy and N_2 adsorption energy as key indicators, with Ru employed as a reference metal. Based on these criteria and considerations of stability and practical applicability, five metals—Ru, Rh, Ni, Ir, and Co—were selected for further comparison. Analysis of the Gibbs free energy profiles for ammonia decomposition on the selected metal surfaces reveals that Ru exhibits the most favorable reaction energetics. However, its high cost limits large-scale application. To address this issue, bimetallic catalysts were explored to reduce noble metal content while maintaining catalytic performance. Among the systems examined, the Ru–Ni catalyst emerged as a promising candidate, showing favorable energetic characteristics for both NH_3 dissociation and N_2 desorption. Overall, this study demonstrates that catalyst screening provides an effective approach for identifying cost-effective and high-performance catalysts for ammonia decomposition, contributing to carbon-neutral hydrogen production.

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HTT5691

Facile Synthesis of High Dispersed Ni Catalyst by Tannic Acid Assisted Impregnation for Low Temperature Ammonia Decomposition

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Ammonia decomposition; Ni-based catalysts; chelation-assisted impregnation; Carbon interlayer; High-dispersion

Abstract Body.

Introduction.

Although the impregnation method is commercially favored for its simplicity, it often results in poorer dispersion than more complex routes (e.g. sol-gel or precipitation). To overcome this limitation, we employed a modified chelation-assisted impregnation approach using tannic acid(TA) to create surface anchor sites and enhance metal dispersion. The formation of carbon-interlayer during carbonization weakens excess metal-support interaction and suppresses solid-solution formation which require harsh reduction conditions to activate.

Methods.

TA/MgO support was prepared by dispersing MgO in distilled water containing 0.5 wt% tannic acid solution at room temperature, followed by centrifugation/washing, and drying at 80 ℃ overnight. NiCMgO catalysts were synthesized by wet impregnation of Ni onto TA/MgO and subsequent carbonization under N_2 at 550 ℃. Reference Ni catalysts were prepared identically using MgO and Al_2O_3 supports.

Ammonia decomposition was tested using 3/8 " quartz tube reactor packed with 0.05g catalysts(0.1g for stability test). The feed composition was NH3:He:Ar=20:5:20 (He as internal standard), and product gas was analyzed by online GC-TCD.

Figure 1. Ammonia decomposition catalyst stability test results of NiCMgO and NiMgO catalysts.

Results and discussion.

The NiCMgO catalysts demonstrated improved metal dispersion and higher ammonia decomposition activity than conventional NiMgO. The carbon interlayer suppressed Ni incorporation into the MgO lattice (solid-solution formation), leading to milder metal-support interactions and facilitating low-temperature reduction. Consequently, NiCMgO exhibited the highest activity with decent thermal stability and an earlier activity onset, highlighting the

potential of this simple impregnation modification for efficient low-temperature catalysts.

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Silica-encapsulated Cu-ZnO nanoparticles for CO2 hydrogenation to methanol

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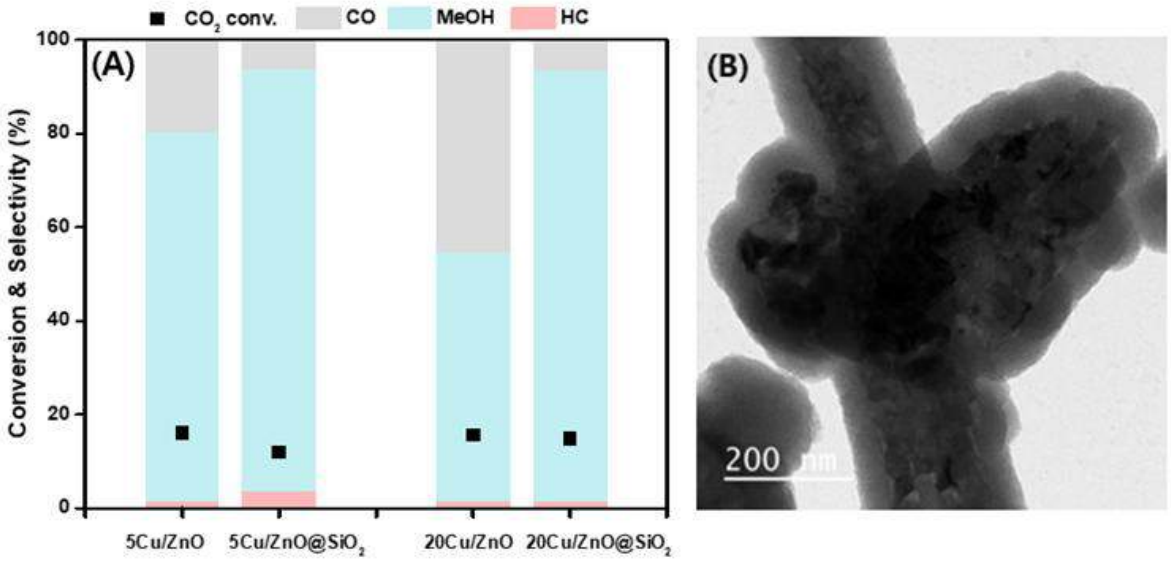
Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: CO2 hydrogenation, Methanol, Core-shell structure, Silica coating, metal sintering

Abstract Body.

Introduction: Commercially available Cu/ZnO/Al_2O_3 (CZA) catalysts are widely utilized for methanol synthesis by COx hydrogenation, however, its lower catalytic activity and stability for CO2 hydrogenation should be solved. The interfacial structures of Cu–ZnO nanoparticles, where metallic Cu sites facilitate H_2 dissociation and oxygen vacant sites in ZnO help CO_2 adsorption to stabilize surface intermediates such as formate, are known to be crucial for higher CO2 conversion [1]. However, the active interfacial structures are easily aggregated through reconstructions under reaction conditions, leading to fast catalytic deactivation. To overcome the phenomena, silica overlayer-coating strategies are largely investigated, where the silica overlayers acted as physical barriers by suppressing sintering of Cu nanoparticles.
Methods: [Synthesis rod-type ZnO] By using a chelating agent of ethylenediamine to form complex with Zn^{2+} ions, the growth of specific crystalline planes was suppressed which allows ZnO to grow preferentially in the [001] direction, resulting in a rod-type morphology. [Synthesis Cu/ZnO] Copper precursor was deposited on the ZnO by a wet impregnation method. [Silica Coating] Silica coating was performed on the Cu/ZnO nanoparticles by using a surfactant-assisted method. CTAB (cetyltrimethylammonium bromide) was first introduced as a cationic surfactant to stabilize and disperse Cu/ZnO nanoparticles, followed by the addition of TEOS (tetraethyl orthosilicate) as silica precursor to form uniform SiO2 coating layers.
Results and discussion: Silica-coated Cu/ZnO@SiO2 catalysts exhibited a significantly enhanced methanol yield and thermal stability. The enhanced catalytic performances were attributed to the effects of stable preservation of Cu-ZnO interfacial sites and stabilization of Cu^+ species [2] with the help of SiO2 coating overlayers. Simple silica encapsulation can solve the deactivation of Cu/ZnO catalysts by improving their thermal stability and water resistance natures. The optimized catalyst (20Cu/ZnO@SiO2) exhibited a higher methanol selectivity of ~87%, while the uncoated catalyst (20Cu/ZnO) showed a minimum methanol selectivity of ~43%. This silica-coated catalyst was demonstrated to stabilize active sites, which were further confirmed by various surface characterization tools.



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ISCRE29 & APCRE11
2026 / SEOUL, KOREA

HTT9702

Enhanced Regenerability of Ru- and Zn-Promoted Mo/MCM-22 for Methane Dehydroaromatization

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: methane dehydroaromatization, MCM-22, regeneration

Abstract Body.
Methane dehydroaromatization (MDA) is widely considered a potential route for the direct conversion of methane into high-value aromatics. Among various catalyst systems, Mo-supported zeolites, particularly ZSM-5 and MCM-22, are most widely utilized due to their superior catalytic performance and shape selectivity. However, achieving long-term stability remains a critical challenge due to rapid deactivation during repeated reaction-regeneration cycles. In this study, we investigated the promotional effects of Ruthenium (Ru) and Zinc (Zn) on Mo/MCM-22 catalysts to overcome these stability limitations.

The catalysts were evaluated over five consecutive reaction cycles at 700 °C. Monometallic catalysts with 4 wt.% and 6 wt.% Mo (6Mo/MCM-22) were first compared to investigate the correlation between Mo loading and catalytic deactivation. To stabilize the high aromatic yield observed at the higher Mo loading, 1 wt.% Ru or 1 wt.% Zn was incorporated into the 6Mo/MCM-22 system via co-impregnation.

While 6Mo/MCM-22 initially exhibited higher benzene, toluene, and xylene (BTX) production than 4Mo/MCM-22, it suffered from severe deactivation, with its performance dropping to 79% by the 5th cycle compared to the first regenerated cycle. 27Al MAS NMR indicates that this deactivation is primarily caused by the irreversible formation of aluminum molybdates ($Al_2(MoO_4)_3$), resulting from the reaction between excessive Mo species and the MCM-22 framework.
In contrast, the Ru-Mo/MCM-22 catalyst maintained 95% of its initial activity, with both Ru-Mo and Zn-Mo bimetallic catalysts demonstrating superior regenerability. Raman analysis revealed a more homogeneous distribution of Mo species in Ru-Mo/MCM-22 compared to 6Mo/MCM-22, suggesting that the addition of Ru effectively enhances Mo dispersion. Interestingly, H_2-TPR analysis showed that the high-temperature reduction peaks were notably absent in the bimetallic catalysts. Instead, they exhibited reduction profiles similar to the more stable 4 wt.% Mo catalyst, suggesting that Ru and Zn help maintain Mo in a more reducible state despite the high loading. This is further supported by TGA results, where the promoters successfully suppressed the sublimation of excessive Mo at temperatures above 800 °C.

It is hypothesized that the promoters reduce the mobility of Mo species, thereby mitigating their migration and subsequent reaction with the zeolite framework to form inactive phases. This stabilization mechanism will be further validated through planned TEM and XPS investigations to confirm the metal nanostructure and oxidation states. These findings

suggest that Ru and Zn provide a robust pathway to stabilize Mo active sites, enabling the use of high-loading Mo catalysts for durable MDA processes without the typical trade-off in regenerability.

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HTP0130

Computational screening of photocatalysts for ammonia synthesis with included excited states

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Photochemical

Keywords: photocatalysis, ammonia synthesis, DFT calculations, excited states

Abstract Body.
Introduction. Ammonia is regarded as an excellent energy carrier and a secure hydrogen storage medium, containing up to 17% hydrogen by weight and offering a competitive cost per unit of stored hydrogen. The industrial production of ammonia via the conventional Haber-Bosch (HB) process is environmentally problematic due to the high energy input required to activate the inert nitrogen molecule and the significant carbon footprint associated with hydrogen production from methane. Photocatalytic ammonia synthesis is a sustainable alternative to the HB process, with the potential to produce ammonia under mild conditions using light as the driving force [1]. In this work, we studied the photocatalytic mechanism of ammonia synthesis in excited states on titanium dioxide (TiO2) photocatalysts modified with selected transition metals, using first-principles calculations combined with microkinetic modelling.

Methods. Spin-polarised density functional theory calculations were performed using VASP. The plane-wave basis set was used with a cutoff energy of 500 eV. The Perdew-Burke-Ernzerhof (PBE) functional was employed for adsorption properties and elucidation of the nitrogen reduction mechanism, while a hybrid functional (HSE06) was selected for more accurate prediction of the electronic properties of the studied catalysts. The Hubbard-U correction was applied to account for on-site Coulomb interactions, and the Grimme-D3 correction was used to include van der Waals interactions. To accurately describe the photocatalytic nitrogen reduction mechanism, it was studied in excited states using time-dependent density functional theory.

Results and discussion. The activation of nitrogen was studied on Mo, Fe, Ru, Os, CoNi, and Tc-doped (TiO2)12 clusters. To investigate the photocatalytic properties of the selected catalysts, we calculated band gaps and photoabsorption spectra, analysed charge density differences, and used Bader charge analysis to study charge transfer for adsorbates. The nitrogen dissociative reaction mechanism was investigated in both the ground state and the first excited state on selected catalysts, which were then compared. On Mo3-(TiO2)12 and Os3-(TiO2)12 catalysts, the second hydrogenation; on Fe3-(TiO2)12 and Co2Ni-(TiO2)12, the nitrogen dissociation; on Ru3-(TiO2)12, the third hydrogenation; and on Tc3-(TiO2)12, the first hydrogenation were identified as the rate-determining steps (RDS) in the ground state, which were reduced in the first excited state. First-principles results were incorporated into a microkinetic model to determine whether ammonia is produced under mild conditions. Using combined first principles and microkinetic modelling, we developed the first

mechanistic insight into photocatalytic ammonia synthesis in excited states on selected catalysts.

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HTP0319

Photocatalytic decomposition of hydrous hydrazine: Experimental and CFD studies

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Photochemical

Keywords: Hydrous hydrazine, photocatalysis, CFD

Abstract Body.

Introduction.

Over the past decades, substantial progress has been accomplished on photocatalytic H2 generation especially through the water splitting reaction [1]. Computational Fluid Dynamics (CFD) is able to capture irradiation profiles and consider the effect of radiation in the reaction rate to capture the decomposition of reactants/generation of products. Aim of this work is the experimental and theoretical study of the photocatalytic decomposition of hydrous hydrazine (HH). A 2-D-axisymmetric model was developed based on the photoreactor system to save computational resources, evaluating irradiation profiles and how HH is decomposed through time, giving good validation from the experimental data.

Methods.

Experimental tests were conducted in a batch photoreactor with the lamp immersed in the medium, using a 0.5 wt% Rh/TiO2 photocatalyst. The effect of HH concentration and HH to photocatalyst ratio were examined. For the simulation of the light intensity distribution inside the reactor, the Radiation Transfer Equation (RTE) was solved, based on the conservation principle applied to a ray along a path through a medium.

(Selected) Results and discussion.

The irradiation intensity profile is shown in Figure 1. A power-law kinetic model was incorporated in the model integrating also the irradiation intensity factor on the reaction rate, where a relatively good validation is observed (Figure 1b). The highest conversion (73.33%) was obtained from the conditions of 90.6 mM and substrate to photocatalyst ratio 25:1.

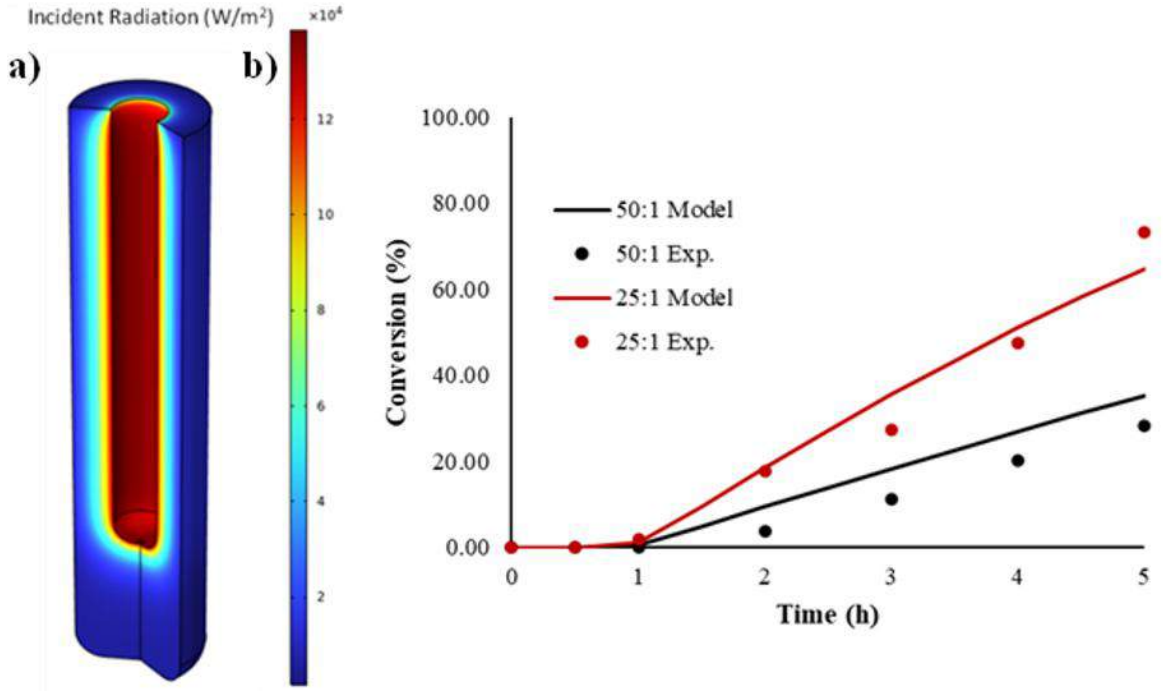

Figure 1. a) incident radiation profile and b) conversion of HH at different HH to photocatalyst ratios.

Conclusions.
Good validation is observed between the model and the experimental results showcasing the ability of the power-law model to predict and describe the behaviour of the photocatalytic reaction system.

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HTP0723

Toward Efficient Photocatalytic Hydrogen Evolution over Pt/g-C3N4: Pt Cocatalyst Evolution, Metal–Support Interactions, and Deactivation Mechanisms

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Photochemical

Keywords: H2 production; photocatalysts; Pt; C3N4; deactivation

Abstract Body.
Introduction. Pt/g-C_3N_4 photocatalysts are widely used for photocatalytic H_2 evolution, yet their activity often decays during operation. Understanding how Pt cocatalyst states and metal–support interactions evolve under reaction conditions is crucial for clarifying deactivation pathways and improving long-term H_2 production stability.
Methods. Bulk g-C_3N_4 (CN) and oxidized g-C_3N_4 (OCN) loaded with Pt cocatalysts were prepared. During photocatalytic H_2 evolution, the structural evolution of both Pt species and the g-C_3N_4 surface was tracked to correlate dynamic changes in cocatalyst dispersion and surface functional groups with activity decay.
Results and discussion. OCN shows superior initial H_2 -evolution activity because abundant O-containing functional groups stabilize highly dispersed Pt species and enhance charge separation. However, these finely dispersed Pt species rapidly agglomerate into large nanoclusters during the reaction, a process promoted by the exfoliated thin-layered structure of OCN. Meanwhile, the progressive loss of O-functional groups weakens the metal–support interaction, further accelerating Pt migration and agglomeration. In contrast, the three dimensional multilayered framework of CN suppresses Pt agglomeration and retains stronger support interactions, leading to higher resistance to deactivation despite lower initial activity. Overall, the fast deactivation of OCN is governed by the synergistic effects of Pt agglomeration and the deterioration of O-functional-group-mediated metal–support interactions.

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HTP5690

Photothermal-Enhanced Bimetallic Ni-CdS Photocatalyst for Dry Reforming of Methane Toward Solar-Driven Hydrogen Production with Reactor Heating Design

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Photochemical

Keywords: dry reforming of methane; bimetallic Ni–CdS; photocatalysis; photothermal effect; reactor design

Abstract Body.
Introduction: Dry reforming of methane (DRM) is an attractive reaction for converting CH_4 and CO_2 into hydrogen-rich syngas; however, conventional DRM is a high-temperature thermochemical process that suffers from severe carbon deposition (coking), leading to catalyst deactivation and poor long-term stability. Lowering the operating temperature is a promising strategy to suppress coking, but this significantly reduces methane activation and overall reaction efficiency. To overcome these challenges, photocatalysis coupled with photothermal effects offers a potential pathway to enable DRM under milder conditions while maintaining catalytic activity.In this study, we investigate a bimetallic Ni-based CdS photocatalyst for photo-assisted DRM, combined with a rational reactor heating design to systematically evaluate temperature effects and catalytic optimization. The primary objective is to establish a measurable reaction baseline under controlled thermal conditions and subsequently elucidate the role of bimetallic Ni cocatalysts in enhancing methane activation and hydrogen production.
Methods: CdS nanosheets were prepared via ligand exchange and decorated with bimetallic Ni species through controlled photodeposition, followed by thin-film fabrication on transparent substrates. Structural and optical properties were characterized using X-ray diffraction (XRD), transmission electron microscopy (TEM), and UV–Vis spectroscopy. Photocatalytic DRM experiments were conducted in a custom-designed photothermal reactor equipped with a transparent irradiation window and integrated heating system. The reactor design enabled precise temperature control and minimized heat loss, allowing systematic investigation of thermal effects under simulated solar irradiation. Initial experiments focused on evaluating the influence of temperature on DRM activity to overcome the intrinsically low reaction rates at room temperature. Once a stable and quantifiable reaction regime was established, the effect of bimetallic Ni cocatalyst composition was examined.
Results and Discussion: The results demonstrate that moderate heating significantly enhances DRM activity while maintaining lower temperatures than conventional thermal

DRM, thereby mitigating coking risks. Further enhancement was achieved through bimetallic Ni decoration, which improved methane activation and hydrogen evolution compared to monometallic systems. The observed performance gains are attributed to the combined effects of photothermal heating, optimized reactor design, and synergistic bimetallic catalytic sites.Overall, this work highlights the importance of integrating temperature management, catalyst design, and photothermal effects to advance low-temperature DRM. The findings provide valuable insights for developing coking-resistant, solar-assisted DRM systems and contribute to sustainable hydrogen production strategies.

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HTE0037

Boosting screening of non-equiatomic high-entropy electrocatalysts by inverse design via active graph learning

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Electrochemical

Keywords: High-entropy electrocatalysts, Inverse design, Graph neural networks, Active learning, Hydrogen evolution reaction

Abstract Body.
High-entropy alloys hold great promise for enhancing the performance of electrocatalysts. However, the rational design and screening of such catalysts are hampered by the vast compositional space and diverse local atomic arrangements involved. Traditional bottom-up deep-learning methods remain constrained by their heavy reliance on datasets generated through density functional theory (DFT), which limits the rapid screening of high-entropy catalysts. To overcome these challenges, we introduce an inverse-design strategy based on an active-learning (AL) framework that integrates conditional generative adversarial networks, atomic graph attention networks, k-nearest neighbors, and high-throughput DFT calculations. This top-down approach reduces the required training dataset size for designing high-performance high-entropy electrocatalysts (HEECs). Using the established AL workflow, we systematically explore the compositional space of HEECs composed of Ni, Co, Fe, Pd, and Pt, and identify optimized non-equiatomic compositions with exceptional hydrogen evolution performance. Furthermore, electronic structure analysis reveals that Pd and Pt serve as the active species, while Ni, Co, and Fe contribute to inducing the “cocktail effect”—a feature that distinguishes HEECs from ordered metals or alloys. Based on these insights, we propose two design principles to guide the discovery of high-performance HEECs: (i) retain Pd/Pt as essential reaction centers, and (ii) utilize Fe, Co, and Ni to enhance entropy and promote cocktail synergy. This AL-driven methodology provides a powerful platform for accelerating the discovery and design of next-generation electrocatalysts。

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2026 / SEOUL, KOREA

HTE0066

Black titania-supported Ir-based high-entropy alloy as a stable electrocatalyst for oxygen evolution reaction in acidic media

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Electrochemical

Keywords: Acidic OER, high-entropy alloy, black TiO2, PEMWE, reconstruction

Abstract Body.
Proton exchange membrane water electrolysis (PEMWE) represents a potential strategy for green hydrogen production. However, its widespread adoption is hindered by sluggish reaction kinetics and the highly corrosive environment of the acidic oxygen evolution reaction (OER). Ir-based high-entropy alloys (HEAs) containing transition metals exhibit promising OER activity, yet their limited stability in acidic media limits their practical applicability.
In this research, a two-dimensional black TiO2 (b-TiO2) material, derived from bronze-phase TiO2(B), is synthesized by directly growing on a carbon cloth (CC) substrate. This defect-rich b-TiO2 material provides robust support for IrM HEA nanoparticles (M = Ni, Co, Fe, and Cu), thereby forming the IrM/b-TiO2/CC electrocatalyst.
The synthesized catalyst exhibits pronounced alloying effects typical of HEAs and enhanced strong metal–support interactions (SMSI), attributed to the defective b-TiO2 support. Under OER operating conditions, the IrM HEA undergoes surface reconstruction, leading to the formation of an IrM@IrOx core–shell structure. The newly generated IrOx shell serves as both an active site and a protective layer, suppressing transition-metal leaching and thereby improving catalyst durability. Consequently, OER analysis in Ar-saturated 0.1 M HClO4 reveals that the IrM/b-TiO2/CC catalyst achieves a low overpotential of 242 mV at 10 mA cm–2 and demonstrates exceptional long-term stability by maintaining performance at 100 mA cm–2 for over 60 hours. Thus, this study has successfully provided an effective approach to improve the activity and stability of HEA catalysts for acidic OER.

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HTE0206

Accelerated Discovery of Optimal NiCoFe Compositions for Oxygen Evolution through Surface-Informed Machine Learning

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Electrochemical

Keywords: oxygen evolution reaction, machine learning, density functional theory, alloy electrocatalysts

Abstract Body.
The development of efficient electrocatalysts for the oxygen evolution reaction (OER) is critical for sustainable hydrogen production through alkaline water electrolysis. However, discovering optimal compositions for multi-element alloy electrocatalysts is time-intensive and resource-consuming due to the vast compositional space that cannot be comprehensively explored through conventional trial-and-error approaches. This study establishes a systematic framework for rational electrocatalyst design by integrating machine learning (ML) with density functional theory (DFT) calculations to accelerate the discovery and optimization of ternary alloy catalysts.
We developed a hybrid computational strategy combining surface configuration information-based ML with DFT calculations to screen NiCoFe ternary alloy compositions. The framework employed 15 cycles of active learning, evaluating 20 NiCoFe surface configurations per cycle, totaling 300 DFT calculations. To minimize computational cost, we utilized scaling relationships and calculated only *O and *OH adsorption energies as critical OER descriptors. Crucially, the ML featurization incorporated detailed surface configuration information, enabling accurate prediction of catalytic performance in complex alloy systems. This represents a significant advancement over conventional ML approaches that rely solely on bulk atomic properties.
The ML-DFT screening successfully identified $Ni_{5.5}Co_{1.5}Fe_{3.0}$ as the optimal composition from the NiCoFe compositional space. Experimental validation confirmed superior OER performance with a Tafel slope of 39.85 mV dec^{-1}, an overpotential of 361 mV at 10 mA cm^{-2}, and a charge transfer resistance of 51.73 Ω. The optimized catalyst maintained stable operation for ~24 hours at 10 mA cm^{-2} with ~96% Faradaic efficiency, outperforming conventional noble metal-based and binary alloy catalysts.
This study demonstrates that incorporating surface configuration information into ML frameworks enables efficient navigation of complex compositional spaces and accurate prediction of electrocatalytic performance. The hybrid ML-DFT strategy provides a resource-efficient, systematic approach for rational catalyst design that transcends empirical methods. This methodology can be extended to optimize diverse multi-element electrocatalyst systems, advancing sustainable water electrolysis technologies for renewable energy

applications.

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HTE0216

A DFT-Based Active Learning Framework for the Identification of High-Performance Multimetallic Alloys for HER

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Electrochemical

Keywords: Multimetallic Alloys, DFT, Active Learning, HER

Abstract Body.
High-entropy alloys (HEAs) attracted considerable interest in the field of electrocatalysis due to their enhanced electrical conductivity, thermal stability, and abundant unique binding sites. Furthermore, HEAs enable the substitution of noble metals with cost-effective alternatives, which is crucial for large-scale production. However, designing HEAs is challenging due to their vast compositional space, making conventional “trial-and-error” methods impractical and sole reliance on density functional theory (DFT) calculations computationally highly expensive.
To significantly reduce computational costs while maintaining high accuracy, we employed an active learning framework integrated with DFT to identify optimal compositions within the multi-elemental design space for the hydrogen evolution reaction (HER). A Gaussian process regressor (GPR) model was used as a learning agent to predict the adsorption energies for each binding site. In each iteration, the model evaluated the uncertainties of predicted values and selected binding sites for DFT calculations to maximize information gain. The computationally predicted optimal compositions were subsequently synthesized using the carbothermal shock (CTS) method on carbon nanofibers to experimentally validate the design.
The developed scheme successfully identified high-performance catalysts with reduced noble metal content from a vast compositional space. Experimental validation confirmed that the synthesized HEAs exhibited excellent catalytic performance with low overpotentials, aligning well with the model's predictions. This study demonstrates the potential of active learning for time-efficient and cost-effective catalyst design.

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HTE0282

Role of Sr Vacancy in Highly Active and Selective Electrocatalytic Urea Synthesis on Fluorine-Doped SrFeO3-δ

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Electrochemical

Keywords: Urea Synthesis, Perovskite, DFT

Abstract Body.
Electrocatalytic urea synthesis is a sustainable alternative to the energy-intensive Bosch-Meiser process (100-300 bar, >400 ℃). SrFeO3-δ (SF) has shown promise as an electrocatalyst in various fields. However, CO2-induced structural deformation reduces its catalytic activity, limiting its application in urea synthesis. In this study, we present an approach to improve catalytic activity for urea synthesis through an A-site cation (Sr) defect in fluorine-doped SF (A-SFF) since the Sr vacancy modulates the electronic structure, while fluorine could improve the structural stability of SF. Our DFT calculations revealed that Sr vacancy formation at SFF (A-SFF) results in a more favorable reaction energy profile for urea synthesis than SFF. Furthermore, we also confirmed that the Sr vacancy modulates the d-band center and charge transfer based on electronic structure analysis, thereby optimizing interactions between reaction intermediates and the catalytic surface for urea synthesis.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

HTE0307

Controlling carbon properties of carbon-supported platinum catalysts prepared from ion-exchange resins as precursors for electrocatalyst applications

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Electrochemical

Keywords: Carbon supported platinum catalyst, ion-exchange resin, electrocatalyst

Abstract Body.
Polymer electrolyte fuel cells (PEFCs) are devices that convert hydrogen into electrical energy and offer various advantages. However, the carbon-supported platinum catalysts used in PEFCs suffer from low power density and poor durability. For the widespread use of PEFCs, the improvement in their activity and lifetime is essential. Therefore, we focused on a method using ion-exchange resins as precursors for carbon supports to solve this problem. This approach allows for highly dispersed metal nanoparticles within the carbon support, thereby suppressing metal agglomeration due to the weak interaction between carbon and metal. Furthermore, carbonization conditions could control the crystallinity of the carbon. In this study, we investigated the feasibility of applying carbon-supported platinum catalysts using ion exchange resin as precursors of electrocatalysts.
Carbon-supported platinum catalysts from ion-exchange resin (Pt@C) were prepared by loading hexachloroplatinate(IV) ion on weakly basic anion-exchange resins and subsequent carbonization of metal-loaded resin in N2 stream at designated temperatures ranging from 600 to 900 °C. Cyclic voltammetry (CV) were performed using a rotating disk electrode (RDE) to evaluate electrochemical properties.
CV revealed no hydrogen adsorption peak at Pt@C carbonized at 600 °C, whereas peaks appeared at 700 °C and above. The electrochemical surface area (ECSA) determined from the hydrogen adsorption peaks, and ECSA of Pt@C carbonized at 800 °C was largest among those carbonized at 700-900 °C. These results suggest a trade-off between electron conductivity and platinum surface area. Focusing on the physical properties of carbon support, a high-angle shift of C(002) peak was observed by XRD, indicating a decrease in the lattice plane spacing of carbon. Additionally, a decrease in the contact resistance of the catalyst powders was observed alongside the high-angle shift of the carbon peak. This indicated that raising the carbonization temperature enhanced the electronic conductivity of the carbon support. On the other hand, Pt crystallite size remained approximately 2-3 nm despite the high carbonization temperature, as observed by XRD. This result suggested that Pt particles were encapsulated in carbon, which effectively suppressed particle growth. In addition, accessible Pt surface area estimated from CO pulsed chemisorption was reduced at high carbonization temperature although Pt loading was unchanged; thus, this suggests that the larger fraction of Pt surface was covered with carbon.
Consequently, the maximum ECSA observed for Pt@C carbonized at 800 °C was achieved through an optimal balance between improved electronic conductivity of carbon and platinum accessibility.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

HTE0609

Synthesis and Electrochemical Characterization of Nitrogen-Doped Carbon-Supported Pt Catalysts for Enhanced ORR Performance in PEMFCs

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Electrochemical

Keywords: electrocatalysis, heavy-duty PEMFC, catalyst layer optimization

Abstract Body.
Hydrogen-based energy systems represent a promising pathway for reducing emissions in heavy-duty and aerospace transportation. Despite recent advances in proton exchange membrane fuel cell (PEMFC) technology, large-scale deployment remains limited by high catalyst costs, durability issues, and mass transport losses. Improving platinum utilization, oxygen transport, and catalyst layer architecture is therefore essential to achieve performance and cost targets. This work presents a systematic investigation of platinum-based electrocatalysts supported on engineered nitrogen-doped porous carbons, aimed at enhancing activity, stability, and mass transport properties for PEMFC applications.
Nitrogen-doped high-surface-area carbon (HSA–NC) supports were synthesized and functionalized with Pt nanoparticles using hydrothermal and polyol-based routes, followed by thermal reduction to improve crystallinity and metal–support interactions. Catalyst inks were formulated with commercial ionomers, with controlled solvent composition and solid content to optimize electrode microstructure. Electrochemical performance was initially evaluated using rotating-disk electrode measurements to assess intrinsic oxygen reduction reaction (ORR) activity and stability. Subsequently, catalysts were tested in gas diffusion layer-supported half-cells (3 cm2 active area) to provide application-relevant screening. Commercial Pt/C catalysts were used as benchmarks.
Comprehensive ex-situ characterization was conducted to analyze morphology, porosity, surface chemistry, and ionomer–catalyst interactions, enabling correlation between structural features and electrochemical performance.
The synthesized nitrogen-doped carbon supports exhibited high specific surface area and tailored pore size distribution, facilitating improved reactant transport. Nitrogen incorporation modified the electronic and surface properties of the carbon matrix, strengthening metal–support interactions and promoting homogeneous Pt nanoparticle dispersion. This resulted in enhanced resistance to particle agglomeration and degradation. Furthermore, nitrogen functional groups favored uniform ionomer coverage through interactions with sulfonic acid groups, leading to an optimized three-phase boundary and improved proton and oxygen transport.
Compared with non-doped catalysts, the developed materials exhibited higher electrochemically active surface area and increased ORR mass activity. Performance was maintained under accelerated degradation protocols, demonstrating improved durability.
Overall, the proposed catalyst design strategy provides an effective route to enhance PEMFC efficiency and stability while reducing noble metal utilization, contributing to the

development of cost-effective hydrogen-based power systems for heavy-duty and aerospace applications.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

HTE0737

Unveiling the Synergistic Effects in a Bridged CuFe Dual-Atom Catalyst for Electrochemical Nitrate Reduction to Ammonia

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Electrochemical

Keywords: dual atom catalyst, nitrate reduction, synergistic effect, differential electrochemical mass spectroscopy, DEMS, ammonia

Abstract Body.
Electrochemical nitrate reduction reaction (NO3RR) represents a promising strategy for sustainable ammonia production. Achieving high-performance NO3RR requires the rational development of efficient catalysts, together with a detailed understanding of reaction mechanisms and the roles of active metals. However, most previous studies primarily emphasize catalytic performance such as Faradaic efficiency and NH3 yield, while mechanistic insights rely largely on theoretical calculations with limited experimental validation. Herein, a highly efficient bridged CuFe dual-atom catalyst (b-CuFe) is prepared, and its reaction mechanism is systematically elucidated through operando differential electrochemical mass spectrometry (DEMS) combined with density functional theory (DFT) calculations. The b-CuFe catalyst follows two distinct NO3RR pathways: a potential-dependent dominant pathway and a potential-independent minor pathway. DEMS and DFT analyses reveal roles of Cu and Fe, where Cu preferentially facilitates NO3- adsorption and activation to NO2-, while Fe promotes subsequent hydrogenation steps toward NH3 formation. As a result of these synergistic effects between Cu and Fe, b-CuFe exhibits substantially enhanced NO3RR activity compared with Cu and Fe single-atom catalysts. Additionally, b-CuFe was implemented in practical membrane electrode assembly (MEA) system, achieving a current density of 200 mA cm-2 at a low cell voltage of 2.0 V while maintaining 90% Faradaic efficiency for NH3 over 100 h of continuous operation. This work provides direct experimental evidence for synergistic effects of CuFe dual-atom effects in NO3RR, offering insights for the rational design of advanced catalysts for efficient electrochemical NO3RR.

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HTE0738

Architected catalyst layer geometry for decoupling mass transport limitations in electrochemical CO2 reduction

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Electrochemical

Keywords: eCO2RR, Multiphysics modeling, local mass transport, catalyst layer design

Abstract Body.
Electrochemical CO2 reduction (CO2RR) to multi-carbon products like ethylene (C2H4) is a vital pathway for closing the carbon cycle and storing renewable energy. While gas diffusion electrodes (GDEs) in flow-cell configurations enable industrially relevant current densities, optimizing the catalyst layer (CL) microenvironment remains a challenge. In conventional GDEs, the interplay between convective flow and diffusive transport often causes suboptimal reactant distribution. Without geometric optimization, rapid bulk flow dominates local transport, preventing a stable, high-concentration reaction zone. This leads to reactant starvation at active sites, limiting the partial current density an Faradaic efficiency for C2 products.
To quantify these phenomena, we developed a 2D multiphysics model using COMSOL Multiphysics. The framework couples electrochemical kinetics with complex species transport in an alkaline flow-cell with an anion exchange membrane (AEM). The model accounts for the multi-step reduction of CO2 to major C1 and C2+ products, as well as the competing hydrogen evolution reaction (HER). To resolve multi-scale transport, gas transport within porous domains was calculated using a combination of Stefan-Maxwell and Knudsen diffusion, with effective diffusivity corrected via the Bruggeman correlation.
A comparative study was performed between a conventional physically mixed model and a synthesized catalyst model with a controlled porous architecture. Simulation results reveal a fundamental disparity in mass transport dynamics. While the mixed model suffers from CO2 starvation due to bulk flow dominance, the synthesized architecture facilitates a retention and react mechanism. The controlled pore structure creates a stagnant diffusion zone that effectively retains high reactant concentrations, allowing CO2 to accumulate at active sites. This geometric optimization resulted in a predicted 74.4 % improvement in peak ethylene partial current density at 600 mA/cm2. Furthermore, sensitivity analysis showed that increasing porosity from 0.1 to 0.5 enhances effective diffusivity be a factor of 11.2, significantly improving reactant supply.
In conclusion, flow-cell configuration is heavily governed by the electrode's spatial arrangement. By engineering CL geometry, we optimized the local mass transport balance, establishing a vital design principle for next-generation GDEs.

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HTE0748

Intermetallic PtBi for Improved Selective Dihydroxyacetone Production via Electrocatalytic Glycerol Oxidation

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Electrochemical

Keywords: Glycerol oxidation, Electrocatalyst, Intermetallic, Biomass conversion, Dihydroxyacetone

Abstract Body.
Dihydroxyacetone (DHA) is a key platform chemical widely used in cosmetic and pharmaceutical applications. The electrocatalytic glycerol oxidation reaction (EGOR) has emerged as a promising and sustainable approach for DHA production. However, EGOR typically suffers from low DHA selectivity and activity, primarily due to an insufficient understanding of the correlation between catalyst properties and selective DHA formation. Additionally, its practical application is limited by low stability resulting from metal leaching under the acidic conditions required for DHA production. In this study, we introduce intermetallic PtBi catalysts supported on activated carbon (i-PtBi@AC) synthesized via a simple thermal annealing method. The ordered atomic arrangement of the intermetallic structure modulates the electronic environment and enhances catalyst stability, thereby promoting the desired reaction pathway and suppressing overoxidation. As a result, i-PtBi@AC exhibits a high DHA selectivity of 81% at 0.54VRHE, which is 5.4 times higher than that of synthesized Pt@AC, and maintains a high current density, leading to an improved DHA production rate. Furthermore, improved stability is confirmed by the suppression of atomic leaching under acidic conditions. This work demonstrates i-PtBi@AC as an efficient and durable electrocatalyst for EGOR and highlights that reaction selectivity can be effectively tuned through electronic structure modulation. These results provide valuable insights for designing electrocatalysts aimed at the selective upgrading of biomass-derived feedstocks.

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HTE0754

Synthesis and Performance Comparison Analysis of PtNi/C with Metal Oxides electrocatalyst for HOR/HER in AEM-URFCs

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Electrochemical

Keywords: PtNi/C with Metal Oxides electrocatalysts, Hydrogen Oxidation reaction, Hydrogen Evolution Reactions, Bifunctional electrocatalysts, Anion Exchange Membrane Unitized Regenerative Fuel Cells

Abstract Body.
Fossil fuels contribute to climate change by emitting greenhouse gases, causing air and water pollution that harms ecosystems and human health. Anion Exchange Membrane Unitized Regenerative Fuel Cells (AEM-URFC) are one of the best renewable energy sources, as it can store energy and convert energy when needed. The sluggish Hydrogen Oxidation reaction (HOR) is the main drawbacks in the alkaline conditions. In this study, PtNi/C with Metal Oxides electrocatalyst was synthesized through hydrothermal and calcination methods and its performance was evaluated for HOR and hydrogen evolution reactions (HER) in AEM-URFCs. Their crystalline structures, the surface morphology, and the chemical and electronic state of the synthesis catalysts (PtNiCeO2, PtNi-Nb2O5 and PtNi-Ta2O5) were investigated through XRD, XPS, BET, and SEM/EDS analysis. Their electrochemical performance was analyzed through EIS, CV, polarization curve, and individual electrode potentials. The polarization curve of the prepared electrocatalyst also compared to the benchmarked noble catalyst.

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HTE0755

In situ electrochemical regeneration of cathode platinum catalysts for performance recovery in degraded PEM fuel cells

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Electrochemical

Keywords: PEMFCs, accelerated stress test, degradation, recovery, recovery mechanism.

Abstract Body.
Abstract: Reversible and irreversible degradation of electrocatalysts is a key barrier to widespread commercialisation of proton exchange membrane fuel cells (PEMFCs). The recovery of performance decline caused by reversible degradation is a crucial topic to enhance the activity and durability of the catalyst for fuel cell electric vehicles. The reversible performance losses caused by platinum oxide formation, impurity ion adsorption, ionomer dehydration and catalyst layer flooding can be recovered with an effective recovery protocol. This study focuses on the environmentally benign, simple, cost-effective recovery process for degraded fuel cells. A post-treatment recovery method involving acid washing and potential application near SHE is applied following an accelerated stress test without cell disassembly. Performance comparisons elucidate the effectiveness of the recovery protocol, revealing enhanced cell performance accompanied by voltage restoration, increased electrochemical surface area, and reduced charge-transfer resistance. The recovery mechanism is primarily attributed to the removal of Pt oxide species and metal ions from both the catalyst surface and the electrolyte membrane, as confirmed by multiple analyses. The recovery strategies provide a viable framework for restoring the performance of degraded PEMFCs.

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HTE0757

Developing Selective Chlorine Evolution Electrocatalysts via Oxidation-State Engineering of Rutile-Type Anodes: A DFT Study

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Electrochemical

Keywords: Density functional theory, Electrocatalyst, Chlorine evolution reaction, Pourbaix diagram

Abstract Body.

Chlorine (Cl_2) is one of the most important commodity chemicals and is used extensively in the production of chemicals, polymers, and pharmaceuticals. Industrial Cl_2 is predominantly generated via the chlorine evolution reaction (CER) at the anode of chlor–alkali electrolyzers, where high catalytic activity and selectivity are crucial for minimizing energy consumption and operating costs. Rutile-type metal oxides such as IrO_2 and RuO_2 have long served as effective anode catalysts; however, their practical implementation is often limited by insufficient selectivity because the competing oxygen evolution reaction (OER) can proceed under CER-relevant electrochemical conditions. This competition lowers the faradaic efficiency toward Cl_2 and yields mixed Cl_2/O_2 product streams that require additional separation, while also accelerating oxidative degradation of anode materials. Here, we investigate heteroatom incorporation into rutile-type oxides as a strategy to enhance CER selectivity while suppressing OER. Using density functional theory (DFT), we first construct potential- and pH-dependent Pourbaix diagrams to determine the thermodynamically stable surface terminations and oxidation states under relevant electrochemical conditions. On the basis of these environment-consistent surface models, we identify key CER intermediates and evaluate plausible CER pathways by comparing the free-energy changes of the elementary steps.

We find that heteroatom incorporation systematically shifts the preferred surface oxidation state and tunes the binding energetics of critical intermediates, thereby modulating the reaction free-energy landscape to favor CER over OER. Overall, our results highlight that accurately defining catalyst oxidation states and surface terminations under operating conditions is essential for mechanistic interpretation of CER selectivity and provides design principles for developing high-performance CER electrocatalysts.

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HTE0776

Synergy in Fe-SAC/Ni-NP@NC for Electrochemical NH_3 Production via Nitrate Reduction

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Keywords: NO_3^- electroreduction; NH_3 production; Fe-SAC; Ni-NP; Hydrogen spillover.

Introduction. Ammonia is a crucial ingredient in the manufacturing of fertilizers, pharmaceuticals, and dyes. Nitrate ions, one of the most prevalent water pollutants worldwide, have emerged as an appealing N source for electrochemical NH_3 synthesis, which is promising to replace Haber-Bosch process. However, it faces substantial challenges due to the strong competition from the hydrogen evolution reaction and the difficulty of simultaneously optimizing the binding energy of intermediates. Our study focuses on the synergistic effects between Fe-SAC and Ni-NP to enhance the electroreduction of NO_3 to NH_3.Fe-SACs (active sites) and Ni-NPs (promoters) were loaded onto MOFs aiming to maximize the hydrogen spillover effect on Ni sites, while simultaneously maintaining the high efficiency of Fe single atoms.

Methods. We induced Fe and Ni using the two-step wet-impregnation method. By utilizing the special structure of MOF to form ionic coordination between Fe and organic ligands, it further enables the formation of Fe-SACs during the following carbonization process. Meanwhile, due to size limitations and sole solvent, Ni is merely adsorbed on the surface, aggregating to nanoparticles during the subsequent carbonization process.

Results and discussion. The optimized Fe-SAC&Ni-NP electrode achieved a FE of 93% and a $Yield_{NH3}$ of 4.520 mg $h^{-1}cm^{-2}$ at -0.5V and -1V vs. RHE, respectively. Furthermore, enhanced stability was observed the Fe-SAC/Ni-NP@NC electrodes that after conducting 20 cycles of testing at -0.5V vs. RHE, the FENH3 remained stable at 85.9%, while the YieldNH3 was sustained at 1.464 mg $h^{-1}cm^{-2}$. This performance stems from the synergistic electronic modulation between Fe sites and Ni-NPs, the physical shielding effect of Ni-NPs[1], and the shortened Fe-N bond length[2].

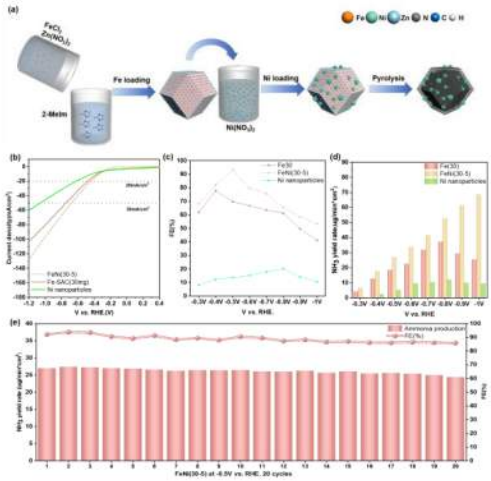

Figure.Synthesis scheme and performance

Acknowledgments

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HMC0197

Molecular Dynamics Simulation of Peptide-Based Cryoprotectant for Enhanced Ice Recrystallization Inhibition Activity

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Abstract Category: Reaction Mechanism and Kinetics - Reaction Mechanism and Kinetics - Computational

Keywords: Cryoprotectants, Molecular Dynamics (MD), Ice Recrystallization Inhibition Activity

Abstract Body.
Cryoprotectants are becoming increasingly important across a wide range of biomedical and biotechnological applications, including organ transplantation, organoid preservation, and oocyte/embryo cryopreservation for infertility treatment. To develop more effective cryoprotectants, it is essential to elucidate their mechanisms at the molecular level—particularly the interfacial phenomena that govern ice recrystallization kinetics—which are often difficult to resolve experimentally. Here, we investigate the molecular mechanism underlying ice recrystallization inhibition (IRI) by a peptide-based cryoprotectant formed by the spontaneous self-assembly of two types of amphiphilic peptides using molecular dynamics (MD) simulations.
To quantify water–peptide interactions near the ice-binding region, we computed hydrogen bond lifetimes and contact durations between water molecules and the ice-binding moieties as molecular-level time-scale descriptors relevant to interfacial water dynamics. The amphiphilic peptide featuring threonine as the ice-binding moiety exhibited longer-lived interactions with surrounding water than the peptide featuring glutamic acid, indicating more persistent hydration dynamics near the threonine-rich surface. To further characterize the local water structure around the hydroxyl groups of the ice-binding moieties, we calculated the averaged local bond order parameter and the tetrahedral order parameter. Both order parameters showed negligible differences between the two peptides. Notably, values were lower than those of bulk water at 250 K, indicating that water molecules in the vicinity of the hydroxyl groups are more disordered than bulk water. these results suggest a possible mechanism for ice recrystallization inhibition (IRI) in which the peptide-based cryoprotectants disrupt the pre-ordering of interfacial water at the boundary between bulk water and the quasi-liquid layer (QLL), thereby hindering ice recrystallization.

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HMC0358

Catalytic Upcycling of Waste Poly(butylene terephthalate): converting non biodegradable plastics into biodegradable ones.

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Homogenous Catalysis

Keywords: Waste plastic upcycling, Homogeneous catalysis, Ir(triNHC), Biodegradable plastic

Abstract Body.

With the increasing amount of discarded plastic waste, it is widely recognized that numerous environmental problems are being exacerbated. Accordingly, significant research efforts have been devoted to the upcycling of waste plastics.

In this study, waste poly(butylene terephthalate) (PBT) was selectively converted into γ-hydroxybutyric acid (GHB) and succinic acid (SA). A kinetic study of the Ir(triNHC) catalyst employed in this process was conducted to determine the reaction orders, providing insight into the roles of the reactants and the catalyst during the reaction. Finally, the synthesized GHB and SA were utilized to prepare biodegradable polymers, namely poly(4-hydroxybutyrate) (P4HB) and poly(butylene succinate-co-terephthalate) (PBST), demonstrating an upcycling strategy from waste plastics to biodegradable polymers.

In conclusion, we developed a novel route for converting waste PBT into biodegradable polymers. Furthermore, a kinetic study of the Ir(triNHC) catalyst revealed distinctive characteristics of the dehydrogenation reaction.

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HMC0375

Catalytic co-upcycling of polylactic acid and polyoxymethylene: Synthesis of 1,3-dioxolan-4-ones

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Homogenous Catalysis

Keywords: waste plastics, PLA upcycling, dioxolanone

Abstract Body.
Recycling or upcycling waste plastics to reduce CO_2 emissions is a major topic in sustainable chemistry. PLA (Polylactic acid), a biodegradable plastic, suffers from difficulties in the degradation process and thermal stability. Herein, we propose a one-pot catalytic co-upcycling strategy of PLA and POM (Polyoxymethylene) to synthesize DOX (1,3-dioxolan-4-one) .

High yields of DOXs were achieved without the use of water-removal devices, in contrast to previously reported methods. Furthermore, various DOX derivatives were successfully obtained in high yields by employing different α-hydroxy acids. The copolymerization of Lactide and DOX afforded a new polymer exhibiting enhanced biodegradability and improved thermal stability compared to PLA, as confirmed by DSC, TGA, and biodegradation tests.

In this work, we developed an efficient strategy to synthesize a new polymer from monomers derived from waste plastics. Not only can DOXs serve as monomers for PHA (Poly α-hydroxy acids) , but they also have potential as green solvents. This study demonstrates that DOXs derived from waste plastics can offer both environmental and economic benefits.

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HMC0468

Esterification of Ammonium formate with Ethanol: Effects of Homogeneous Acid Catalyst and Water Removal

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Homogenous Catalysis

Keywords: esterification, ammonium formate, ethyl formate, acid catalyst, water removal

Abstract Body.
Formic acid has attracted increasing attention as a representative product of CO2 conversion; however, its direct utilization remains limited due to the lack of established downstream conversion pathways. In many CO and CO2 conversion routes, particularly biological processes, formic acid is predominantly produced and handled in the form of formate salts rather than as free formic acid. Therefore, the development of efficient conversion routes for readily available formate species is essential for advancing formic-acid-based chemical platforms. Ethyl formate has recently gained attention as an environmentally favorable solvent and chemical intermediate and is conventionally produced via acid-catalyzed esterification of formic acid and ethanol. In this study, ammonium formate was investigated as an alternative formic acid source for the synthesis of ethyl formate. Unlike conventional esterification systems, this reaction requires in situ generation of formic acid while simultaneously producing water, making reaction conditions critical for efficient ester formation.
Esterification reactions were carried out using ammonium formate and ethanol in the presence of sulfuric acid as a homogeneous acid catalyst under reflux conditions. The effects of sulfuric acid loading relative to ammonium formate, reflux time, reflux temperature, and water removal using a molecular sieve (3A) were investigated. After the reaction, volatile components were separated by reduced-pressure evaporation, and ethyl formate was quantitatively analyzed using gas chromatography (GC).
Reflux time had little effect on ethyl formate formation, whereas reaction temperature and sulfuric acid loading led to noticeable differences. A relatively higher ethyl formate formation was observed at a sulfuric acid loading of 1.1 equivalents relative to ammonium formate. Furthermore, the addition of molecular sieve (3A) increased ethyl formate formation by approximately 12 % under identical conditions. Without 3A, higher temperatures were relatively favorable, whereas the presence of 3A shifted favorable conditions toward lower temperatures, resulting in approximately 18 % higher ethyl formate formation compared to higher-temperature conditions. These results indicate that reaction conditions, together with effective removal of water generated during the reaction, play an important role in shifting the reaction equilibrium toward ethyl formate formation in ammonium-formate-based esterification systems.

Poster Presentation

Hydrogen

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HYP0062

Development of a Microkinetic Model for Photocatalytic Hydrogen Evolution via Methanol Photoreforming and Water Splitting

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Abstract Category: Hydrogen - Hydrogen Production

Keywords: Microkinetics, Photocatalysis, Hydrogen, DFT

Abstract Body.
Photoreforming of organics offers a solar-driven sustainable route to produce hydrogen from organic waste. Mechanistic studies using quantum mechanical methodologies are crucial for interpreting experimental phenomena at the atomic level, elucidating reaction barriers, electronic structure, and adsorption energies. In this work we present a microkinetic model that was developed to describe hydrogen production via methanol photoreforming under UV and visible light [1]. The model combines DFT calculations with experimental data to elucidate the reaction mechanism and simulate hydrogen evolution in a batch reactor over metal-loaded TiO2 catalysts.

DFT calculations were performed using the 5.4.4 version of the Vienna Ab initio Simulation Package (VASP). A microkinetic model was developed to integrate insights from experimental findings and computationally derived rate coefficients, providing a detailed kinetic characterization of the photoreforming mechanism. Each elementary reaction step was assumed to be reversible, with no a priori assumption on the rate determining step.

Methanol shows a moderate barrier for methoxy formation (0.39 eV) and a low barrier for formaldehyde formation (0.16 eV), identifying CH_2O as a key intermediate that enables multiple oxidation pathways. Water contributes through the moderately accessible generation of hydroxyl radicals (0.43 eV), while oxygen radical formation is less favourable (0.66 eV). Radical coupling leads to exothermic formic acid formation, whereas formaldehyde oxidation yields CO and its hydroxylation produces CO_2. The DFT-informed microkinetic model reproduces experimental hydrogen production trends (Figure 1) [2], indicating that CH_2O formation closely follows H_2 evolution and represents the most kinetically favourable oxidation route. Across all investigated metals, O_2 evolution is negligible, and CO/CO_2 production remains minimal. This combined theoretical–experimental approach provides mechanistic insight into the elementary steps governing methanol photoreforming and highlights key intermediates controlling selectivity and efficiency in solar-driven hydrogen production.

Figure 1. H2 production from methanol over metal-loaded anatase. Symbols and dashed

lines represent experimental and simulated hydrogen productions, respectively.

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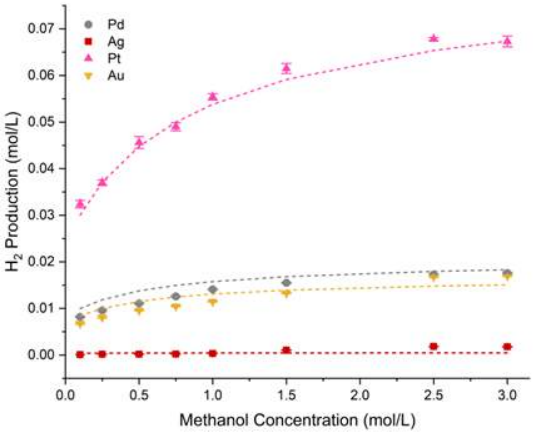

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HYP0168

Low-Loading Platinum Surface Modification of Solid Oxide Cell Electrodes Using Plasma Enhanced Atomic Layer Deposition

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Abstract Category: Hydrogen - Hydrogen Production

Keywords: Plasma-enhanced atomic layer deposition, Solid Oxide Cell, Electrode Engineering

Abstract Body.
Introduction.
Solid oxide cells (SOCs) are promising electrochemical systems for efficient energy conversion and storage due to their fuel flexibility and high efficiency; however, their practical deployment is limited by insufficient performance at intermediate temperatures (500–700 °C) and high electrode costs. To address sluggish fuel electrode kinetics while minimizing noble metal usage, plasma-enhanced atomic layer deposition (PEALD) is employed as an effective atomic-scale surface engineering strategy, enabling conformal catalyst deposition with precise thickness control and high material utilization.
Methods.
Ni–YSZ fuel electrodes were modified by depositing ultrathin Pt catalysts using plasma-enhanced atomic layer deposition with controlled deposition cycles to achieve ultralow Pt loadings. The microstructure and composition were characterized by electron microscopy and spectroscopy techniques, while electrochemical performance was evaluated at 700 °C under fuel cell and electrolysis modes. Density functional theory calculations were conducted to elucidate the catalytic role of Pt at the electrode interface.
Results and discussion.
The PEALD modified Ni–YSZ electrodes exhibited significantly enhanced electrochemical performance in both fuel cell and electrolysis modes, with an optimal Pt loading achieved at 10 deposition cycles, yielding up to an 18–20% improvement compared to bare electrodes at 700 °C. Despite the ultralow Pt loading, the modified electrodes demonstrated excellent durability with negligible performance degradation during extended operation under humidified hydrogen conditions. The improved activity and stability are attributed to the nanoscale dispersion of Pt catalysts and their distinct stabilization behavior on Ni and YSZ phases, which collectively enhance hydrogen reaction kinetics while suppressing catalyst coarsening.

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HYP0209

Synthesis of single atom and atomic cluster catalysts by chemical vapor deposition technique

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Abstract Category: Hydrogen - Hydrogen Production

Keywords: chemical vapor deposition (CVD), single atom catalyst, atomic cluster catalyst, dry reforming of methane

Abstract Body.

Introduction. With the recent increasing concerns regarding climate change, worldwide interest has been focused on the technologies that convert methane (CH4) into valuable compounds such as hydrogen (H2). The dry reforming process is a highly valuable method that utilizes carbon dioxide (CO2) and methane (CH4), two major greenhouse gases, as feedstocks to produce hydrogen(H2) or synthesis gas(H2+CO). This process was initially proposed by J. Lang and others in 1888 and has been under investigation for about 135 years. However, despite extensive research, its widespread commercialization remains elusive due to the issue of catalyst deactivation caused by coking, which occurs simultaneously with the main reaction pathways.

Methods. For the preparation of Ni/Al2O3 catalysts for the dry reforming of methane process, γ-Al2O3 (Sigma Aldrich, BET surface area 162.91 m2/g, 99.5%) was utilized. To achieve this, a chemical vapor deposition (CVD) process was employed, where various nickel precursors, such as nickel(II) bis(2,2,6,6-tetramethyl-3,5-heptanedionate), nickel(II) acetylacetonate, or nickel tetracarbonyl compounds, were vaporized within a vaporization chamber. Nitrogen gas was then employed to transfer the vaporized nickel species to the reactor, ensuring that Ni molecules were deposited onto the surface of the alumina support.

Results and discussion. The Ni/γ-Al2O3 catalyst prepared by CVD method was observed by TEM, which shows that the single-atomic Ni particles are uniformly dispersed on the γ-Al2O3 support. This catalyst exhibited a mass activity (hydrogen yield per catalyst unit mass) at least ten times higher than that of nano-sized Ni catalysts (particle size 2~3 nm) which was prepared by conventional wet impregnation methods. The single-atomic Ni catalyst exhibits long-term stability, retaining more than 90% of its initial activity over 3-day reaction.

Acknowledgments

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ISCRE29 & APCRE11
2026 / SEOUL, KOREA

HYP0239

Bench-Scale Demonstration of Thermocatalytic Methane Pyrolysis over Low-cost SUJ2 Steel Beads with Active-Site Identification

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Abstract Category: Hydrogen - Hydrogen Production

Keywords: Methane pyrolysis; Solid catalyst; Oxidative regeneration; Turquoise hydrogen; scale-up H2 production

Abstract Body.
Introduction. Methane pyrolysis is a feasible route for scale-up hydrogen production, generating solid carbon as a valuable by-product [1]. However, from a commercial perspective, conventional powder catalysts are limited by rapid deactivation, high pressure drop, and poor scalability. To address these operational and economical limitations, this study investigates a bench-scale fixed-bed reactor for methane pyrolysis employing low-cost SUJ2 steel beads as a catalytic medium. Catalytic tests were performed at 800–1000 oC under CH4/N2 atmospheres, examining the effects of temperature, flow rate, and regeneration on methane conversion and stability.
Methods. A fixed bed filled with 0.82 m SUJ2 steel beads were packed into a vertical 1.0 m reactor. Methane pyrolysis was carried out at temperatures of 800–1000 °C, with methane flow rates between 0.1 and 1.0 LPM. The effects of temperature, flow rate, and regeneration cycles on catalytic performance were systematically investigated. Oxidative regeneration was conducted by treating deactivated beads in air at elevated temperature, followed by subsequent pyrolysis. Post-reaction analysis of the beads and recovered carbon was performed using XRD, SEM-EDS, TEM, Raman spectroscopy, TPO, and XPS to correlate surface evolution with catalytic activity.
Results and discussion. For 1st pyrolysis at 1000 oC and 1 LPM flow rates, resulted in the 22.2% methane conversion, whereas after the regeneration in air the ~99% conversion was observed successfully. The enhanced methane conversion is attributed to the surface deformation of SUJ2 and redistribution of the surface metallic species. This allows the increase in the in-situ formation of Fe3C species determined by the DFT studies as an active species for methane adsorption and diffusion. The detailed study of effect of oxidative regeneration on the surface of SUJ2 was established by SEM-EDS, XPS, XRD analysis. Both XPS and XRD of the carbon recovered from the reactor confirmed the existence of Fe3C species as a dominant impurity alongside the Fe0.

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HYP0300

Engineering Advanced BiVO4 Photoanodes for Efficient Photoelectrochemical Water and Ethylene Glycol Oxidation

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Abstract Category: Hydrogen - Hydrogen Production

Keywords: BiVO4 photoanode; photoelectrochemistry; water oxidation; ethylene glycol oxidation

Abstract Body.
Introduction. Bismuth vanadate (BiVO4) is a leading photoanode material for solar-driven water splitting due to its visible-light absorption and stability in alkaline media, though its performance is limited by poor charge transport and slow oxygen evolution kinetics. [1-3] Methods. In this study, we developed advanced BiVO4 photoanodes by integrating a NiO hole transport layer and a FeOOH co-catalyst to enhance charge separation and catalytic efficiency. BiVO4 thin films were synthesized via spin-coating with optimized parameters for nanoporous morphology, high crystallinity, and strong light absorption. NiO layer was deposited by reactive sputtering to improve interfacial charge extraction and provide a stable scaffold for FeOOH, which was electrodeposited to accelerate oxygen evolution. We fabricated four configurations: pristine BiVO4 (BVO), BVO/NiO, BVO/FeOOH, and BVO/NiO/FeOOH and evaluated them by XRD, FESEM, and photoelectrochemical testing under AM 1.5G illumination (100 mW cm-2). PEC measurements were conducted in 1 M KBi buffer for water oxidation and in a mixed electrolyte with 10 vol% ethylene glycols (EG) for organic oxidation. Results and discussion. BVO/FeOOH and BVO/NiO/FeOOH achieved photocurrent densities of ~2.3 and ~1.8 mA cm-2 at 1.23 VRHE for water oxidation, around eightfold and sixfold higher than pristine BVO, confirming improved interfacial charge transport and catalytic performance. For EG oxidation, pristine BVO yielded the highest photocurrent (~3.5 mA cm 2), suggesting possible competing catalytically active sites on unmodified sample. All photoanodes exhibited higher photocurrents for EG oxidation than for water, highlighting the kinetic favorability of organic oxidation. These results emphasize the importance of interfacial engineering and requirement of further detailed surface analysis to attain optimized PEC performance. Building on this platform, the high-performing BVO photoanode was be integrated with a halide perovskite photovoltaic absorber to construct an artificial leaf device for unassisted solar fuel production. This monolithic tandem system is also designed to couple solar energy harvesting with selective oxidation reactions, aiming for high solar-to-fuel conversion efficiency.

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HYP0314

Thermal depolymerization of waste polypropylene: effects of steam and CO2 on producer gas composition and tar reforming

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Abstract Category: Hydrogen - Hydrogen Production

Keywords: CO2, Gasification, Steam, PP, bench-scale fixed-bed system

Abstract Body.
Gasification of waste polypropylene (PP) with various additives was carried out using CO2 as a gasifying agent in a bench-scale fixed-bed gasifier. In the first stage of this study, the gasification performance of PP was evaluated based on syngas production at a specific CO2/C (mole/mole) ratio. The optimal CO2/C ratio was determined based on the H_2 /CO (vol/vol.%) ratio in the syngas, as an H_2 /CO ratio of 2–2.5 is required for the use of syngas as an alternative gaseous fuel in environmentally friendly combustion engine operation. The optimum CO2/C ratio was determined to be 0.3, at which an H2/CO ratio of 2.4 (mole/mole). Although this H2/CO ratio is suitable for downstream applications, the tar concentration remained at 90 mg/Nm³, indicating that additional tar treatment is required. In the second stage, steam-assisted gasification was performed to reform tar and enhance hydrogen production. The S/C (mole/mole) ratio was evaluated based on tar content and H_2 /CO in syngas. In the final stage, a higher operating temperature was applied in the fixed-bed gasifier to assess the overall performance of the bench-scale system. Activated carbon was added in a fixed bed gasifier with mesh 10 for tar cracking and production of hydrogen for all experiments. The CO_2 conversion was calculated over a 120 min experimental period to evaluate the extent of CO_2 consumption during gasification.

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2026 / SEOUL, KOREA

HYP0315

Thermal Depolymerization–Assisted Conversion of Polypropylene Pyrolysis Oil and Biomass toward Hydrogen-Rich, Low-Tar Producer Gas

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Abstract Category: Hydrogen - Hydrogen Production

Keywords: Mixed plastic waste. Thermal reorganization, K2CO3-assisted processing, Hard carbon, Pyrolysis char

Abstract Body.

Upcycling mixed plastic waste into battery-relevant carbon materials is a promising strategy for addressing both plastic pollution and the growing demand for sustainable electrode materials. However, carbon derived from mixed plastics via conventional chemical activation routes is typically optimized for a high specific surface area. This often results in excessive microporosity and surface chemistry that are unfavorable for battery anode applications. Here, we investigated a K2CO3-assisted thermal reorganization approach to convert mixed polyethylene (PE), polypropylene (PP), polystyrene (PS), and polyethylene terephthalate (PET) waste into hard carbon, emphasizing controlled structural evolution rather than aggressive activation. The process consists of sequential thermal treatments under defined temperature regimes. Mixed plastic feedstocks were first pre-carbonized at 500–700 °C to generate a stable carbon precursor framework. The resulting char is subsequently subjected to K2CO3-assisted thermal treatment at 800–900 °C under an inert atmosphere, where alkali-mediated thermal effects are employed to promote carbon framework rearrangement while suppressing excessive pore development. After the removal of residual inorganic species, a final high-temperature re-carbonization step at 1200–1600 °C is applied to stabilize the reorganized carbon structure. This study focuses on elucidating how alkali-assisted thermal processing and high-temperature stabilization influence the structural evolution of mixed-plastic-derived carbon, rather than targeting ultra-high surface areas. Structural characterization was used to track changes in carbon ordering and pore characteristics as a function of the processing conditions. Electrochemical evaluation was conducted in Li-, Na-, and K-ion half-cell configurations to assess the general applicability of the resulting carbons across different alkali-ion storage systems without preselecting a specific battery chemistry. By decoupling carbon framework reorganization from the conventional activation-driven design, this study provides a systematic experimental basis for transforming mixed plastic wastes into hard-carbon-type materials for rechargeable battery applications. Furthermore, the proposed approach enables the identification of the most suitable ion-storage system based on the intrinsic carbon structure.

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HYP0334

Comparative Study on Purification Processes of Carbon from Hydrocarbon Pyrolysis Using a Liquid-Metal Bubble Column Reactor

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Abstract Category: Hydrogen - Hydrogen Production

Keywords: Turquoise hydrogen (H2), Propane pyrolysis, Liquid metal, Carbon byproduct, Purification process

Abstract Body.
Introduction. Turquoise hydrogen production via hydrocarbon pyrolysis has emerged as a next-generation clean hydrogen pathway, enabling simultaneous production of hydrogen and solid carbon without direct CO_2 emissions [1]. Liquid-metal bubble column reactors are particularly advantageous due to their high heat-transfer capability and resistance to carbon fouling (coking). However, the inevitable presence of residual metal on the carbon by-products hinders downstream valorization, thereby necessitating purification for high-value utilization. To address this challenge, we investigate three post-treatment protocols for carbon recovered from liquid-metal based propane pyrolysis.

Methods. Carbon from propane pyrolysis (0.1 LPM, 900 °C) in a liquid-metal bubble column reactor (40 mm i.d. × 1,100 mm height) was purified by (i) water–hexane interfacial separation with ultrasonication/centrifugation (ii) acid leaching (1 M HCl or mixed acids (HCl:HNO3)), and (iii) high-temperature vacuum heat treatment (1200–1400 °C). Morphology, crystallinity, and impurity evolution before and after purification were evaluated using SEM–EDS, TGA, XRD, Raman, XRF, and TEM.

Results and discussion. Following purification, the carbon content increased from 70.9 wt% to as high as 98 wt%. Among the three processes, high-temperature vacuum treatment achieved the highest Sn removal efficiency, effectively eliminating Sn from both external surfaces and interlayer regions, and it also showed potential to induce partial graphitization. Comprehensive structural analyses confirmed that the as-recovered propane-pyrolysis carbon byproduct is primarily turbostratic carbon with characteristics close to carbon black [2]. Consequently, we identify high-temperature vacuum heat treatment as the most effective method to purify and valorize hydrocarbon-pyrolysis carbon by-products, thereby facilitating their downstream utilization.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

HYP0336

Enhancement of Methane Pyrolysis Conversion Using Oxidized Liquid Metals

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Abstract Category: Hydrogen - Hydrogen Production

Keywords: Turquoise hydrogen; Methane pyrolysis; Redox reaction; Liquid metal; Partial Oxidation;

Abstract Body.

Introduction.

Liquid-metal-based methane pyrolysis offers high heat-transfer capability and uniform gas–liquid contacting, effectively mitigating the deactivation issues caused by carbon accumulation on solid catalyst.[1] However, conventional (pure) pyrolysis still suffers from drawbacks such as the need for high reaction temperatures, a substantial external heat-supply burden, and conversion limitations depending on the catalyst and reaction environment. To address these limitations, this study introduces a redox-driven liquid-metal system in which the medium is pre-oxidized with air. By utilizing the liquid metal as an oxygen carrier, this approach aims to lower the energy barrier and significantly enhance methane conversion

Methods.

This study is conducted in a liquid-metal bubble column reactor at 800–1000 °C, employing Sn, Sn–Ni (3 wt.%), and Sn–Ga (3 wt.%) as the liquid-metal compositions. The liquid metal is pre-oxidized with air for 30 min at the same temperature, followed by CH4 injection, and the (i) methane conversion, (ii) hydrogen selectivity, and hydrogen production (yield) are quantitatively compared under each condition. Reactions are carried out at atmospheric

pressure with fixed flow rates of 0.1 LPM for both air and CH4, and the outlet gas composition is analyzed using NDIR to calculate conversion and selectivity. Through this approach, the effects of oxidation pretreatment and alloy composition on reaction performance are systematically evaluated.

Results and discussion.

Under Methane conversion increased under pre-oxidation conditions compared with the non-oxidized liquid-metal case. However, transient increases in CO/CO2 and H2O formation may occur, potentially lowering hydrogen selectivity; therefore, balancing improved conversion with maintained hydrogen selectivity is a key discussion point. Overall, this study compares the effects of oxidation pretreatment and alloy composition on methane conversion and hydrogen productivity, aiming to identify optimal operating conditions that enhance performance while minimizing COx co-production.

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HYP0352

Methane Pyrolysis over Fe-based Catalysts in a Fluidized Bed Reactor: Experimental Evaluation and Predictive Performance Modeling under Variable Operating Conditions

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Abstract Category: Hydrogen - Hydrogen Production

Keywords: hydrogen, catalytic methane pyrolysis, fluidized bed, CNTs, reactor modelling, DoE

Abstract Body.
Introduction. Hydrogen production plays a crucial role in enabling the energy transition. Among emerging technologies, thermal methane decomposition (TMD) has gained increasing attention. In this process, methane is converted into solid carbon and “turquoise hydrogen” [1]. This study investigates catalytic methane cracking as a sustainable route for H2 and carbon nanotubes (CNTs) generation and focuses on both the experimental evaluation and predictive performance modeling of a fluidized-bed reactor (FBR).
Methods. An iron–alumina catalyst with a 40% iron loading and tailored textural properties was synthesized via Wet-Impregnation (WI) synthesis [2]. A comprehensive characterization campaign (H2-TPR, XRD, BET, Raman, FESEM, TEM, EDX) was performed to elucidate structural and morphological features. Time-on-stream and kinetic analyses were carried out in a packed-bed reactor to determine catalyst deactivation and reaction kinetic parameters. Furthermore, a Design of Experiments (DoE) approach was applied in a fluidized-bed reactor to systematically evaluate how combinations of reaction conditions influence the resulting carbon yield. A dynamic MATLAB model of the FBR was then developed.
Results and discussion. Structural characterization (XRD, Raman, TEM) was correlated with catalytic performance. Although reductive pretreatment generates metallic iron, this phase is transient under pyrolysis conditions. Catalytic tests revealed that deactivation is governed by the formation of Fe3C and the progressive encapsulation of active sites. A new deactivation model was developed to describe this decay trend. Fluidized-bed tests were conducted at fixed mass catalyst, total flow rate and under varied temperatures and CH4/H2 concentrations, following a DoE framework (Fig.1). These trials demonstrated that carbon yield reaches a maximum at intermediate temperature and H2 concentrations, indicating that carbon-growth nature strongly influences the extent of deposition. Raman and TEM studies provided further insights into the structural evolution of carbon responsible for this behavior. Overall, the results support the development of an efficient TMD process for low-carbon H2 and CNTs production.

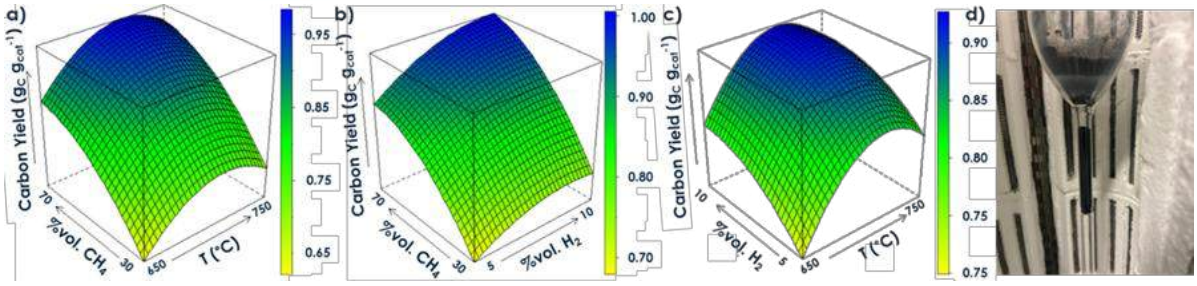

Figure 1 a,b,c) Response surfaces showing the interaction between temperature, methane concentration, and hydrogen concentration derived from the DoE model and d) a picture of the used FBR

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HYP0550

Kinetic Study and Structural Characterization of Covalent Triazine Framework-Based Catalysts for Catalytic Methane Decomposition

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Abstract Category: Hydrogen - Hydrogen Production

Keywords: CTFs, catalytic methane decomposition, turquoise hydrogen, onion shell, kinetics

Abstract Body.
Introduction. Thermo-catalytic methane decomposition (TMD) offers a cleaner alternative in hydrogen and solid carbon co-production without COx formation. Covalent Triazine Frameworks (CTFs) represent a promising class of carbon-based catalysts which ensure structural versatility and high thermal stability[1]. This study examines TMD performance over CTFs catalysts and their role as iron-containing supports for 'turquoise hydrogen' production.
Methods. A CTF catalyst with high specific surface area and intrinsic micro- and mesoporosity was synthesized. The bare sample (CTF) was also used as support for the deposition of iron nanoparticles via Wet Impregnation (CTF-FeWI) and Metal Vapor Synthesis (CTF-FeMVS). A comprehensive characterization campaign (XRD, BET, FESEM, TEM, EDX) was performed to elucidate structural and morphological features. Ramp and kinetic tests were carried out in a packed-bed reactor to determine the catalytic activity and reaction kinetic parameters.
Results and discussion. Results reveal marked differences in Fe nanoparticles (NPs) size and dispersion between the two catalysts, strongly affecting initial activity and deactivation during TMD. In CTF-FeWI, larger Fe-NPs promote partial carburization of active sites, leading to higher reaction rate and the formation of thicker graphitic carbon layers. Conversely, smaller and highly dispersed iron particles in CTF-FeMVS are rapidly encapsulated by carbon, leading to lower initial activity and a deactivation trend characteristic of carbon-based systems (Fig.1a,b), comparable to bare CTF. Kinetic tests indicate that iron impregnation increases the apparent activation energy and pre-exponential factor, consistently with higher density of active sites and a CH4 dissociation-limited mechanism, typical of iron. In contrast, rapid metal encapsulation in CTF-FeMVS (Fig.1c,d) shifts the reaction toward a typical carbon growth-driven mechanism. These results highlight a novel class of carbon-supported catalysts for TMD and H2 production.

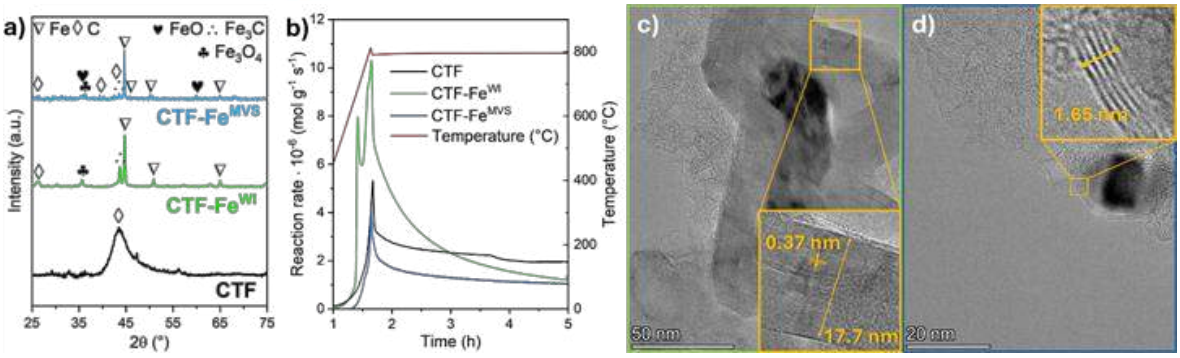

Fig.1 a) XRD of spent catalysts and b) reaction rate profiles; c)-d) TEM images of spent CTF-FeWI and CTF-FeMVS.

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HYP0418

Catalyst Design and Optimization for Methane-to-Hydrogen Conversion Using $FeCo/Al_2O_3$

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Keywords: Hydrogen; Methane Decomposition; Fe-Co Catalyst; Carbon Nano Tubes (CNTs); Density Functional Theory (DFT); Response Surface Methodology (RSM)

Introduction. Catalytic decomposition of methane presents a promising route for producing hydrogen and carbon nanotubes (CNTs). While Fe is the most cost-effective catalyst for this process [1]. Fe in the presence of Co shows the synergistic effect. FeCo supported on alumina demonstrated superior catalytic activity, indicative of the promotional effect of Co on Fe [2]. However, the optimal catalyst composition and reaction conditions for the catalytic decomposition of methane remain unexplored. The aim of this study is to explore the optimum reaction conditions and catalyst composition for maximum methane conversion. The parametric optimization with a less number of experiments was done using Response Surface Methodology (RSM) [3]. The rate-determining step, i.e. disassociation of the first C-H bond of methane was studied by Density Functional Theory (DFT) using Vienna Ab initio Simulation Package (VASP) for catalytic decomposition of methane with different Fe-based bimetallic.

Methods. $FeCo/Al_2O_3$ catalysts were prepared by impregnating porous gamma alumina with nitrate salts of iron and cobalt and reduced *in-situ* during experiments. These catalysts were then evaluated for their methane decomposition activity using a fixed-bed reactor setup.

Results and discussion. This study focused on optimizing maximum CH_4 conversion using an iron-cobalt supported on alumina catalyst ($FeCo/Al_2O_3$). From the DFT, it was found that Fe-Ni can be a better catalyst for this reaction [4, 5]. However, the limitation of stability and early deactivation are concerns for this catalyst. Therefore, Co provided better catalytic stability with Fe [2]. The effects of methane partial pressure (0.4-0.8 atm), reaction temperature (700-800°C), and iron content within the FeCo bimetallic composition (50-100%Fe) were investigated on the methane conversion. The catalysts were synthesized by the wetness impregnation method. A Central Composite Design (CCD) of experiments was employed to guide 20 experiments, assessing the % CH_4 conversion [3]. A quadratic polynomial model was developed using Design Expert software to predict the optimal conditions for methane cracking, maximizing conversion of methane. Response surface methodology was applied to determine the optimum reaction conditions and catalyst composition for achieving the maximum CH_4 conversion percentage. Characterization techniques (XRD, BET, Raman, HRTEM, FESEM-EDX) revealed the formation of various CNT structures under optimal conditions. These findings offer valuable insights for the development of more efficient catalysts for sustainable methane cracking processes to produce hydrogen and CNT.

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HYP0454

Mechanochemically synthesized Ni/Al2O3 catalysts with pore structure modification for catalytic methane decomposition

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Abstract Category: Hydrogen - Hydrogen Production

Keywords: Catalytic methane decomposition, Mechanochemical synthesis, Nickel on alumina, pore structure

Abstract Body.

Introduction.

In recent years, catalytic methane decomposition has emerged as a promising strategy for hydrogen production, offering both zero-CO2-emission operations [1] and economic viability through the synthesis of high-value carbon nanotubes [2]. Since carbon is a primary product of catalytic methane decomposition, its deposition on the catalyst surface inevitably results in a loss of catalytic activity over time. Consequently, a regeneration process to separate the catalyst from the carbon is essential. However, in cases of tip-growth mechanisms, carbon removal directly leads to the loss of active metals. Therefore, it is crucial to induce base-growth carbon formation on the catalyst surface. Enhancing the metal-support interaction (MSI) is critical for promoting the base-growth mechanism, as it ensures that the active metals remain firmly anchored to the support during carbon formation [3]. In this study, Ni/Al2O3 catalysts with enhanced metal-support interactions were synthesized via a mechanochemical one-pot method and applied catalytic methane decomposition.

Methods.

Ni/Al2O3 catalysts were synthesized following the procedure described in previous work [4]. The H2O/AlP ratio, calcination temperature was adjusted to optimize the pore structure, metal-support interaction, and Ni particle size. Catalytic methane decomposition was carried out in a 1/4-inch fixed-bed reactor. Catalytic methane decomposition was evaluated at 550 ℃ following in-situ reduction, with 50 % CH4/N2 gas supplied at a gas hourly space velocity (GHSV) of 12,000 mL gcat-1·h-1 [5].

Results and discussion.

The pore size distribution of one-pot synthesized Ni/Al2O3 catalyst varies with H2O/AlP ratio. This variation in pore size not only affects the support structure but also influences the chemical states of Ni. Pore size variation demonstrates comparable effects on catalyst activity and stability. Initially, negligible activity differences were observed among catalysts, however, the catalyst with larger pores exhibited a markedly slower decline in CH4 conversion and H2 yield as the reaction proceeded.

Acknowledgments

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ISCRE29 & APCRE11
2026 / SEOUL, KOREA

HYP0456

Microwave-induced Ni exsolution on MgO for carbon nanotube growth via methane pyrolysis

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Abstract Category: Hydrogen - Hydrogen Production

Keywords: Methane pyrolysis, Hydrogen, Carbon nanotube, Exsolution, Microwave

Abstract Body.

Introduction.

Methane pyrolysis is a CO2-free pathway for hydrogen production that directly decomposes methane into hydrogen and solid carbon. When oxide-supported metal catalysts are used, carbon nanotubes (CNTs) can be simultaneously produced, offsetting hydrogen production costs. In particular, CNT formation predominantly occurs when metallic Ni particle sizes are in the range of 7–40 nm [1, 2]. Nonetheless, catalyst activation under thermal reduction conditions often induces metal agglomeration, leading to reduced CNT yield and quality. Microwave (MW)-induced exsolution is explored in this study to control Ni particle size. This strategy has been reported to promote oxygen vacancy formation and lower reduction temperature in perovskite oxides, enabling exsolution under milder conditions and potentially mitigating metal agglomeration [3]. While MgO is widely used as a commercial support due to its low cost and high thermal stability, controlled exsolution on this simple oxide remains challenging. Therefore, this work evaluates CNT production during methane pyrolysis over Ni/MgO catalysts activated by MW exsolution.

Methods.

MW exsolution was performed in a MW cavity resonator operating in the TE111 mode at ~2.45 GHz under a 4% H2/N2 atmosphere. Sample temperature and outlet gas were monitored by IR pyrometers and mass spectrometer (HPR-20, Hiden Analytical), respectively.

Results and discussion.

Uniformly distributed Ni particles (5–20 nm) were exsolved on MgO under MW irradiation, as shown in Figure 1. The MW-exsolved Ni/MgO exhibited higher activity in methane pyrolysis than thermally exsolved case. Highly crystalline carbon structures were identified by Raman spectroscopy, and CNT structures were directly confirmed by SEM. These results indicate that MW exsolution effectively promotes CNT growth by controlling Ni particle size.

Acknowledgments

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ISCRE29 & APCRE11
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HYP0461

Synergistic Effects of Ce and Zr Incorporation in CaNiO3-Based Catalysts for Enhanced Activity and Stability in Methane Dry Reforming

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Dry reforming, Mixed Ni oxide, Ce-Zr co-introduction, High activity & durability

Abstract Body.

Introduction

The utilization of CO2 and CH4 as feedstocks for the production of value-added chemicals has attracted considerable attention as an approach to simultaneously mitigate greenhouse gas emissions and enhance carbon resource efficiency. Among the available routes, dry reforming of methane (DRM) offers a direct pathway to convert CO2 and CH4 into synthesis gas with a near-unity H2/CO ratio, which is suitable for various downstream chemical processes.

However, the DRM reaction is thermodynamically demanding, requiring elevated temperatures that often result in rapid catalyst deactivation due to carbon accumulation and metal particle agglomeration [1]. Although Ni-based catalysts are commonly employed because of their favorable activity and economic advantages, their susceptibility to coke formation remains a critical challenge. To address this issue, numerous strategies have been explored, including tuning support composition, introducing promoters, and reinforcing metal–support interactions, particularly through oxide supports exhibiting enhanced basicity and oxygen transport capability [2].

Methods

The Ce-Zr co-doped mixed oxide Ni catalyst was synthesized via a citric acid-assisted Sol-Gel method using metal nitrate precursors dissolved in deionized water. After gelation and drying 180oC, the obtained powder was calcined in air at 800oC. Catalytic test was performed with 0.1g of catalyst, followed by DRM at 800 oC using a CH4/CO2/N2(47.5/47.5/5) feed stream.

Results and discussion

In this work, Ce and Zr were simultaneously incorporated into a CaNiO3-based catalyst to enhance catalytic activity and extend catalyst lifetime for the dry reforming of methane. The introduction of Ce and Zr was intended to improve oxygen mobility, strengthen metal–support interactions, and suppress carbon deposition under harsh DRM conditions. The structural properties and catalytic performance of the modified catalysts were systematically investigated to elucidate the synergistic effects of dual Ce and Zr incorporation on activity and stability.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

HYP0489

Kinetic Analysis and Catalytic Effects of Methane Pyrolysis on Sn-based Binary Molten Metal Catalysts

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Abstract Category: Hydrogen - Hydrogen Production

Keywords: Methane pyrolysis, Turquoise hydrogen, Molten metal catalyst, Reaction kinetics, Binary alloy

Abstract Body.
Introduction.
Methane pyrolysis offers a CO2-free route for hydrogen production, fundamentally differing from gray and blue hydrogen pathways [1]. Molten metal catalysts further enhance this process by enabling spontaneous carbon separation and suppressing reactor fouling [2]. In this study, Sn-based binary alloys are systematically compared to quantify kinetic parameters, including apparent activation energy (Ea) and pre-exponential factors (A), and to elucidate the origins of catalytic enhancement.
Methods.
In this study, pure Sn and binary alloys of Sn-Ga (9:1), Sn-Ni (95:5), Sn-Mg (95:5) were tested in a bubble column reactor between 800 and 1000 ℃. Methane was injected through a nozzle, and effluent gases were analyzed via NDIR spectroscopy. Nitrogen (N2) was utilized as an inert internal standard to correct for total molar changes due to the pyrolysis reaction, ensuring accurate calculation of conversion rates. Based on the experimental data, Arrhenius plots were constructed to derive the kinetic parameters for each alloy system.
Results and discussion.
Kinetic analysis revealed that the introduction of binary alloying elements significantly reduced the apparent activation energy relative to pure Sn. Most notably, the Sn-Ga (9:1) alloy exhibited the lowest Ea of 98.48 kJ/mol, compared to 125.74 kJ/mol for Sn-Ni (95:5) and 125.69 kJ/mol for Sn-Mg (95:5). This superior performance of Sn-Ga is attributed to Ga-induced changes in gas-liquid interfacial properties (e.g., surface tension and wetting), which effectively lowers the apparent kinetic barrier [3].
These results explicitly confirmed that the selected alloying elements enhance reactivity by reducing the energy barrier. Thus, this work elucidates the intrinsic catalytic activity through kinetic analysis, surpassing the limitations of simple comparisons based on apparent conversion.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

HYP0628

Enhance Hydrogen Production via steam methane reforming in a Membrane Reformer: Effect of the key process parameter

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Abstract Category: Hydrogen - Hydrogen Production

Keywords: Membrane Reformer; Membrane Separation; Steam Methane Reforming; Annealing; PEM fuel cell

Abstract Body.

Introduction.

Hydrogen production created a new energy vector for mobile and stationary energy sources. However, hydrogen enters the economy only when used safely. The safe storage and transportation of hydrogen is a 'holly-grail' of the whole hydrogen-based economy. . The on-demand and on-site production of the hydrogen production can solve this problem. Hydrogen is produced in large quantities by conversion processes, such as methane steam reforming, autothermal reforming (ATR), and partial oxidation (POx). Among them, methane steam reforming is widely used industrially because it provides the highest hydrogen yield and cost of hydrogen produced is less than $2.The current work proposes a membrane reformer (MR) technology, which have a potential to produce on-site and on-demand ultra-pure hydrogen by using methane as a feed. Ni/Al2O3 catalyst is used for methane steam reforming reaction and Pd-Ag membranes are used for hydrogen separation. Both membrane and catalyst is packed in the same column in a shell and tube heat exchanger assembly. The effect of temperature, pressure, steam to methane ratio and inlet flowrate on the performance of MR is studied in terms of methane conversion, hydrogen flux and hydrogen recovery.

Methods.

A Nickel nitrate hexahydrate was used as the nickel precursor. γ-Al_2O_3 was employed as the catalyst support due to its high surface area and thermal stability. The catalyst was prepared by wet impregnation. A membrane was prepared using Electroless Pore-Plating (ELP-PP), Pd-Ag on an α-Al2O3 tube [2].

Results and discussion.

The experiment was performed at different flow rates, temperatures, and pressures, with the catalyst at 500-700 °C and a pressure range of 0.5-4 bar. The inlet flow rate of methane varied from 200 ml.min-1 to 700 ml.min-1. The steam-to-methane ratio was varied from 1:2 to 1:4 to assess methane conversion as a function of the steam-to-methane ratio. The higher the methane conversion was. The membrane reformer was used to test the membrane at different pressures by varying the pressure while maintaining a constant temperature, to observe the effect on membrane performance, resulting in hydrogen purity > 99.5%. High permeation flux was obtained. Membrane testing was performed for 100 h, and the membrane remained stable for the duration.

Acknowledgments

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2026 / SEOUL, KOREA

HYP0637

Methane pyrolysis and C-valorization in steelmaking sector: a multi-scale investigation over Fe-based catalyst

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Abstract Category: Hydrogen - Hydrogen Production

Keywords: COx-free hydrogen, CH4 pyrolysis, iron catalyst, scale-up, steelmaking

Abstract Body.

Introduction. Catalytic Methane Pyrolysis (CH4 = 2H2+C(s), DH°=75 kJ/mol) is emerging as viable strategy to produce COx-free hydrogen along with solid carbon. In this work, Fe-Al2O3 catalysts were prepared and tested for CH4 pyrolysis in different reactor configurations to guide process optimization. Integrated solid characterization was used to elucidate mechanisms governing C-growth, with emphasis on spent properties to assess its potential valorization in steelmaking as reducing agent for waste-iron recovery.

Methods. Fe-Al2O3 (5-100wt.%Fe) catalysts were prepared by fusion-decomposition method from nitrate salts. Pyrolysis reaction was conducted in thermogravimetric balance (TG, 0.004g), packed (PBR, 0.75g) and fluidized (FBR, 3.5g) bed reactors, at varying temperature, feed composition, spatial velocity. Fresh, reduced, spent catalysts were characterized (e.g. BET, XRD, SEM, TEM, Raman, TPO). The reduction potential of spent-catalyst was also assessed via carbothermal conversion of FexOy into Fe0, using waste mill-scale as Fe-bearing feedstock [1] (FexOy+yC(s) = xFe0+yCO(g)). For this purpose, spent-catalyst and mill-scale were pelletized together and heated up to 1500 °C (100vol.%Ar).

Results and discussion. Thermogravimetric analyses identified the equimolar Fe-Al2O3 (52wt.%Fe) the best formulation in terms of activity and C-accumulation capacity. This catalyst was further tested in PBR, showing a rapid decrease in CH4 conversion at increasing CH4 feed (10-95vol.%) and temperature (725-850 °C) due to formation of encapsulating-C. Stable operations were demonstrated by reducing the GHSV to 1 NL/h/gcat at 750 °C, achieving the highest C-load of 5 gC/gcat. A dynamic reactor model was developed in order to predict C and H2 productivity in a wide operating range. Afterwards, CH4 pyrolysis was investigated in FBR, which allows to overcome PBR clogging problems through stable bubbling fluidization regime, thereby enabling longer experiments, spent discharge and post-characterization. The formation of highly ordered and pure MWCNTs (IG/ID>2) was observed, leading to a growth in particle size (100-400 μm), and reduced density (700-35 kg/m3). Such spent-materials also exhibited promising reduction degree (>80%) and iron recovery ratio when tested in the carbothermic smelting processes of mill-scale above 1375 °C.
These findings highlight the quality of Fe-Al2O3 catalysts, combining high H2 productivity and C-load essential for process commercialization [2]. They also produce valuable Fe-C hybrid materials, which can theoretically replace iron ore and anthracite in steel manufacturing, opening to the potential synergy between hydrocarbon pyrolysis and

steelmaking. Furthermore, the integration of bio-streams as feedstocks would further enhance these advantages by producing COx-negative H2 and increasing the market value of carbon.

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HYP0679

Enhanced Visible-Light-Driven Hydrogen Production over CuLi1/3Ti2/3O2 / Li4Ti5O12 / TiO2

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Abstract Category: Hydrogen - Hydrogen Production

Keywords: Photocatalysis, Hydrogen production, Heterojunction, Visible-light-driven, Charge separation

Abstract Body.
Introduction. Visible-light-driven hydrogen evolution is vital for sustainable energy. CuLi1/3Ti2/3O2 (CLTO) is a promising narrow-bandgap (~2.1 eV) photocatalyst active up to 600 nm [1, 2]. However, rapid charge recombination limits its efficiency. The purpose of this study is to construct ternary heterojunctions with chemically stable Li4Ti5O12 (LTO) and TiO2 to overcome this limitation, focusing on the optimization of lithium and titanium stoichiometry.
Methods. The composites were synthesized via a conventional solid-state reaction method by varying the excess amounts of Li2CO3 and TiO2 precursors. The structural, morphological, and optical properties of the obtained powders were characterized by XRD, FESEM, FTIR, and UV-Vis diffuse reflectance spectroscopy. Photocatalytic hydrogen evolution was evaluated using sulfide/sulfite sacrificial agents and a Ru cocatalyst under visible light.
Results and discussion. XRD and FESEM confirmed the formation of agglomerated ternary composites with an optical band gap of ~2.1 eV. Crucially, the optimized composite (with 15% excess Li2CO3 and 5% excess TiO2) achieved a high hydrogen evolution rate of 1,045 μmol·g-1·h-1, significantly outperforming pristine phases [1]. This enhancement is attributed to the in-situ formation of a CLTO/LTO/TiO2 heterojunction. A cascading energy alignment promotes spatial charge separation, effectively suppressing recombination.
Conclusions. This work demonstrates that controlling Li/Ti stoichiometry is an effective strategy to engineer CLTO-based heterojunctions. The optimized CLTO/LTO/TiO2 composite exhibits superior photocatalytic performance, offering a promising pathway for efficient solar hydrogen production.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

HYP0713

Enhanced Photocatalytic Hydrogen Production via Interfacial Charge Transfer in Graphene Quantum Dot-Modified K4Nb6O17 Nanocomposites

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Abstract Category: Hydrogen - Hydrogen Production

Keywords: Photocatalytic Hydrogen Evolution, Potassium Niobate, Graphene Quantum Dots, Interfacial Engineering

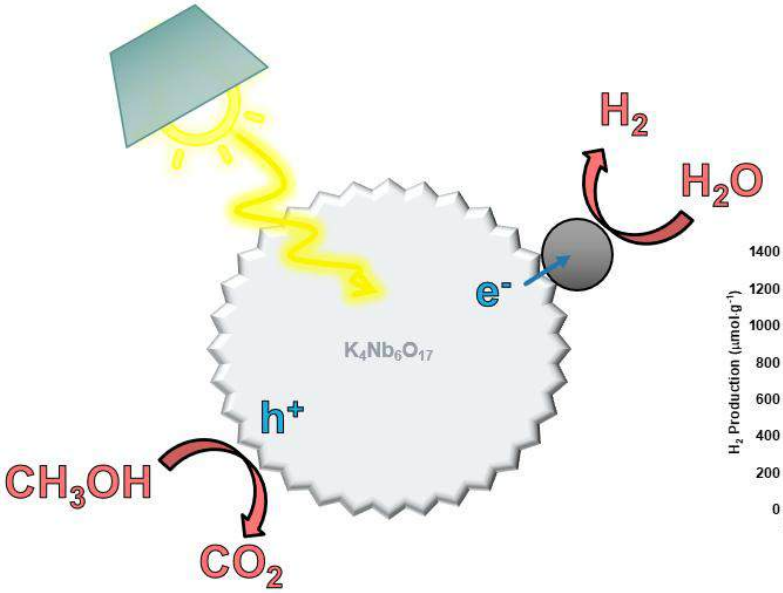
Abstract Body.

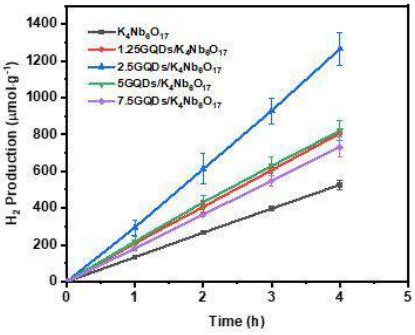
Photocatalytic hydrogen production is a promising strategy for sustainable solar-to-fuel conversion; however, the efficiency of layered potassium niobate (K4Nb6O17) is significantly limited by rapid charge carrier recombination and restricted light utilization. This study aims to overcome these kinetic limitations by integrating graphene quantum dots (GQDs) onto the K4Nb6O17 surface to serve as efficient interfacial electron acceptors and improve overall photocatalytic performance.

A series of GQD-modified K4Nb6O17 were synthesized via a hydrothermal method with controlled GQD loadings (1.25, 2.5, 5.0, and 7.5 wt%). The structural, morphological, and electronic properties of the synthesized materials were comprehensively characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM), Transmission electron microscopy (TEM), high-resolution X-ray photoelectron spectroscopy (XPS), and UV-Vis diffuse reflectance spectroscopy (DRS). Photocatalytic activity was evaluated by measuring hydrogen evolution rates under simulated solar irradiation.

Characterization results confirmed the uniform anchoring of GQDs on the K4Nb6O17 host without perturbing its crystalline framework. The photocatalytic activity exhibited a volcano-type dependence on GQDs loading, with the optimal 2.5 wt% composite achieving a maximum hydrogen evolution rate of 243.3 μmolg-1h-1, representing a 1.86-fold enhancement compared to pristine K4Nb6O17. Although the optical band gap remained unchanged at ~3.6 eV, XPS analysis revealed a negative shift in Nb 3d binding energies, indicating the formation of a built-in electric field that promotes directional electron transfer from the niobate to the GQDs.

This study demonstrates that the enhanced photocatalytic activity originates from efficient interfacial charge separation driven by the built-in electric field, rather than band gap engineering. The findings highlight the critical role of GQDs in suppressing electron-hole recombination and provide a robust strategy for interface-driven performance optimization in wide-bandgap photocatalysts for sustainable energy applications.


H2
H2O
e-
K4Nb6O17
h+
CH3OH
CO2


K4Nb6O17
1.25GQDs/K4Nb6O17
2.5GQDs/K4Nb6O17
5GQDs/K4Nb6O17
7.5GQDs/K4Nb6O17
H2 Production (μmol g-1)
Time (h)
0
200
400
600
800
1000
1200
1400
0
1
2
3
4
5

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

HYP0727

Enabling Visible-Light-Driven Overall Water Splitting through Cocatalyst-Assisted Kinetics and Optical Concentration

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Abstract Category: Hydrogen - Hydrogen Production

Keywords: Overall water splitting, Visible-light photocatalysis, Cocatalyst engineering, CdS nanoplatelets

Abstract Body.
Introduction. Electrochemical water splitting has been extensively studied and is widely regarded as the most technologically mature route toward hydrogen production. However, achieving long-term carbon neutrality ultimately requires direct solar-driven water splitting without external electrical inputs. In this context, photocatalytic overall water splitting (OWS) offers a compelling pathway, yet studies on visible-light-driven OWS remain exceptionally rare. Thermodynamically, a semiconductor with a bandgap exceeding 1.24 eV is sufficient to drive water splitting; however, practical demonstrations of OWS have been predominantly limited to wide-bandgap (>3.0 eV) ultraviolet-responsive materials. This apparent discrepancy arises primarily from kinetic limitations in charge transfer, particularly the sluggish oxygen evolution reaction (OER), which severely suppresses overall reaction rates under visible-light excitation. In wide-bandgap photocatalysts, large energetic offsets between band-edge positions and water redox potentials are introduced to compensate for these kinetic deficiencies, thereby enabling OWS. However, this strategy inherently confines solar utilization to the ultraviolet region, imposing a fundamental limitation on achievable efficiency. Consequently, realizing OWS under visible-light irradiation requires new approaches that can overcome kinetic bottlenecks.
Methods. CdS nanoplatelets were employed as a visible-light-responsive photocatalyst, and both hydrogen evolution reaction (HER) and OER cocatalysts were introduced to construct a kinetically optimized material. Building upon this material, optical concentration was employed as a central strategy to increase the charge supply rate. Photocatalytic performance was evaluated under scavenger-assisted conditions, where OER kinetic barriers are effectively removed, and under pure water conditions, where OER kinetics dominate.
Results and discussion. Dual-cocatalyst configuration enables simultaneous acceleration of reduction and oxidation reactions. Optical concentration was allowing kinetic barriers—unattainable under one-sun illumination—to be systematically overcome. To elucidate the kinetic origin of visible-light-driven OWS, photocatalytic performance was compared under scavenger-assisted conditions, where OER kinetic barriers are effectively removed, and pure water conditions, where OER kinetics dominate, as a function of optical concentration. The stark contrast between the near-linear or saturated response observed under scavenger-assisted conditions and the super-linear enhancement of overall water splitting under

concentrated illumination directly demonstrates that overcoming sluggish OER kinetics is the decisive factor for enabling visible-light-driven OWS.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

HYP0739

Process Design of Ammonia-Natural Gas Dual-Fuel Fuel Cell Systems for DC Power Demand

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Abstract Category: Hydrogen - Hydrogen Production

Keywords: Solid Oxide Fuel Cell, Ammonia, Hydrogen, Fuel flexibility

Abstract Body.
As the demand for direct current (DC) power scales rapidly due to the expansion of AI and data centers, there is a critical need for stable, low-carbon distributed power sources. This study proposes a process design for a high-efficiency fuel cell system utilizing a composite composition of ammonia (NH3) and natural gas (NG) as a bridge technology toward a carbon-neutral economy.
To achieve this, a dual-fuel power generation system process was designed by integrating a Solid Oxide Fuel Cell (SOFC) stack, a fuel processor, and optimized heat exchangers. Recognizing that NG-based SOFC systems are already established as commercial products, this study utilizes the existing commercial system design as a baseline, modyfing the Balance-of-Plant (BOP) and stack configuration to support the transition to the NH3-NG dual fuel.
To explore the operational feasibility of this dual-fuel system, Aspen Plus simulation is employed to model the integrated system, including a fuel processor and a high-temperature SOFC stack. A sensitivity study regarding the reactant composition ratio have been conducted, accounting for the different reforming reactions and steam requirements of the dual-fuel conditions. Operational scenarios are developed based on these reaction characteristics to minimize thermal loss between components, particularly through heat and mass analysis results. This process ensures high energy efficiency and carbon reduction, providing a strategic technical solution that can be utilized before clean ammonia achieves full price competitiveness in the global market.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

HYP0750

Cathode Ionomer Optimisation for Anion Exchange Membrane Electrolysers Operating at Low Electrolyte Concentrations.

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Abstract Category: Hydrogen - Hydrogen Production

Keywords: Anion Exchange Membrane (AEM), Oxygen Evolution reaction, Hydrogen Evolution reaction, Ionomer, Electrochemical characterization

Abstract Body.

Introduction:

Anion exchange membrane electrolysers (AEMWEs) offer a promising pathway towards cost-effective hydrogen production. AEMWEs have some inherent properties which still requires development,. Here in, we are working on optimizing interface between AEM and cathode electrode at low electrolyte concentrations, by varying the Ionomer to carbon ratio in the cathode electrode ink. Different electrochemical characterization techniques are used to evaluate the performance such as Linear sweep voltammetry, Electrochemical Impedance spectroscopy and Distribution of Relaxation times.

Methods:

Three different catalyst inks were prepared with Ionomer to carbonE ratios, 0.3, 0.5, 0.7, using Pt/Vulcan carbon (Tanaka-TEC10V50E) as catalyst and PiperION®, 20 wt% Ionomer dispersion. The catalyst and ionomer solution are dispersed in solvents (Water:Isopropanol) to make a 1 wt% solid ink solution. To prepare the catalyst layer, the catalyst ink is spray coated directly onto the Porous Transport Layer (PTL) with loading of 0.45± 0.02 mgPt cm-2. Spray coating is done at a temperature of 55-60 °C. This process is repeated until the required loading is reached. The electrodes are then assembled together with membrane and anode and made a single cell. These single cells are tested to obtain polarization curves, Impedance plots. DRT analysis is done for fitting impedance data.

Results and discussion.

It is observed from the polarization curves that as we increase the ionomer content, the electrochemical performance of the cell is decreasing. This trend can also be proved from impedance analysis. EIS spectra show that the high frequency resistance increases with increase in ionomer to carbon ratio[2]. Furthermore, there is a reduction in size of the semicircular arcs of I/C = 0.3 as compared to 0.5 and 0.7 and relatively no change in between 0.5 and 0.7.

Future work includes to test the Ionomer to carbon ratio of 0.1 and without ionomer in the electrode to obtain a benchmark. Additionally to test the durability of these electrodes.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

HYP0758

Elucidating the Active Sites in Iron Ores for Catalytic Methane Decomposition

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Abstract Category: Hydrogen - Hydrogen Production

Keywords: Methane pyrolysis, Hydrogen, Fe-based catalyst, Iron ore catalyst

Abstract Body.
Introduction. Catalytic methane decomposition (CMD) is an environmental process that produces hydrogen and solid carbon without CO2 emissions [1]. Natural iron ores are cost-effective catalysts that offer a practical integration with iron-making processes, where the produced hydrogen can serve as a clean reducing agent [2]. This study investigates the catalytic activity of natural iron ores for CMD and aims to identify the nature of the active sites in iron-based catalysts during the reaction. By analyzing the phase transformation of the ore, the role of evolved iron species in methane decomposition is identified to optimize the integrated process.
Methods. CMD experiments were performed in a fixed-bed reactor at 900 °C using Goethite, Hematite, and Marra Mamba iron ores. The CH4 conversion and H2 yield were monitored to evaluate the catalytic performance. The structural evolution of the crystalline phases was analyzed via X-ray diffraction (XRD) at different reaction stages. Carbon properties were investigated using TGA, TEM, and Raman spectroscopy to correlate the state of the iron catalyst with carbon growth
Results and discussion. The iron ore catalysts exhibited distinct catalytic behaviors depending on the pre-treatment conditions. Without pre-reduction, an induction period was observed, during which the formation of iron carbide (FexC) appeared to trigger increase activity. In contrast, pre-reduced catalysts showed high initial methane conversion due to the presence of metallic iron (Fe0) as the active sites, however suffered from rapid deactivation. XRD analysis confirmed the correlation between these iron phases and their respective catalytic stability. Furthermore, TGA, TEM, and Raman analyses revealed that the crystallinity and morphology of the produced carbon were significantly influenced by the specific mineral composition of the iron ore. These results provide critical insights into selecting the optimal active phase for stable hydrogen and carbon production.

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2026 / SEOUL, KOREA

HYS0072

Kinetic Modeling of the Reversible Formate/Bicarbonate System for Hydrogen Storage over Pd-based Catalysts

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Abstract Category: Hydrogen - Hydrogen Storage (LOHC, NH3, MeOH etc)

Keywords: Hydrogen storage, Kinetic modeling, Heterogeneous catalysis, Formate/bicarbonate system, Pd-based catalysts

Abstract Body.

Purpose

The formate/bicarbonate system is a promising liquid organic hydrogen carrier (LOHC) for reversible hydrogen storage under mild and intrinsically safe conditions. While some experimental studies have demonstrated its potential, the absence of robust kinetic models still limits process design and scale-up. This work aims to develop a comprehensive kinetic model capable of describing both hydrogen release from aqueous formate mixtures and hydrogen storage via bicarbonate hydrogenation. Particular attention is devoted to the role of catalyst load and operating conditions (temperature, pressure, concentration) in view of process engineering and reactor design.

Methods

Kinetic experiments were conducted using a Pd-based heterogeneous catalyst supported on TiO_2 , adopting nanopowder and micropowder formulations. Both formate dehydrogenation and bicarbonate hydrogenation were studied over a range of temperatures, pressures, and reactant concentrations relevant to practical operation.

Mechanistic kinetic models were developed within a heterogeneous catalysis framework, considering different reaction pathways and adsorption mechanisms, including Langmuir–Hinshelwood and Eley–Rideal formulations with associative and dissociative hydrogen adsorption. Model parameters were estimated by nonlinear regression of experimental data. Model discrimination and validation were performed using statistical indicators such as the residual sum of squares, confidence intervals of fitted parameters, and Fisher's F-test to assess the significance of model improvements.

Results

The proposed kinetic models accurately describe both hydrogen release and uptake within the formate/bicarbonate cycle, capturing the influence of operating conditions and catalyst load on reaction rates. The comparison between nano- and micro-sized Pd-based catalysts supported on TiO_2 catalysts highlights marked differences in apparent kinetics. Models explicitly accounting for surface adsorption phenomena provide a superior fit to experimental data, particularly for hydrogen-involved elementary steps, confirming the key role of surface coverage in governing the overall reaction rates.

Conclusions

A unified kinetic framework for the reversible formate/bicarbonate cycle for hydrogen storage system has been developed and validated. The model provides a valuable tool for process engineering, reactor design, and optimization of hydrogen storage and release systems

based on aqueous formates mixtures.

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HYS0100

Simulation-guided design of a 3D printed vapor-liquid separator with integrated heat exchange for CO2-to-Methanol synthesis

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Abstract Category: Hydrogen - Hydrogen Storage (LOHC, NH3, MeOH etc)

Keywords: Additive Manufacturing, CFD, Phase separation, Heat exchange, CO2-Hydrogenation

Abstract Body.
Methanol is expected to play an important role in the long-term storage and long-distance transportation of renewable energy. Its synthesis can be carried out with CO2 as the main carbon source; however, higher levels of CO2 decrease the equilibrium conversion compared to CO-rich feeds. Product separation after the reactor can be used in combination with either multiple reactor stages or recycling flows to improve the process economics. The key for an efficient process lies in reheating the unreacted gas phase after the condensation of liquid products to allow reignition of the reaction after separation. Thus, heat management becomes crucial.
In this work, a design for a highly integrated unit was realized, which can be printed using additive manufacturing. The device combines the concept of plate heat exchange and a condensation unit by using directly printed porosity. A 2D-CFD model was developed to simulate a central repetitive unit of the 3D printed part and guide the design of the device. Fluid flow, mass transport and heat transfer in the fluid, porous and solid phases were solved in parallel. The vapor-liquid equilibrium at each point of the geometry was calculated using Soave-Redlich-Kwong equation of state. Mixture-averaged properties were used to model the fluid properties of density, viscosity, heat capacities, and thermal conductivity in a pseudo-homogeneous approach. Further, Fuller-Schettler-Giddings's method for binary diffusion coefficients was applied to consider diffusion effects.
Figure 1 a) depicts a scheme of the implementation of the repetitive key element in the CFD simulation. The sensitivity analyses for nine different design parameters, presented in Figure 1 b), show that more than 75 % of the product can be condensed and below 7 K of temperature loss for the reaction gas is possible in the chosen design space. The height of the heat exchanger plates and the height of the porous layer show the highest influence. Resulting from this study a real device employing the presented concept was developed. The digital twin was further used to design an up-scaled unit, achieving condensation and reheating in a 50 kg h-1 reactor exit flow. The simulations show the potential of 3D printing in combination with simulation to design highly integrated and multi-hierarchically structured devices, allowing the coupling of multiple functionalities into one object.

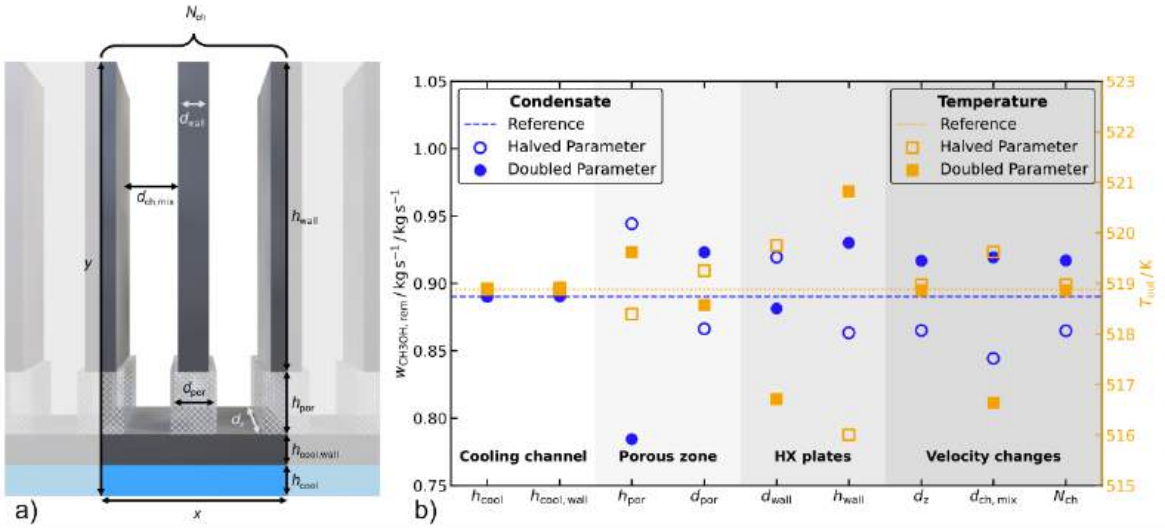

Figure 1: a) Schematic representation of the simplified repetitive key element in the CFD-model. b) Fraction of methanol and outlet temperature of the vapor phase for varying design parameters.

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HYS0262

CO2-derived carbons for enhanced hydrogen desorption in magnesium-based hydrogen storage

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Abstract Category: Hydrogen - Hydrogen Storage (LOHC, NH3, MeOH etc)

Keywords: Carbon dioxide utilization; Hydrogen storage; Magnesium hydride; Carbon morphology; Hydrogen desorption kinetics; Magnesiothermic reduction

Abstract Body.
This study proposes a carbon-centered approach to improve hydrogen desorption kinetics in magnesium-based hydrogen storage materials using carbons derived from carbon dioxide with designed structures. Tubular and sheet-like carbon architectures were synthesized via magnesiothermic reduction of CO2, enabling the conversion of a greenhouse gas into value-added solid carbon with controlled dimensionality. These CO2-derived carbons were compared with commercial carbon black as additives in Mg-based hydrogen storage composites. The central hypothesis is that carbon structure plays a key role in hydrogen desorption kinetics by influencing contact, heat transfer, and hydrogen diffusion. Mg composites with the same carbon content were prepared using 0D carbon black, 1D carbon tubes, and 2D carbon sheets. Hydrogenation was carried out at 320 °C under 30 bar H2, followed by temperature-programmed desorption up to 400 °C at atmospheric pressure under identical heating conditions. Ni was additionally introduced to examine synergistic interactions between carbon architecture and hydrogen activation sites. The results demonstrate that CO2-derived tubular and sheet-like carbons evidently lower the onset temperature for hydrogen desorption and accelerate desorption kinetics compared with carbon black, while maintaining comparable hydrogen storage capacity. Tubular carbon exhibits the most pronounced kinetic enhancement, likely due to its continuous one-dimensional transport network, whereas sheet-like carbon provides extensive interfacial contact that facilitates hydrogen diffusion. This work establishes CO2-derived carbons as functional components in advanced hydrogen storage systems and highlights a viable pathway for integrating carbon capture with hydrogen energy technologies.

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HYS0277

Continuous (de)hydrogenation of NEC/12H-NEC in a micro-packed bed reactor for hydrogen storage

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Abstract Category: Hydrogen - Hydrogen Storage (LOHC, NH3, MeOH etc)

Keywords: Liquid organic hydrogen carrier, micro-packed bed reactor, hydrogen storage, N-ethylcarbazole

Abstract Body.
Liquid organic hydrogen carrier (LOHC) is a potentially economical and secure method for hydrogen storage. However, due to the slow reaction rate and limited mass and heat transfer in hydrogenation and dehydrogenation of LOHCs, harsh conditions and high loadings of precious metal catalysts are needed[1,2]. Designing a cost-effective hydrogenation and dehydrogenation process for LOHCs is still a significant challenge.
In our work, a continuous flow system based on a micro-packed bed reactor is developed for the selective hydrogenation and dehydrogenation of N-ethylcarbazole (NEC) and dodecahydro-N-ethylcarbazole (12H-NEC). For NEC hydrogenation, 1% Ru/Al2O3 exhibits the best catalytic performance with 100% conversion of NEC and 99% selectivity to 12H-NEC under a mild reaction condition of 80 ℃ and 4 MPa. 1% Pd/Al2O3 shows the highest catalytic activity in 12H-NEC dehydrogenation reaction, achieving 100% conversion of 12H-NEC and 92% yield of NEC at 180 °C. Long-term stability test shows that the continuous reaction system exhibits good stability. Further, efficient nickel catalysts were developed for hydrogenation and dehydrogenation reactions. Similar or even better results were obtained under the same reaction conditions.

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HYS0368

LH2 BOG Cold Energy Recovery for Integrated N2 and CO2 Liquefaction

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Abstract Category: Hydrogen - Hydrogen Storage (LOHC, NH3, MeOH etc)

Keywords: LH2 BOG, cryogenic integration, CO2 liquefaction, N2 liquefaction, 4E analysis, blue hydrogen CCUS

Abstract Body.
Liquid hydrogen (LH2) storage tanks inevitably generate boil-off gas (BOG) at low temperatures (~20 K) due to heat leaks, posing energy waste and safety challenges. Conventional approaches focus on costly BOG reliquefaction or fuel utilization, overlooking its exceptional cryogenic potential. This study proposes an innovative process that harnesses LH2 BOG cold energy for the integrated liquefaction of nitrogen (N2, 77 K boiling point) and carbon dioxide (CO2, 216 K at 5.2 bar) derived from blue hydrogen production carbon capture utilization and storage (CCUS), filling a critical research gap in multi-fluid cryogenic energy integration.
The proposed system employs a sequential heat exchanger train where BOG serves as the primary cold sink: first pre-cooling N2 feed streams, then condensing CO2 in a cascade configuration. Preliminary steady-state simulations in Aspen HYSYS V14 demonstrate technical feasibility, achieving substantial energy savings compared to standalone N2 Claude cycle and CO2 mixed-refrigerant processes. The low temperature driving force (ΔT_{min} = 5 K) enables high exergy efficiency while minimizing compression work. Comprehensive 4E (energy, exergy, economic, environmental) analysis reveals: 25-35% exergy efficiency improvement, 20-30% specific energy reduction, levelized cost of CO2 liquefaction (LCO2) dropping to $40-50/ton (22% savings vs. benchmarks), and 12-18% lower global warming potential through avoided emissions. For a representative 44 kton LH2 terminal (0.2% daily BOR), BOG cooling duty matches full N2 requirements for terminal operations and partial (40-50%) CO2 load from adjacent 30 ton/day blue H2 production. This sustainable BOG valorization strategy not only mitigates LH2 storage losses but also enhances blue H2 project economics by creating revenue from CO2 liquefaction products. The process supports net-zero hydrogen infrastructure, offering scalable pathways for CCUS integration in emerging LH2 export terminals.

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HYS0400

Joule-Heated Reactor for Efficient Hydrogen Production via Ammonia Decomposition

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Abstract Category: Hydrogen - Hydrogen Storage (LOHC, NH3, MeOH etc)

Keywords: Joule-Heated Reactor, Hydrogen Production, Ammonia decomposition

Abstract Body.
In the context of achieving carbon neutrality through hydrogen energy, ammonia (NH3) has emerged as a key carrier owing to its high hydrogen storage density and excellent transport efficiency. This study proposes an electrified reactor-based ammonia decomposition process utilizing Joule-heating to circumvent the heat transfer limitations inherent in conventional external heating systems. By directly supplying electrical energy to the catalyst-packed reactor, energy losses were significantly mitigated, enabling the system to rapidly reach the activation threshold of over 500°C from ambient conditions. To maximize hydrogen production efficiency, the impact of critical design and operational parameters—specifically reactor length and space velocity (SV) on ammonia conversion rates was systematically investigated. Furthermore, the thermal performance was enhanced by configuration of the thermal insulator. Experimental results demonstrated that high ammonia conversion and exceptional energy utilization efficiency could be achieved through the precise modulation of power input to optimize localized thermal distribution. Consequently, this work provides a robust technical foundation for the design of high-efficiency electrified processes tailored for decentralized hydrogen production infrastructure.

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HYS0579

First-Principles Study of TiFe Surfaces for Solid-State Hydrogen Storage

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Abstract Category: Hydrogen - Hydrogen Storage (LOHC, NH3, MeOH etc)

Keywords: Surface magnetism, Hydrogen storage, First-principles calculations

Abstract Body.

TiFe alloys are widely studied as hydrogen storage materials; however, their practical performance is strongly limited by surface oxidation and activation issues. Since these processes are governed by surface structure and energetics, a detailed understanding of TiFe surfaces is essential. Previous theoretical studies have largely focused on idealized surface models and have paid limited attention to surface termination effects. In this work, we systematically investigate TiFe surfaces with different terminations using first-principles calculations and demonstrate that surface magnetism plays a critical role in determining surface energetics, equilibrium nanoparticle morphology and hydrogen adsorption behavior.

First-principles calculations were performed within density functional theory using the Vienna Ab initio Simulation Package (VASP). Spin polarization was included in all calculations. Surface energies for various terminations were evaluated by explicitly separating cleaving and relaxation contributions. Hydrogen adsorption energies were evaluated on spin-polarized surface models.

Spin-polarized, termination-resolved calculations reveal pronounced differences between Ti-terminated and Fe-terminated TiFe surfaces. While the Ti-terminated surface remains nearly non-magnetic, the Fe-terminated surface develops significant spin polarization with ferrimagnetic ordering. Using spin-polarized surface energies, we construct the Wulff shape of TiFe nanoparticles and find a substantial stabilization of high-index facets compared to previously reported morphologies. In addition, hydrogen adsorption energies are found to depend strongly on surface termination. These differences originate from magnetism-induced modifications of both surface geometry and electronic structure.

Our results demonstrate that the combined treatment of surface asymmetry and magnetism is essential for accurately predicting surface properties. This computational framework including magnetism provides a reliable approach for other alloys containing magnetic elements.

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HYS0708

Integrated design of ammonia-based solid oxide fuel cell system preventing nickel nitride degradation

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Abstract Category: Hydrogen - Hydrogen Storage (LOHC, NH3, MeOH etc)

Keywords: Hydrogen, Ammonia, Solid oxide fuel cell (SOFC), Nitridation prevention, Gas separation process, Power generation

Abstract Body.
Hydrogen is widely recognized as a clean energy source, and ammonia is regarded as a promising hydrogen carrier. Solid oxide fuel cells (SOFCs) can supply sufficient heat for ammonia decomposition due to their high operating temperatures, making them a viable option for ammonia-based power generation. However, Ni-based anodes suffer from nitridation during direct ammonia utilization, posing a major obstacle to long-term operation.

Conventional approaches, such as employing noble metal catalysts (e.g., Ru) in external reactors or modifying SOFC designs, either lack scalability for large-scale power production or require further development. Moreover, as SOFC research increasingly focuses on lowering operating temperatures to reduce thermal stress, the nitridation behavior also changes, necessitating optimized prevention strategies.

In this study, nitridation prevention is investigated from a process design perspective by regulating the anode inlet stream composition. Based on the concept of nickel nitriding potential, optimal inlet conditions are identified and integration with gas separation processes is proposed. This approach provides a systematic strategy to prevent nitridation and enhance the feasibility of ammonia-based SOFC systems for sustainable power generation.

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HYS0710

Spray-reliquefaction using subcooled LH2 tanks in import hydrogen terminals

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Abstract Category: Hydrogen - Hydrogen Storage (LOHC, NH3, MeOH etc)

Keywords: BOG, Pressurizing, Subcooled tank, Integrated process

Abstract Body.
(BOG) generation is an inherent challenge in liquid hydrogen (LH_2) import terminals due to continuous heat ingress during storage and handling. Conventional BOG management strategies typically rely on compression and re-liquefaction systems, which increase both energy consumption and operational complexity. In this study, a novel spray-reliquefaction concept utilizing subcooled LH_2 storage tanks is proposed as an alternative BOG mitigation strategy for import hydrogen terminals. The proposed system employs a subcooled LH_2 tank as a thermal sink, where subcooled liquid hydrogen is sprayed into the vapor space of a saturated storage tank. Through direct contact heat transfer between the subcooled spray and the BOG, vapor condensation is induced without the need for additional compressors or cryogenic refrigeration units. A thermodynamic model is developed to evaluate BOG generation, heat transfer characteristics, and re-liquefaction performance under varying liquid levels and operating pressures. The results demonstrate that the spray-reliquefaction approach effectively suppresses BOG generation by maintaining the tank pressure within allowable limits while significantly reducing energy consumption. Compared to conventional compressor-based systems, the proposed configuration exhibits lower specific energy consumption (SEC) and enhanced operational flexibility. Furthermore, the integration of subcooled LH_2 tanks enables stable long-term storage and improved safety margins for large-scale hydrogen import terminals. This study confirms that spray-reliquefaction using subcooled LH_2 tanks is a promising and energy-efficient solution for BOG management in future liquid hydrogen infrastructure.

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HYS0729

Enhanced Hydrogen Tolerance of Co-Y/CNT Composite Catalysts for Ammonia Decomposition

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Abstract Category: Hydrogen - Hydrogen Storage (LOHC, NH3, MeOH etc)

Keywords: Ammonia decomposition, Hydrogen, Cobalt, Carbon nanotubes

Abstract Body.
Introduction. Ammonia (NH3) is a promising carbon-free hydrogen carrier, yet non-noble metal catalysts like cobalt are often hindered by “hydrogen poisoning”, where adsorbed hydrogen atoms competitively occupy active sites.1 This study focuses on a cobalt-yttrium (Co–Y) oxide catalyst and carbon nanotube (CNT) composite to address this limitation. The primary objective is to enhance hydrogen tolerance by facilitating the migration and desorption of hydrogen species through a hybrid composite framework.
Methods. The CoY-CNT composites were synthesized via a one-pot co-precipitation and heat-treated at 500 °C under Ar to yield a CoO–Y2O3–CNT hybrid structure. Catalytic activities were measured in a fixed-bed reactor at 400 to 700 °C with GHSV of 30,000 mL·gcat−1·h−1. The interaction between hydrogen and the catalyst surface was analyzed through H2-TPD.
Results and discussion. The addition of CNTs resulted in a measurable improvement in catalytic performance. At 500 °C, the NH3 conversion increased from 42% for the pristine CoY catalyst to 49% for the CoY-CNT composite (Figure 1a). This enhancement in activity is fundamentally supported by a notable shift in the hydrogen reaction order, which increased from −1.1 to −0.9 upon the incorporation of CNTs. This shift provides evidence of a reduced inhibitory effect of hydrogen on the active sites, effectively improving the catalyst’s hydrogen tolerance. H2-TPD profiles further corroborated these findings, showing a distinct desorption peak between 500 °C and 600 °C (Figure 1b). This suggests that the composite structure effectively promotes the desorption of hydrogen atoms from the catalyst surfaces.
Conclusions. The CoY–CNT composite effectively mitigates hydrogen poisoning through facilitated interfacial hydrogen migration, offering a robust strategy for designing high-performance, non-noble metal catalysts.

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HYS0730

Design of Pd catalysts for liquid organic hydrogen carriers

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Abstract Category: Hydrogen - Hydrogen Storage (LOHC, NH3, MeOH etc)

Keywords: Liquid organic hydrogen carrier (LOHC); Pd catalyst; Dehydrogenation; Promoter

Abstract Body.
Introduction. Liquid organic hydrogen carriers (LOHCs) represent a safe and efficient medium for reversible hydrogen storage, enabling practical deployment of hydrogen energy technologies. However, developing catalytic systems that allow low-temperature, reversible dehydrogenation with high stability remains a critical challenge.

Results and discussion. In this study, we present a comprehensive approach to designing Pd-based catalysts by tailoring the physicochemical properties of metal–support interfaces. Through rational modification of oxide supports—via incorporation of promoters, defect engineering, and structure control—we systematically modulate electronic interactions and hydrogen-related surface behaviors. Charge transfer phenomena, surface acid–base tuning, and hydrogen spillover are leveraged to promote reversible hydrogen activation and facilitate dynamic adsorption–desorption processes [1-3].
For example, Pd loaded on hierarchical titanate nanosheets (Pd/HTN) were found to be suitable catalysts for reversible single catalyst for hydrogenation–dehydrogenation cycles [1]. Pd/HTN shows 5.70 wt% H_2 uptake over 6 h and 5.46 wt% of H_2 release over 8 h, close to the maximum hydrogen storage capacity of the NMID-based LOHC system. It demonstrated stable hydrogen storage and release performance over 5 consecutive hydrogenation–dehydrogenation cycles without any decrease in activity. The defective surface of Pd/HTN lowers the electron density of Pd, which acts as an active site, resulting in a hydrogen spillover effect that enhances the hydrogenation ability of the Pd catalyst.
This integrative catalyst design strategy offers insights into achieving both efficient hydrogen release and storage in N-heterocyclic LOHC systems. Our findings underscore the potential of support engineering as a general platform to realize practical, low-temperature reversible LOHC processes using earth-abundant catalytic materials.

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HYS0760

Metal-graphitic carbon composite for efficient nitrite reduction reaction

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Abstract Category: Hydrogen - Hydrogen Storage (LOHC, NH3, MeOH etc)

Keywords: Metal-carbon composite, Electrocatalysis, Nitrite reduction, Ammonia synthesis

Abstract Body.
Purpose. Hydrogen production via methane pyrolysis is a promising eco-friendly technology, but it generates solid carbon byproducts containing residual metal catalysts that typically require costly purification. This study aims to recycle these byproducts by directly utilizing the unpurified cobalt-carbon composite (Co@C) as an efficient electrocatalyst for the nitrite reduction reaction (NO2-RR) to produce ammonia.
Methods. Co@C composites were synthesized by performing methane pyrolysis in a fixed-bed reactor at high temperature. For comparison, Fe@C, Ni@C, and commercial carbon-supported cobalt catalysts(Co/C) were also prepared. The physicochemical properties were characterized using TGA, SEM, XRD, and Raman spectroscopy. The electrocatalytic performance for ammonia synthesis was evaluated via nitrite reduction in a alkaline electrolyte.
Results. The synthesized Co@C consisted of cobalt nanoparticles encapsulated by highly crystalline graphitic carbon layers. Despite having a lower specific surface area compared to Co/C, Co@C exhibited superior catalytic performance. At optimized potentials, Co@C achieved a remarkable ammonia Faradaic efficiency and a high yield rate, significantly outperforming Co/C and other metal-carbon composites. The high graphitization of the carbon shell enhances electron transfer and suppresses the competing hydrogen evolution reaction.
Conclusion. We demonstrated that cobalt-carbon composites derived from methane pyrolysis serve as highly selective and active electrocatalysts for ammonia synthesis without the need for metal removal. This approach offers a dual advantage of cost-effective hydrogen production and the development of sustainable electrode materials for the nitrogen cycle.

ISCRE29 & APCRE11
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HYS0762

Steam-Iron Process for Thermochemical Hydrogen Storage over Fused Fe-based materials

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Abstract Category: Hydrogen - Hydrogen Storage (LOHC, NH3, MeOH etc)

Keywords: Steam-iron process; Hydrogen storage; Red-Ox cycles

Abstract Body.
Introduction. Hydrogen is attracting growing interest as an efficient and clean energy carrier. To overcome H_2 storage challenges, the steam–iron process has emerged as a promising solution. Here H2 is indirectly stored and released through cyclic reactions of charging where Fe_3O_4 is reduced to metallic Fe ($Fe_3O_4 + 4H_2$ à $3Fe + 4H_2O$), and discharging where Fe is oxidized by water vapor, generating H2 ($3Fe + 4H_2O$ à $Fe_3O_4 + 4H_2$)[1]. This work investigates the steam–iron process over Fe-based materials prepared by fusion–decomposition [2].
Methods. Fe-based materials with varying Fe loading were prepared by fusion-decomposition of the nitrate precursors. Reduced and oxidized samples were characterized by BET, SEM, XRF, XRD. Redox experiments were carried out in TGA and packed-bed reactor.
Results and discussion. The textural characterization of the fused materials (Fig. 1a) indicates appreciably high surface area (30-50 m2/g), mesoporosity and small Fe-crystallites (< 30 nm), suggesting an adequate Fe dispersion. Isothermal and T-ramping reductions in TGA (Fig. 1b) reveal the positive effect of temperature on the Degree of Reduction (DOR), but also its time-dependence. Indeed, the kinetics of reduction are complex and their comprehension is crucial for the efficiency of the entire process. Based on our results, they positively depend on Fe dispersion and H2 partial pressure, but negatively on H2O content. Besides, it was observed that lower reduction temperature leads to faster subsequent oxidation (Fig. 1c). This suggests that the reduction conditions affect the oxidation kinetics by modulating the Fe accessibility. Ongoing research aims at identifying optimal temperature and gas-phase conditions for reduction and oxidation, as well as developing comprehensive kinetics to address reactor design.

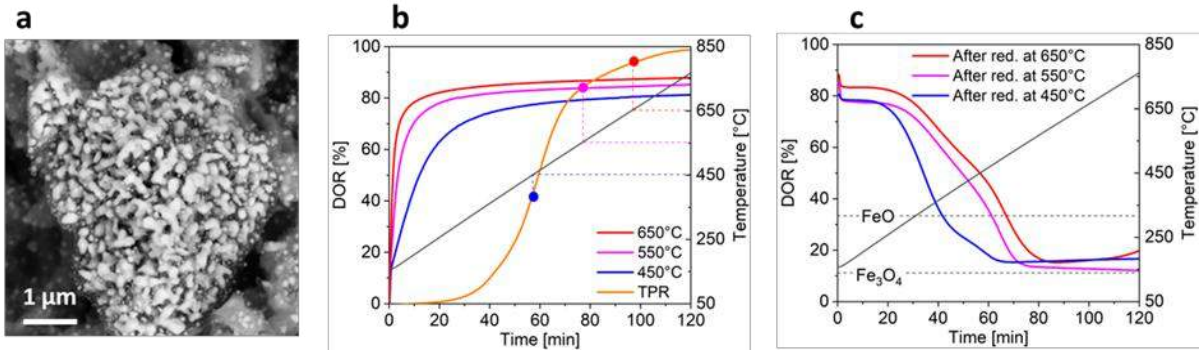

Figure 1. a) SEM images of the reduced Fe-based storage materials; b) Effect of

temperature on reduction of Fe_2O_3 to Fe; c) Effect of reduction temperature on temperature-programmed oxidation from reduced sample to Fe3O4. Temperature program: 150à800°C, 5°C/min; total flow rate: 150 Nml/min.

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HYT0735

Quantitative Risk Assessment on LH2 receiving Terminal

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Abstract Category: Hydrogen - Hydrogen Transportation

Keywords: Liquified Hydrogen Receiving Terminal, Liquified Hydrogen(LH2), Quantitative Risk Assessment(QRA), Qualitative Risk Assessment, Hazard Identification, , Liquid Hydrogen Infrastructure, Hydrogen Economy

Abstract Body.
This study conducted a quantitative risk assessment (QRA) for a large-scale liquefied hydrogen (LH_2) receiving terminal, assuming future import expansion. To this end, a steady-state model was constructed for the terminal process, comprising a 10,000 m³ spherical vacuum-insulated storage tank, a BOG recompression and recondensation system, an evaporator, and transmission pipelines. BOG behavior and process conditions reflecting actual operating conditions were derived. Subsequently, through HAZID, representative leak and rupture scenarios were selected, focusing on the storage tank, recondenser, high-pressure pump, and vaporizer. Individual Risk (IR) and Societal Risk (SR) were quantified by combining thermal radiation and overpressure effects, human casualty assessment using the Probit function, and failure frequency, ignition probability, meteorological, and population density data. Analysis results showed that large leak and rupture scenarios involving high-pressure pumps and vaporizers contributed most significantly to IR and SR, while contributions from storage tanks and recondensers were relatively low. The overall risk level fell within the ALARP (As Low As Reasonably Practicable) range according to international standards. This indicates that while further risk reduction is possible through additional protective measures and design improvements, safety at a technically and economically acceptable level can be achieved. The results of this study are expected to serve as foundational data for future risk-based design of liquefied hydrogen receiving terminals, setting safety objectives, establishing risk mitigation measures, and developing domestic safety standards for liquefied hydrogen infrastructure.

Poster Presentation

Net-zero CO_2 Technologies

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

CDC0160

Characterization of Side Reactions in Onboard Aqueous Amine CO_2 Absorbents

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Capture

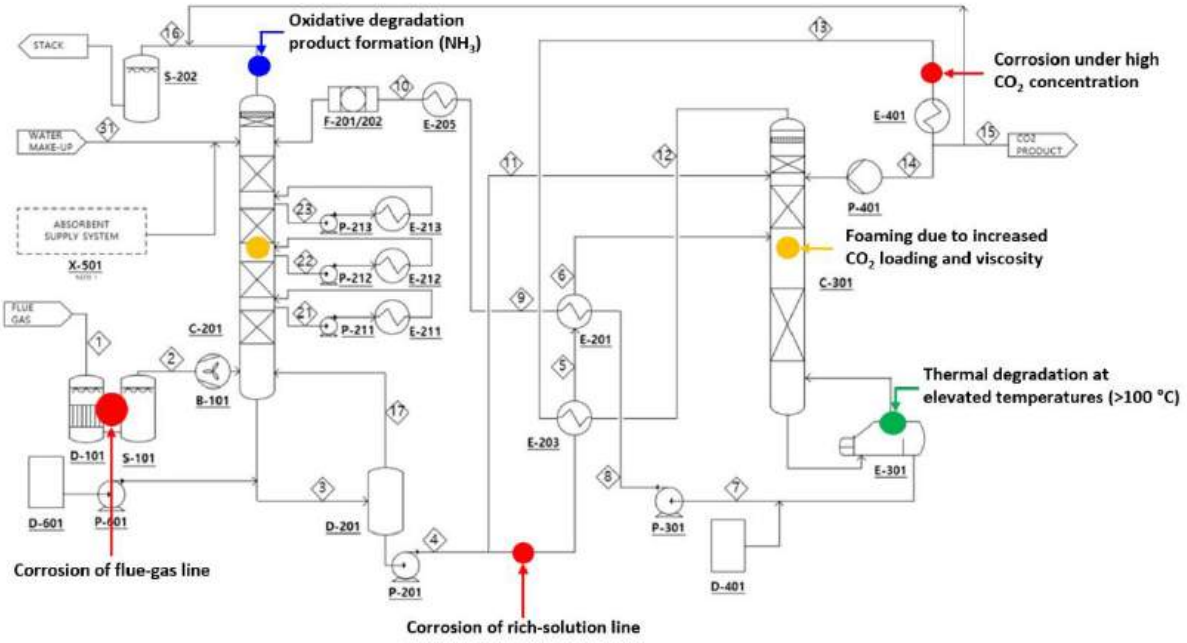
Keywords: CO_2 capture, Amine absorbent, Solvent degradation, Corrosion, Foaming

Abstract Body.

The maritime industry, which accounts for approximately 3% of global carbon emissions, is actively advancing technologies that directly capture CO_2 from ship engine exhaust to mitigate releases to the atmosphere and to marine ecosystems. Among the available carbon capture options, post-combustion capture using amine absorbents is considered a practical route for onboard implementation because it can be integrated with existing exhaust systems. In real ship operation, however, exhaust gas contains not only CO_2 but also impurities such as NOx, SOx, and particulate matter, and the composition can vary with engine load and fuel quality. These contaminants can drive undesired side reactions in amine-based absorption processes, leading to oxidative and thermal degradation of the solvent, corrosion of process equipment, and foaming behavior. Such phenomena may cause absorbent loss, deterioration of CO_2 capture performance, increased maintenance demand, and in severe cases operational instability and equipment damage.

In this study, we quantitatively compared impurity-driven side reactions using a lab-scale amine absorption system operated with simulated flue gas. Oxidative degradation was evaluated by monitoring ammonia (NH_3) formation as a representative indicator produced after reaction between the amine solvent and dissolved oxygen originating from the exhaust gas. Corrosion was assessed by analyzing the concentration of dissolved metal ions released from SUS304 stainless steel and carbon steel coupons, which are widely used as structural materials in absorption equipment and piping. Foaming characteristics were evaluated through measurements of foam stability and surface tension, providing insight into foaming tendency and persistence under process-relevant conditions.

After establishing the baseline severity of degradation, corrosion, and foaming under simulated exhaust conditions, we further investigated the feasibility of applying mitigation additives, including corrosion inhibitors and antifoaming agents, to reduce these adverse reactions in amine solvents. Ultimately, this work aims to support stable long-term operation and to provide technical foundations for the commercialization of large-scale CO_2 capture systems for maritime applications.


Oxidative degradation product formation (NH_3)
Corrosion under high CO_2 concentration
Foaming due to increased CO_2 loading and viscosity
Thermal degradation at elevated temperatures (>100 °C)
Corrosion of flue-gas line
Corrosion of rich-solution line
STACK
WATER MAKE-UP
ABSORBENT SUPPLY SYSTEM
X-501
FLUE GAS
CO2 PRODUCT
S-202
F-201/202
E-205
P-213
E-213
P-212
E-212
P-211
E-211
C-201
B-101
D-101
S-101
D-601
P-601
D-201
P-201
E-201
E-203
P-301
D-401
E-401
P-401
C-301
E-301

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CDC0207

Unveiling the Molecular Origins of Cation-Specific Effects on CO2 Capture in Alkali Glycinate Solutions

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Capture

Keywords: carbon capture, molecular simulation, amino acid

Abstract Body.
Counter cations dictate the CO2 capture efficiency of amino acid salt (AAS) solvents, yet the governing molecular mechanisms remain elusive. This knowledge gap hinders the rational design of AAS systems for controlling precipitation and absorption. We employed molecular dynamics simulations to quantify the roles of potassium, sodium, and lithium cations in aqueous glycine solutions. Our results reveal that cation identity directly governs CO2 capture kinetics and transport properties. Notably, potassium solutions outperform lithium systems. Especially, potassium ions extend the CO2–amine interaction time by twofold and increase CO2 diffusivity by over 10%. These macroscopic enhancements stem from lower cation charge density, which fundamentally alters the dynamics of solvent and solute species, alongside their hydration structures. Our findings match experimental observations and provide a molecular blueprint for tuning AAS solvents to design next-generation carbon capture technologies.

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CDC0223

Sub-ambient Temperature Direct Air Capture using CALF20

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Capture

Keywords: Sub-ambient temperature, Direct Air Capture, Metal organic frameworks

Abstract Body.
The atmospheric concentration of CO2 continues to increase, intensifying the need for scalable and energy-efficient direct air capture (DAC) technologies. Conventional DAC processes typically rely on adsorption at ambient conditions followed by high-temperature regeneration, leading to high energy consumption and capture costs. Sub-ambient DAC provides an alternative strategy by exploiting the exothermic nature of CO2 adsorption, enabling CO2 capture at low temperature and release at ambient conditions with reduced regeneration energy. In addition, the availability of waste cold energy from LNG regasification terminals in South Korea offers a practical opportunity to implement lowtemperature DAC without additional cooling demand. In this context, metal–organic frameworks (MOFs), with their high surface areas and tunable adsorption properties, are promising candidates for sub-ambient DAC. Among them, CALF-20 has shown favorable CO2 adsorption performance at low concentrations. This study investigates CO2 capture on CALF-20 at −25 °C under ambient air-level CO2, followed by desorption at room temperature.

Prior to breakthrough experiments, CALF-20 was activated at 150 °C under N_2 flow for 2 h. The activated sample was packed into a fixed-bed column and immersed in an antifreeze bath connected to a chiller set at −25 °C. After temperature equilibration, a gas mixture containing 400 ppm CO2 balanced in He was introduced. Upon CO2 saturation, the inlet gas was switched to N_2 , and the column temperature was gradually increased to 25 °C to induce desorption. Outlet CO2 concentrations were continuously monitored using an infrared gas analyzer (LI-COR).

At 25 °C and 400 ppm CO2, CALF-20 exhibited a low adsorption capacity of 0.04 mmol g^{-1}. In contrast, at −25 °C under the same CO2 concentration, the adsorption capacity increased significantly to 0.71 mmol g^{-1}, reflecting the exothermic nature of CO2 adsorption. During the desorption step, nearly complete release of the adsorbed CO2 was achieved at ambient temperature. This highly reversible adsorption–desorption behavior indicates that CO2 uptake in CALF-20 is dominated by physisorption, resulting in a low regeneration energy requirement. These results highlight the potential of sub-ambient DAC using CALF-20,

particularly when coupled with LNG cold-energy utilization, as an energy-efficient pathway for direct air capture.

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CDC0362

Discovery of Membrane Materials for CO2 Capture via Material-Process Integrated Framework

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Capture

Keywords: CO2 capture, membrane system, machine learning

Abstract Body.
Membrane systems offer advantages such as high energy efficiency, process simplicity, and a compact equipment footprint. However, material performance is constrained by the permeability-selectivity trade-off. In this study, we systematically identify promising polymer membrane materials from a process economic perspective using a material-process integrated framework that includes (i) machine-learning based gas permeability prediction, (ii) process optimization and techno-economic analysis, (iii) large scale screening. First, using permeability data for 353 polymers as training data, we compared 8 models and selected a GNN (Graph Neural Network) based Chemprop model that achieved the highest coefficient of determination. The trained model is then applied to predict gas permeabilities for 12,000 synthetically available polymers and 4,000,000 virtual polymers. Next, the permeability-selectivity space is discretized into a logarithmic grid, and process optimization and techno-economic analysis are performed at each grid point. At each grid point, we optimize a two-stage membrane process configuration, membrane area, operating pressure to minimize cost. Based on these results, we train a gaussian process regression surrogate model to predict process cost as a function of permeability and selectivity. Case studies are conducted for CO2 capture process. For CO2 capture, we consider two flue gas cases, cement calciner process flue gas for high CO2 concentration and refinery boiler flue gas for low CO2 concentration. We find polymers that are economically promising at the process level, rather than using property-only metrics.
Acknowledgement: This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (RS-2025-00515836) and by the Korea Institute of Energy Technology Evaluation and Planning (KETEP) and the Ministry of Trade, Industry & Energy (MOTIE) of the Republic of Korea (No. RS-2024-00441791)

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CDC0363

Comparative Energy Analysis of Thermally and Electrochemically Regenerated Direct Air Capture Systems

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Capture

Keywords: Direct Air Capture, Electrification, Bipolar Membrane Electrodialysis

Abstract Body.
In the last year, the average surface temperature of the earth was 1.5 °C above preindustrial levels, excessing the temperature limit of the Paris Agreement in 2015. This temperature increase is mainly induced by greenhouse gas including methane, nitrogen and carbon dioxide. To mitigate these emissions, Carbon Capture, Utilization and Storage (CCUS) technologies have been developed to isolate and utilize carbon dioxide from concentrated emission sources, such as industrial sites and power plants. Direct Air Capture (DAC) is a novel CCUS approach capturing CO2 from atmosphere, which plays a role in offsetting CO2 emission from distributed sources as well as removing already accumulated atmospheric CO2. However, DAC systems require broad area and large process facilities to absorb CO2 from diluted air, causing substantial capital investment. Also, conventional DAC system requires significant thermal energy, which can lead to additional CO2 emissions during energy generation and partially offset the amount of net CO2 captured. Recently, electrochemically driven CO2 regeneration has emerged as an alternative approach that can substitutes thermal energy with electrical energy, enable the integration of liquid-based DAC with renewable energy systems, and offer the potential to reduce energy consumption. In this study, the energy performance and operational characteristics of a KOH-based DAC process coupled with a bipolar membrane electrodialysis (BPMED) regeneration system were analyzed, and conventional thermally regenerated DAC was compared with electrically driven DAC configurations. The DAC system was simulated using the commercial process simulator Aspen Plus 14.0, while the BPMED stack was modeled and integrated with DAC process using MATLAB. Using these models, the sensitivities of key operation variables containing current density, solvent concentration and load ratio were systematically analyzed to explore potential pathway for performance improvement. In addition, the DAC-integrated designing and operating strategies for effective system coupling were identified considering absorption efficiency of air-contactor and CO2 release performance within BPMED stack.
This work was supported by a Korea Institute of Energy Technology Evaluation and Planning (KETEP) grant funded by the Korea government (MOTIE) [grant number RS-2022KP002700 (20224C10300050)] and by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT). (RS-2025-00515836)

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CDC0416

CFD and experimental studies of CO_2 solubility using novel deep eutectic solvents

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Keywords: CO_2 absorption; deep eutectic solvents; CFD studies; solubility of CO_2

Introduction

The CO_2 can be released into the atmosphere via different processes such as pre- combustion, post-combustion and oxyfuel. Thus, the development of a CO_2 capture technologies is crucial. The development of computational fluid dynamics (CFDs) models can optimize reactor and operation conditions, thus saving time and resources [1]. In this work CO_2 absorption was carried out in various choline chloride-based deep eutectic solvents (DESs) such as ChCl:MEA, ChCl:DEA, ChCl:Urea and ChCl:Gly using the experimental set-up of Figure 1a. The purpose of this study is to investigate theoretically and experimentally the solubilities of CO_2 in each DES.

Modelling methodology

A CFD model was developed to predict the CO_2 concentration distribution at the gas- liquid interface during the absorption into the DES, using COMSOL Multiphysics 6.2 software. A 2D system batch reactor system was taken into consideration for the development of the model. The CO_2 concentration field was obtained by using the Transport of Diluted Species and due to the batch nature of the system convective transport was neglected, and the species conservation equation can be described as:

$$\nabla \cdot (-D_i \nabla c_i) = R_i \quad (1)$$

where c_i is the molar concentration of each species (mol m^{-3}), D_i the molecular diffusion coefficient (m^2 s^{-1}) and R_i expresses the sum of each components rate expressions (mol m^{-3} · s^{-1}).

Selected results and discussion

Figure 1b presents the steady-state CO_2 concentration distribution in the gas phase under batch conditions near the gas-liquid interface. Ongoing work focuses on the transport properties in the liquid phase to predict quantitative prediction of CO_2 concentration in DES at time-dependent conditions. Thus, the experimental values of Henry's constant and diffusivity will be found and calculate the values of CO_2 solubility and compare them with the modelling values.

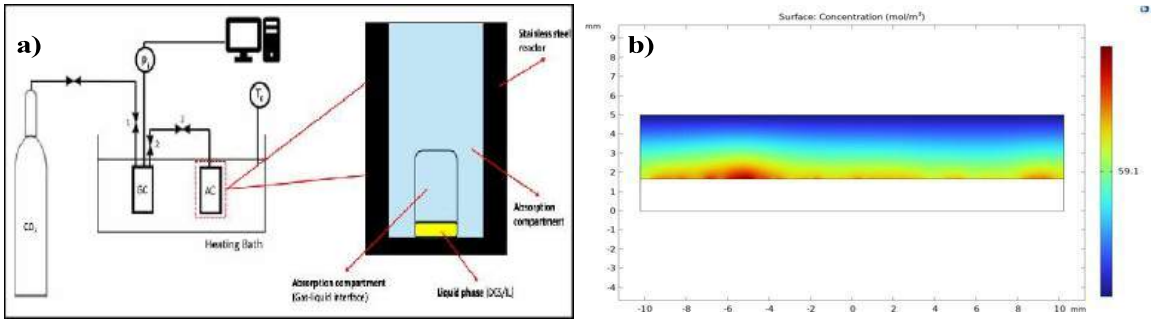

Figure 1. a) Gas absorption experimental set-up; gas compartment (GC), absorption compartment (AC), pressure transducer (PI) and temperature controller (TC). **b)** Steady-state CO_2 concentration profile across the gas-liquid interface.

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CDC0592

Epoxy-Functionalized Tetraethylenepentamine for Direct Air Capture

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Capture

Keywords: Direct Air Capture, Amine-Functionalization, Oxidative Degradation

Abstract Body.

Introduction. Amine-based adsorbents have been extensively investigated due to the their high selectivity and high CO2 sorption capacities at low partial pressure. Polyethyleneimine(PEI) is the most commonly used amines owing to amine-rich structure and low volatility. However, high-molecular-weight and viscosity of PEI result in the pore blocking, which reduce amine efficiency and limit diffusion capability. Tetraethylenepentamine (TEPA) is a promising alternative as it offers distinct advantages, including lower viscosity, cost-effectiveness and especially higher CO2 capacity due to its low tertiary amine content. Nevertheless, the low oxidative stability of TEPA caused by volatilization and amine leaching is still challenging. Herein, we studied functionalized TEPA via grafting epoxide to selectively convert primary amines into secondary amines, thereby suppressing degradation pathways and improving structural stability. This study aims to elucidate the relationship between chain length of the epoxide, CO_2 adsorption capacity, adsorption kinetics, and long-term cyclic stability.

Methods. The adsorption-desorption profiles were collected by a thermogravimetric analyzer (TGA). The adsorbents were pretreated at 100 °C for 1 h under the He flow. Adsorption was carried out under 0.04% CO2 in He balance at 25 °C. After adsorption, the gas was switched to pure He flow for 15 min, and the temperature was raised to 70 °C. To assess their oxidation stabilities, a gas mixture (0.04% CO2 and 20% O2 in He balance) was used in the adsorption process at 25 oC.

Results and discussion. The epoxide-functionalized TEPA was impregnated into the fumed silica. 50wt.% TEPA/fumed silica showed the largest CO2 uptake of 9.1 wt.%, whereas Epoxy-TEPA/fumed silica showed lower CO2 uptake of 7.6 wt.%. The decrease of CO2 uptake is attributed to the decrease in primary amine portion after the epoxide functionalization. A series of five adsorption–desorption cycles were conducted to investigate the regeneration capabilities of prepared sorbent. There was an obvious reduction in the CO2 uptakes, especially TEPA/fumed silica, weight loss rate reached 16.5% after 5 cycles. On the other hand, adsorption capacity of Epoxy-TEPA/fumed silica relatively stable, with a decrease of 2.8 wt.% compared to the initial CO2 uptake, Confirming the effect of epoxy functionalization in enhancing cyclic stability. Meanwhile, the CO2 working capacities were similar for both samples, but desorption kinetic was faster on Epoxy-TEPA/fumed silica. Whereas 20 min was needed to desorb adsorbed CO2 on TEPA/fumed silica, 7.5 min was

required for Epoxy-TEPA/fumed silica. Moreover, accelerated aging experiment is ongoing to investigate stability against urea formation and oxidative amine degradation.

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CDC0620

CFD and experimental studies for CO2 capture using amine and deep eutectic systems

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Capture

Keywords: CFD modelling, CO2 capture, Amines/DES, experimental validation

Abstract Body.

Introduction.

The reduction of CO2 emissions remains a major challenge for process design and separation engineering. The need to find and develop new CO2 technologies is essential. Experimental work integrated with CFD modelling is a new approach to optimize reactor design and reaction conditions [1]. In this study, CFD models were developed for CO2 removal using various conventional and emerging absorbents such as NaOH, MEA, DEA, ChCl:MEA, ChCl:Urea, ChCl:DEA, ChCl:Gly to advance the CO2 capture efficiency of DES and compare it with the conventional solvents.

Methods.

A theoretical CFD model was developed based on our novel reactor design to study the effect of the parameters that influence CO2 capture between conventional and unconventional solvents, using COMSOL Multiphysics 6.2. The two-dimensional stationary model was carried out to couple diffusion, mass transfer, reaction kinetics and simulate the flux of CO2 through the membrane and into the liquid phase.

Results and discussion.

Figure 1 indicates the CO2 removal efficiency of both conventional and unconventional solvents as a function of volumetric gas flow rate. An increase in gas flow rate entails in reduced residence time of CO2 in the gas phase, thus, a decrease in CO2 removal ability. Ongoing studies focus on the validation of the modelling results with the experimental data using our experimental setup. Additionally, current work focuses on the optimization of reactor design and reaction conditions.

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CDC0663

Development of a Kinetic Model for a Scalable CO2 Capture Unit Using a Sustainable Na2CO3/Al2O3 Solid Sorbent

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Capture

Keywords: CO2 Capture, Kinetic Modeling, CFD Simulation, Solid Sorbents.

Abstract Body.

Introduction. To accelerate the transition to a low-carbon economy, this research targets the development of a cost-effective, circular CO2 adsorption system. While commercial options exist, this study focuses on sodium carbonate supported on alumina (Na2CO3/Al2O3) as a superior sustainable alternative due to its low cost, operational safety, and ease of synthesis. The primary objective was to establish a precise hot flow kinetic model to predict the sorbent's behavior in dynamic environments, serving as the critical physics input for future computational fluid dynamics (CFD) simulations.

Methods. Experimental breakthrough curves were used to calculate specific adsorption rates based on mass balance principles. To ensure the model is geometrically independent and scalable, volumetric flow rates were converted to superficial gas velocity, with a fixed water vapor concentration of 2.4% included to satisfy reaction requirements.

Results and discussion. The developed semi-empirical model as shown in Fig. 1 achieved high accuracy (R^2 = 0.9150), identifying flow velocity as the primary driver of adsorption (reaction order y ≈ 1.029), while confirming the reaction is exothermic with a low activation energy (E_a = -2.61 kJ/mol). Although the maximum capacity of Na2CO3/Al2O3 (55.33 mg/g) was slightly lower than the commercial reference Lewatit VP OC 1065 (70.63 mg/g), its kinetic behavior proved highly responsive and suitable for fluidized-bed systems. This validated kinetic framework will be directly integrated into CFD simulations to optimize reactor geometry and hydrodynamics. This approach allows for the virtual testing of largescale circulating-fluidized bed systems, ensuring efficient design before physical implementation.

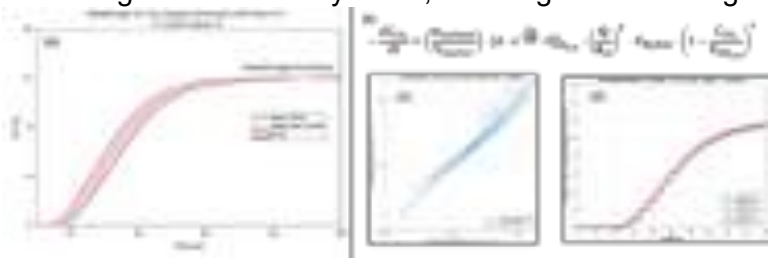

Fig. 1. CO2 adsorption analysis and modeling: (a) breakthrough performance, (b) a semiempirical equation, (c) parity analysis, and (d) validation of experimental vs. predicted concentration profiles.

Acknowledgments: The Program Management Unit for Competitiveness (PMU-C), Office of National Higher Education Science Research and Innovation Policy Council (NXPO), Thailand, is acknowledged for partial financial supports to this project.

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CDC0711

Synthesis and functionalization of 2D Imine based COF for CO2 Capture

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Capture

Keywords: Covalent organic frameworks, CO2 adsorption, Imine-linked framework, Rapid synthesis

Abstract Body.
Introduction: Population growth and excessive human activities have caused a rapid increase in atmospheric CO2, leading to serious global climate change. Conventional CO2 capture methods, such as liquid absorption and pressure swing adsorption, are effective but often limited by high energy demand, cost, and poor long-term stability. Recently, covalent organic frameworks (COFs) have emerged as promising porous crystalline materials for CO2 adsorption due to their high surface area and structural stability. In this study, an imine-linked COF synthesized from 1,3,5-tris(4-aminophenyl)benzene and terephthaldehyde is investigated. To improve practicality, a mild solvothermal method using a mixed solvent system is adopted, reducing synthesis time from 72 hours to 16 hours while maintaining high crystallinity and porosity.
Methods: The COF was synthesised via a mild solvothermal condensation of 1,3,5-tris(4aminophenyl) benzene and terephthaldehyde following the reported method. A mixed solvent system of n-butanol, acetic acid, and water was used, and the reaction was carried out at 70 °C for 16 hours under stirring. The resulting solid was purified, washed, and dried before characterisation.
Results and discussion: Following the reported synthesis strategy, the as-prepared TABP–PDA COF is expected to exhibit high crystallinity and well-defined porosity despite the significantly reduced reaction time. Powder X-ray diffraction (PXRD) patterns are anticipated to display sharp low-angle reflections in the 2θ range of approximately 3–8°, confirming the presence of long-range structural order. Nitrogen adsorption–desorption analysis is expected to reveal a high Brunauer–Emmett–Teller (BET) surface area in the range of ~600–1000 m2 g−1, accompanied by a combined Type I/IV isotherm, indicative of microporous and small mesoporous features. The pore size distribution is anticipated to show a dominant pore diameter of approximately 1.6–2.5 nm. Furthermore, the material is expected to demonstrate good thermal and chemical stability comparable to COFs synthesised via conventional solvothermal methods.
Acknowledgements: The authors gratefully acknowledge the support and facilities provided by their respective institutions for carrying out this research. Appreciation is also extended to colleagues and laboratory staff for their technical assistance and valuable discussions.

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CDC0741

Hydrophobic Amine System for Ru-Catalyzed CO_2 Hydrogenation to Formate and Amide Derivatives

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Capture

Keywords: CO_2 Hydrogenation , Hydrophobic Amine , Biphasic Catalysis

Abstract Body.

The integration of CO_2 capture and catalytic hydrogenation offers a promising pathway for the sustainable synthesis of value-added C1 products; however, conventional homogeneous systems suffer from major downstream limitations, particularly in the separation and recovery of amines and dissolved catalysts. These challenges complicate catalyst recycling, reduce process efficiency, and hinder industrial applicability. In this study, a hydrophobic amine was employed as a dual-function medium for CO_2 capture and subsequent hydrogenation to formate and formamide derivatives. Owing to its hydrophobic nature, it exhibited efficient CO_2 uptake while simultaneously enabling a biphasic reaction environment. Catalyst loading conditions were systematically optimized to achieve improved catalytic performance and efficient substrate conversion under the studied hydrogenation environment. Under hydrogenation conditions in the presence of a ruthenium pincer catalyst, the reaction system showed a dominant trend toward formate formation. This work highlights the potential of hydrophobic amines to overcome amine and catalyst separation bottlenecks while integrating CO_2 capture, catalytic conversion, and phase-assisted separation within a single process framework.

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CDC0744

Direct Knitting of Ru-MACHO into Hierarchical Porous Organometallic Polymers: Linker Engineering for Enhanced CO2 Hydrogenation

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Capture

Keywords: Direct knitting, Hydrogenation of CO2, Porous organometallic polymers, Ru-MACHO

Abstract Body.

The valorization of CO2 into value-added chemicals, such as formic acid and methanol, is essential for establishing carbon-neutral energy systems. To date, the Ru-MACHO catalyst has been recognized for exhibiting the highest activity in the hydrogenation of CO2 to formate and methanol. However, for industrial applications, Ru-MACHO must be heterogenized to facilitate the separation and purification of final products. In this study, RuMACHO was heterogenized via a Friedel–Crafts direct knitting strategy using triphenylmethane (TPM), diphenylmethane (DPM), and bibenzyl (BB) linkers to construct porous organometallic polymer (POMP) networks. This approach yielded catalysts with welldispersed Ru active sites and hierarchical porosity; notably, the integration of TPM significantly increased the specific surface area (SBET) compared to linker-free systems. Structural and catalytic evaluations in amine-assisted CO2 hydrogenation revealed that these organic linkers enhanced framework rigidity and active-site exposure. Among the synthesized materials, Ru-MACHO-POMP-TPM demonstrated the highest activity and durability, followed by Ru-MACHO-POMP-DPM and Ru-MACHO-POMP-BB. All linkermodified catalysts outperformed both the linker-free system and the homogeneous precursor in terms of stability and recyclability. These findings underscore the critical role of linker engineering in optimizing the performance of heterogenized organometallic frameworks for sustainable CO2 conversion.

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2026 / SEOUL, KOREA

CDC0745

Visible-Light-Driven Photoanode Design for Photoelectrochemical Regeneration of Amine-captured CO2

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Capture

Keywords: CO2 capture, photoelectrochemical, amine regeneration

Abstract Body.
Carbon capture is a key strategy for achieving negative emissions, and electrochemical carbon capture has emerged as a promising alternative to conventional thermal regeneration. Systems based on hydrogen oxidation and hydrogen evolution reactions enable CO2 desorption and amine regeneration; however, their practical implementation is limited by high energy consumption. Herein, an anion exchange membrane (AEM)-based photoelectrochemical process is proposed to enhance amine recovery by integrating photocatalysis with electrocatalysis. Among photocatalytic materials capable of harvesting visible light, BiVO4 is a promising photoanode material owing to its suitable bandgap, chemical stability, and low cost; however, its practical photoelectrochemical performance is often limited by poor charge transport and interfacial recombination. To address these limitations, a BiVO4/ TiO2 photoanode supported on carbon felt (CF) is developed, where TiO2 functions as an electron-transport layer and CF provides a conductive scaffold, resulting in improved charge separation and anodic stability under illumination. This work demonstrates how rational photoanode engineering can enable photo-assisted CO2 desorption in electrochemical carbon capture systems.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

CDU0015

Application of RSM and Machine Learning for Predicting the Interaction of Key Parameters Governing Calcium Leaching for Indirect Mineralization of Cement Kiln Dust

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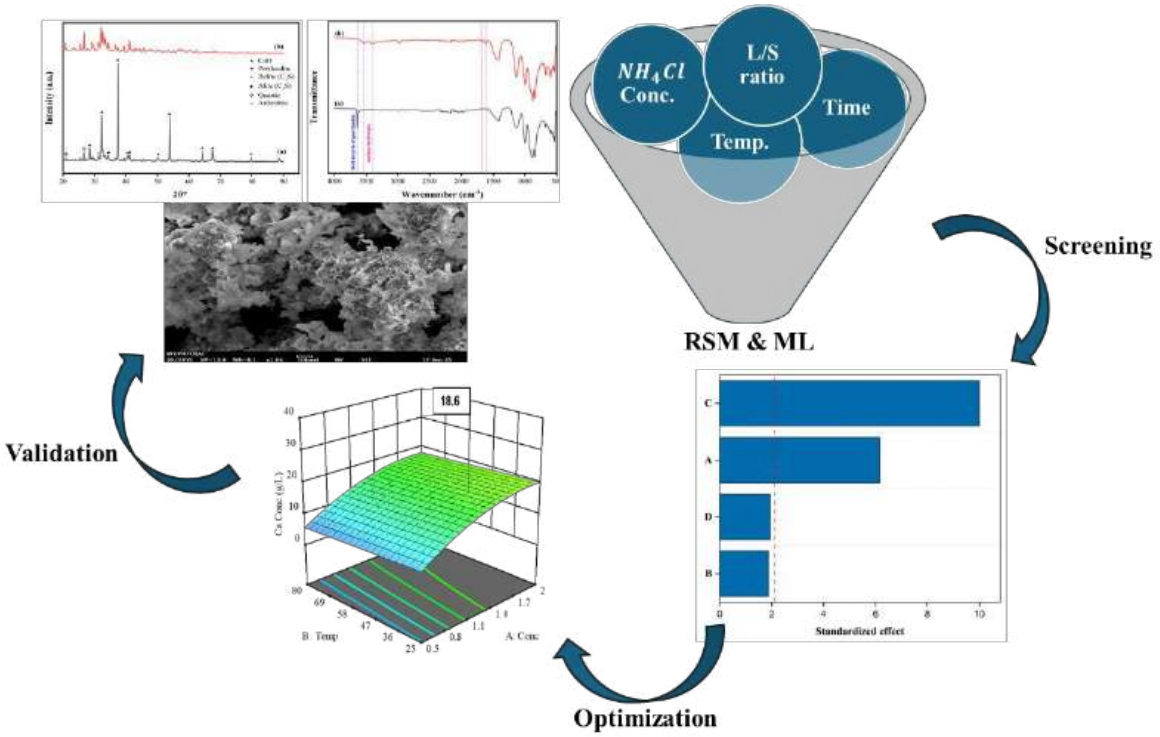
Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: Carbon, Sequestration, Modeling, Artificial intelligence, Waste utilization

Abstract Body.

Due to the increase in CO_2 emissions, there is heightened interest in applications that provide long-term sequestration via indirect mineralization. A crucial aspect involves leaching ions from the source, such as cement kiln dust (CKD). This work uses response surface methods and machine learning approaches to improve leaching parameters and examine their interaction for calcium leaching using ammonium chloride. RSM model (R^2 = 0.814) identified statistically significant terms (p < 0.0001) and predicted an optimal concentration of Ca at 18.6 g/L. Machine learning models were trained and cross-validated to identify nonlinearities that polynomial response surface methodology was unable to detect. The predictions exhibited higher accuracy (R^2 = 0.94; RMSE = 1.5-2.5). The assessment of feature significance ranked the variables as follows: liquid-to-solid ratio, NH_4 Cl concentration, temperature and time. Solid residue under optimal leaching conditions was analyzed using X-ray diffraction (XRD) and Fourier-transform infrared spectroscopy (FTIR), indicating substantial dissolution and confirming the successful extraction of calcium under the optimized conditions. Subsequently, the carbonation of the leached samples was done, resulting in the formation of pure calcium carbonate. Analyses using XRD and FTIR indicated that the process resulted in the formation of vaterite. Scanning electron microscopy (SEM) revealed that the observed shape was typically aggregated and nearly spherical. The rapid precipitation and efficient transformation of dissolved calcium indicate that the optimized leachate serves as a robust foundation for future mineralization. The integrated workflow, RSM-ANOVA for enhanced parameter optimization, and machine learning for accurate prediction improved calcium recovery from CKD and facilitated the synthesis of carbonates. These findings demonstrate a viable pathway to valorize cement-industry byproducts and advance circular, low-carbon manufacturing.


Intensity (a.u.)
Transmittance
Wavenumber (cm⁻¹)
NH4Cl Conc.
L/S ratio
Time
Temp.
RSM & ML
Screening
Standardized effect
Optimization
Validation
18.6
Cs Conc (g/L)
B: Temp
A: Conc

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

CDU0092

Energy-efficient CO_2-to-formate conversion coupled with glycerol oxidation using electrodeposited $BiVO_4$ photoanodes under concentrated light

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: Photoelectrochemical co-valorisation; glycerol oxidation; CO2 reduction; electrodeposited BiVO4 photoanodes.

Abstract Body.

Introduction. Photoelectrochemical (PEC) CO_2 conversion is an energy-efficient alternative to conventional electroreduction ($ERCO_2$), enhanced by $BiVO_4$ photoanodes with strong visible-light absorption and favourable OER kinetics [1]. When $BiVO_4$ is electrodeposited on FTO and operated under back-side illumination, current densities up to −23 mA cm^{-2} have been reported for systems using a CO_2 gas-phase feed and a Bi/C GDE dark cathode. Under these conditions, formate concentrations of 41.4 g L^{-1} with a Faradaic efficiency of 86% were achieved [2]. Further reductions in overall energy consumption can be realized by implementing alternative oxidation reactions at the photoanode, such as the glycerol oxidation reaction (GOR). This strategy offers two main advantages: a lower anodic potential and the production of value-added chemicals, dihydroxyacetone (DHA) [3].

Methods. In this context, electrodeposited $BiVO_4$-based photoanodes, with a buried Bi gradient to act as an electron transport layer [4], demonstrated remarkable performance, reaching current densities of −83 mA cm^{-2} under a constant bias of −1.8 V vs. Ag/AgCl. When the GOR with the BiVO4-based photoanodes is coupled with $ERCO_2$ to formate in liquid phase (0.5 M KCl + 0.45 M $KHCO_3$) using a Bi/C GDE, Faradaic efficiencies of up to 65% and 84% toward formate were obtained under illumination at constant −45 and −90 mA cm^{-2}, respectively, representing an improvement of more than 12% compared to dark operation. Additionally, the photoanode generated high-value products such as DHA, glyceraldehyde, and formate, achieving a combined FE of 50%, which significantly surpasses previously reported values for Pt dark anodes (21% total FE for GOR) at -90 mA cm-2 [5].
Results and discussion. In terms of energy efficiency, the system reached approximately 28% under illumination versus 22% in the absence of light, underscoring the effectiveness of photoanode integration in enhancing $ERCO_2$ performance. To further explore this potential,

the effect of solar light intensity is evaluated (up to 14 suns employing a solar concentrator) to determine the extent to which additional photon flux can improve energy efficiency, formate production, and its effect on the GOR product selectivity. Ultimately, this work shows that the combined implementation of electrodeposited $BiVO_4$ photoanodes with GOR leads to a substantial enhancement in energy efficiency, two of the main bottlenecks in the scaling up of PEC processes.

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CDU0093

From Nb2O5 to Oxynitrides: Impact of ammonolysis on the photoelectrochemical properties of thin films

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: Thin film, oxynitrides, ammonolysis, photoelectrochemistry, bandgap.

Abstract Body.
Introduction. In the critical ongoing transition towards renewable energy technologies, the development of robust semiconductors capable of efficiently harvesting solar energy remains a top priority. Among potential materials, niobium oxide (Nb2O5) stands out as a promising candidate due to its exceptional chemical stability. However, its practical application in solardriven processes is severely hindered by a wide bandgap, which restricts light absorption almost exclusively to the ultraviolet region, thereby limiting its solar conversion efficiency [1]. Methods. To address these challenges, this work presents a comprehensive strategy to convert porous Nb_2O_5 thin films into active niobium oxynitrides, serving as efficient photoanodes for photoelectrochemical (PEC) water oxidation. Specifically, 1 cm2 photoanodes are fabricated via dip-coating in a precursor niobium solution, followed by a thermal treatment and a subsequent controlled ammonolysis process. This synergistic approach combines two levels of materials engineering. First, the structuring of pore morphology to significantly increase the active surface area [2], and second, the partial substitution of oxygen atoms in the crystal lattice with nitrogen to precisely adjust the electronic structure and reduce the material's bandgap [3].
Results and discussion. A thorough physicochemical characterization validates these modifications. Structural analysis using XRD and Raman spectroscopy assessed crystallinity and lattice changes, while SEM examined the porous morphology. As well, XPS confirmed the surface chemical composition and effective nitrogen incorporation. A PEC filter-press reactor equipped with the developed photoanodes and operating under front illumination is applied for water oxidation. Carbon-supported Bi nanoparticles (Bi/C) are used as the cathode for the selective production of formate ($HCOO^-$) from CO_2 reduction. The catholyte (0.5 M KCl and 0.45 M $KHCO_3$ aqueous solutions) operates under a continuous CO_2 flow of 200 mL min^{-1}, whereas the anolyte contains 0.5 M $KHCO_3$; both electrolytes are circulated at 0.57 mL min^{-1}. The compartments are separated by a Nafion 117 membrane, and a leakfree Ag/AgCl reference electrode is employed. PEC tests include CP, LSV and EIS to investigate charge transport and bandgap, and oxygen production is quantified using microgas chromatography. The results are compared with our recent work on the development of BiVO4- based photoanodes for water oxidation [4]. This study amins to demonstrate that the ammonolysed films exhibit superior PEC activity compared to the pristine oxide, thereby validating this approach for optimising niobium-based photoanodes.

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CDU0135

Carbon capture and conversion to value-added products using a novel biphasic absorbent system

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: CO2 capture, Mineralization, Ionic Liquids, Carbonates, Ethanol

Abstract Body.

Introduction. Carbon capture and storage (CCS) is a key strategy for mitigating large-scale CO_2 emissions, with the potential to reduce over 6 Gt CO_2 annually by 2050. Although amine-based scrubbing is the most mature capture technology, its high regeneration energy demand remains a major limitation. Biphasic solvents offer a promising energy-efficient alternative by separating into CO_2-rich and CO_2-lean phases after absorption, enabling selective regeneration of only the rich phase [1]. This significantly reduces regeneration energy while allowing the captured CO_2 to be directly utilized for mineralization [2] to convert industrial waste to mineral carbonates or conversion into value-added fuels such as methanol and ethanol.

Methods. CO_2 absorption was performed in a biphasic amine system by bubbling CO_2 at 60 mL min^{-1} for 1 h into 100 mL of absorbent containing 10 wt% polyamine absorbent, 30 wt% water, and 60 wt% isopropanol. Absorption was carried out at 30–70 °C with stirring at 400 rpm until constant mass was achieved. The CO_2-saturated solution spontaneously separated into a CO_2-rich lower phase and a CO_2-lean upper phase. The CO_2-rich phase was isolated and used either for mineralization with CaO or blast oxygen furnace slag at ambient to 85 °C for 1 h, or for catalytic hydrogenation. For hydrogenation, the CO_2-rich phase was reacted with a Cu-based catalyst in a high-pressure batch reactor under 20 bar H_2 at temperatures up to 170 °C for 3–5 h, followed by product analysis.

Results and discussion. The solid products were analyzed using FTIR for functional groups, XRD for crystalline structure, TGA for mineralization efficiency, and FESEM for morphological features. Meanwhile, the liquid products were examined using NMR spectroscopy to determine their chemical composition, providing a comprehensive understanding of both solid and liquid phases.

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2026 / SEOUL, KOREA

CDU0167

Redox cycling of CH4 reforming and CO2 splitting over SrFeO3 with Ce doping effects on carbonation and stability

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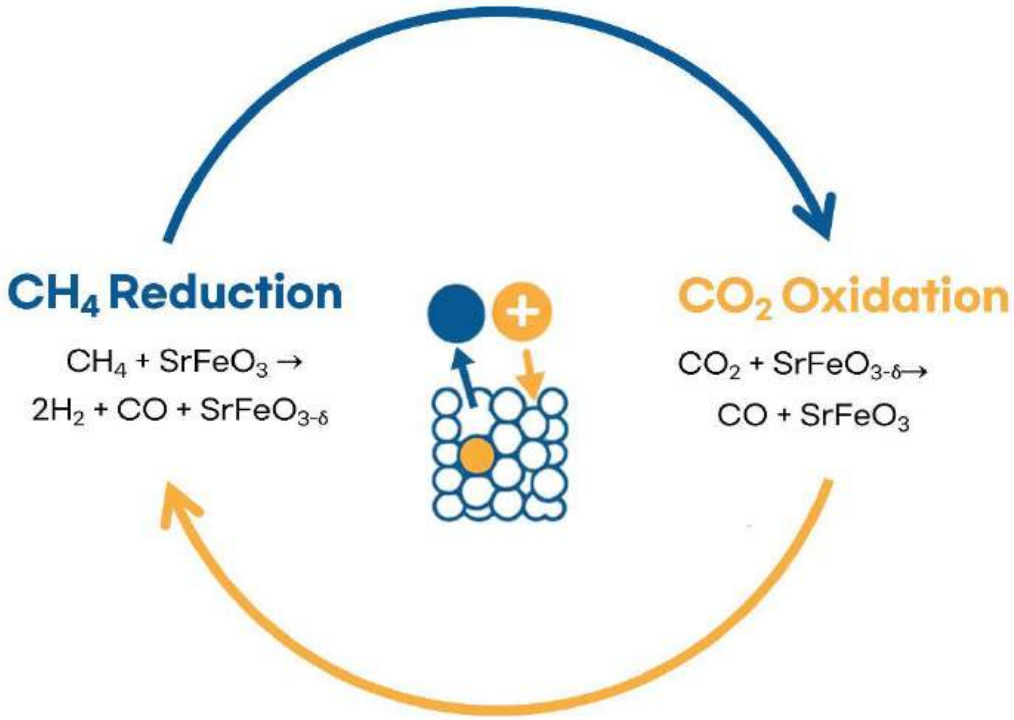
Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: Redox, methane reforming, CO2 splitting, synthesis gas, metal oxides

Abstract Body.
Perovskite-type SrFeO3 has been widely considered a promising oxygen carrier for CH4 reduction – CO2 splitting owing to its high oxygen mobility and reversible redox behavior. The CH4 reduction – CO2 splitting redox cycle enables simultaneous syngas (H2/CO) production and CO2 utilization as a reactant, rendering it an attractive pathway for carbon capture and utilization. However, under high CO2 atmospheres, Sr2+ at the A-stie of SrFeO3 can readily form thermodynamically stable SrCO3. Such carbonate formation can block surface active site and inhibit oxygen transport, thereby degrading redox reversibility and resulting in decreased reactivity and reduced long-term stability upon repeated cycling. Previous studies indicate that Ce doping can promote oxygen vacancy formation and latticeoxygen mobility and may improve phase stability and sintering resistance during long-term operation. Based on this literature, Ce-doped SrFeO3 was synthesized, and the effect of Ce doping on Sr carbonation behavior and redox performance during CH4 reduction – CO2 splitting was evaluated.
SrFeO3 and Ce-doped SrFeO3 were prepared via a sol–gel method. Experiments were conducted at 900 °C with a fixed CH4 concentration while the CO2 concentration was varied stepwise. Each CH4 reduction and CO2 splitting was conducted for 30 min, followed by an N2 purge for 60 min. To examine surface reaction pathways and carbonation behavior during cycling, in-situ DRIFTS was employed to observe the formation and accumulation of carbonate species and reaction intermediates as a function of CO2 concentration. Structural and chemical-state changes before and after reaction were examined by XRD and XPS, respectively, and microstructure and elemental distributions were analyzed by SEM/EDS. XRD patterns of the fresh SrFeO3 and Ce-doped SrFeO3 showed similar major diffraction features, indicating that the perovskite was retained upon Ce doping. In addition, no distinct carbonate-related reflections were detected for the fresh samples, which provide an initial baseline for assessing carbonate formation and accumulation induced under CO2 during cyclic redox. The Sr carbonation behavior of SrFeO3 and Ce-doped SrFeO3 is comparatively investigated, and the influence of Ce doping on surface reaction pathways and structural stability under CH4 reduction – CO2 splitting redox cycling conditions is evaluated by integrating in-situ and ex-situ characterizations.



Acknowledgement
This work was supported by “Syngas and Olefin Production Demonstration Technology Development Using By-product Gas and CO2” (Project No. RS-2022-NR068678) through the National Research Foundation (NRF) funded by the Ministry of Science and ICT (MSIT), Republic of Korea.

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CDU0179

Integrated CO2 capture and Utilization for CO production from ambient level CO2 using K/Al2O3

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: Keywords: Direct Air Capture (DAC); RWGS; transition-metal-free; potassium carbonate

Abstract Body.
Introduction. The reverse water–gas shift (RWGS) reaction is a pivotal pathway for converting CO2 into CO; however, it traditionally necessitates high operating temperatures (500–700 °C) and employment of transition-metal catalysts. Integrated CO_2 capture and utilization (ICCU) via dual-function materials (DFMs) offers a promising alternative by coupling CO_2 sorption with in situ conversion, effectively lowering the RWGS temperature to ≤500 °C. Despite these advances, most ICCU studies have focused on concentrated CO_2 streams, leaving the conversion of atmospheric level CO2 (~400 ppm) largely unexplored. In this study, we developed a transition-metal-free, potassium-based DFM for ICCU-driven production of CO from highly dilute CO_2. Furthermore, we evaluated the catalytic performance under realistic feed conditions, especially investigating the inhibitory effects of of O_2 and humidity.

Methods. The performance of a 15wt.% K2CO3-impregnated γ-Al_2O_3 DFM was evaluated in a fixed-bed reactor (0.15 g catalyst). Prior to each run, the DFM was pretreated at 450 °C for 2 h under 5% H_2/He (150 mL·min^{-1}), followed by a He purge to eliminate residual H_2. The ICCU cycle consisted of two steps at 450°C: (1) a capture step using 0.04% CO_2/He (150 mL·min^{-1}) for 2 h, and (2) a subsequent RWGS step under 5% H_2/He (150 mL·min^{-1}) for 2 h. To simulate ambient air conditions, O2 (20%) and water vapor (introduced via a bubbler) were selectively added to the feed during the capture step while maintaining the total flow rate and temperature constant.

Results and discussion. Carbonate-derived K/Al_2O_3 DFMs demonstrated effective CO production from atmospheric-level CO_2 (~400 ppm) at 450 °C. A series of DFMs with varying K loadings were synthesized to optimize performance. Among the samples tested, the 15 wt% K/Al_2O_3 DFM achieved the highest performance, delivering >90% CO_2 conversion with

100% CO selectivity under dry O_2-free conditions. Under an O_2-containing atmosphere, while the CO_2 capture capacity remained comparable to O_2-free conditions, the CO_2 conversion decreased by 42.7%. Furthermore, the introduction of humidity led to a 50.6% decline in CO_2 uptake relative to dry conditions. Overall, these findings demonstrate that K/Al_2O_3 DFMs can effectively drive highly selective ICCU from dilute sources without transition metals, although the observed performance degradation under O_2 and moisture underscores the need for more robust, impurity-tolerant DFMs for practical applications.

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2026 / SEOUL, KOREA

CDU0187

Design and Optimization of an Integrated Thermochemical CO2/H2O Co-splitting and Methanation for Green Methane Production

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: Green methane, CO2/H2O co-splitting, Methanation, Integrated process design

Abstract Body.
Introduction. Green methane from renewable energy and recycled carbon sources is an attractive carbon-neutral fuel because it is compatible with existing gas infrastructure. However, most power-to-methane concepts produce H2 in a separate electrolysis unit, which adds system-level burdens associated with storage, and transport. In addition, direct coupling of electrolysis with pressurized methanation is complicated due to differentialpressure constraints. Two-step thermochemical H2O splitting offers an alternative H2 route that can be more readily integrated with high-pressure operation. In addition, CO_2/H_2O cosplitting can generate CO together with H_2, thereby enhancing methanation. However, the water-gas shift reaction may increase CO2 byproduct formation. Therefore, the intermediategas composition must be optimized to maximize CH4 yield while minimizing CO2 byproduct and residual H2.
Methods. We design and experimentally demonstrate a lab-scale integrated green methane production process by coupling thermochemical co-splitting with Fe0.45(MgCoMn)0.55Oy, and methanation with Ni/Al2O3 catalyst using a fixed total carbon basis (CO + CO2). Results and discussion. We map the effects of the CO:CO2 and H2:(CO+CO2) ratios on CH4 yield, CO2 byproduct, and unreacted H2, and identify an optimal composition window and identify a representative target composition of CO:CO2:H2 ≈ 1:3:4 under the present operating condition. Then the target CO:CO2:H2 composition is converted to the upstream co-splitting step by determining the required CO2/H2O feed ratio and total flow rate to generate the desired mixture. This framework links methanation performance targets to thermochemical syngas production and thus provides quantitative composition specifications for future redox materials and reaction designs.
Acknowledgments
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2026 / SEOUL, KOREA

CDU0229

Highly efficient direct air CO2 capture and methane production over Rhodium-Modified LDH Dual-Functional Materials.

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: Direct air capture, Dual-functional materials, Integrated CO2 capture and utilization, Rhodium-Modified LDH

Abstract Body.

Purpose

Dual-functional materials (DFMs) that integrate CO2 capture and catalytic conversion offer a promising route for carbon-circular energy systems. However, most conventional DFMs are evaluated under high CO2 concentrations (5–15%), which does not reflect the requirements for direct air capture (DAC). This study investigates Rh-incorporated MgAl layered double hydroxide (LDH)-derived mixed oxides designed for ultra-dilute CO2 (400 ppm) capture and subsequent low-temperature methanation. The objective is to develop a material with high adsorption affinity and catalytic efficiency under ambient-level CO2 conditions.

Methods

Rh-modified MgAl-LDHs were synthesized through a one-pot hydrothermal route and calcined at 400 °C to produce highly dispersed mixed metal oxides. The CO2 uptake capacity was measured using NDIR-based breakthrough analysis, and CH4 production was quantified via GC-FID. The integrated DFM cycle consisted of three stages: H2 activation at 320 °C, CO2 capture at 250 °C (400 ppm), and isothermal methanation in H2 at 250 °C. To evaluate practical robustness, the materials were exposed to simulated air (20% O2) and humidified streams.

Results

At a CO2 concentration of 400 ppm, the Rh-modified DFMs exhibited substantial adsorption capacities, reflecting the high thermodynamic affinity of the LDH-derived basic sites for CO2 under dilute conditions. During the subsequent hydrogenation step, the materials achieved over 80% CO2 conversion with high methane selectivity between 250–320 °C. This suggests an efficient coupling between the basic sites of the LDH matrix and the Rh active sites for low-temperature catalysis. Notably, the DFM maintained its performance even after exposure to 20% O2, showing that the material remains stable and active under oxygencontaining conditions. Tests under humidified streams further indicated that H2O did not significantly inhibit the capture or conversion process. Long-term stability was confirmed through 10 consecutive capture/methanation cycles, where both CO2 breakthrough capacity and CH4

yield remained stable without detectable degradation. These results highlight the material's ability to handle the impurities and dilute concentrations inherent in direct-air applications.

Conclusions

This study demonstrates that Rh-incorporated LDH-derived mixed oxides are effective DFMs for 400 ppm CO_2 capture and low-temperature methanation. The materials are stable under 20% O_2 and humidified conditions, addressing key challenges for practical carbon recycling from the atmosphere. By enabling both capture and conversion at 250 °C, these DFMs offer a pathway to reduce energy consumption in carbon utilization processes. These findings support the feasibility of using LDH-derived materials for scalable and carbonneutral energy production.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

CDU0249

Scaling up CO_2 Electroreduction to Formate for Industrial Pilot Plant demonstration

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: CO2 electroreduction; Pilot plant; Scale up; Formate

Abstract Body.
Introduction. The electrochemical reduction of CO2 into value-added chemicals has gained significant traction as a sustainable strategy for carbon utilization and renewable energy storage. Among various products, formate is particularly attractive due to its diverse industrial applications and its potential as a high-density liquid hydrogen carrier [1,2]. While laboratory-scale advances have achieved Faradaic efficiencies (FE) above 90%, transitioning this technology to industrial environments requires addressing critical engineering challenges associated with scaling and long-term stability. This work presents the design, construction, and experimental validation of a 100 cm2 electrolyzer prototype integrated into a pilot plant capable of processing 2 L·min-1 of CO2.
Methodology. The electrolyzer was constructed using an Ir-MMO anode, a Nafion 117 membrane, and a Bi2O3-based GDE [3], working with a 1 M KCl liquid catholyte and 1.5 M KOH anolyte. The pilot plant incorporates automated data acquisition systems, including gas analyzers and sensors for flow and temperature, aimed at developing a digital twin. Results and discussion. Initial performance tests across current densities ranging from 45 to 300 mA·cm-2 identified 200 mA·cm-2 as the optimal operating point, achieving a maximum FE for formate of 92%. However, stability tests conducted over 20 cumulative hours (5 hours per day) revealed a degradation trend, as seen in Figure 1, with formate FE dropping from 75% on the first day to 26% on the fourth. This decline is attributed to the deactivation of GDE due to salt deposition, flooding, or catalyst detachment.
To enhance the competitiveness of this technology, future research must focus on stackbased configurations to increase production capacity and GDE optimization to extend operational life. Furthermore, improving energy efficiency by coupling CO2 reduction with alternative oxidation reactions, such as glycerol oxidation, could significantly reduce cell potential and operational costs. This study provides a foundational step toward the industrial deployment of CO2 electrolysis systems.

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CDU0308

Rational design of Cu-MWW catalyst for enhanced CO2 conversion

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: Cu-MWW; CO2 conversion; Methanol synthesis; RWGS reaction

Abstract Body.

Introduction. The incorporation of metal species into zeolitic frameworks is a common strategy in catalyst design, as the coordination environment and dispersion of metal strongly influence catalytic performance. Borosilicate MWW-type (B-MWW) zeolite is attractive due to its layered nature and facile heteroatom substitution, leading to the formation of metallosilicates with enhanced external surface area and accessible active sites [1]. Copper incorporation into zeolite framework can stabilize Cu species in defined coordination environments and effectively disperse the active metals [2]. In this study, Cu-MWW was explored as catalytic materials for CO2 conversion, with emphasis on the role of the MWW framework in regulating Cu accessibility and catalytic behavior for sustainable carbon transformation.

Methods. Cu-MWW catalysts were prepared via a one-pot hydrothermal treatment of BMWW(P) using different concentrations (0.01–1.00 M) of aqueous Cu(NO3)2 solutions, followed by washing, drying, and calcination, and finally denoted as Cu-MWW(x), where x represents the Cu precursor concentration.

Results and discussion. Figure 1 compares the CO2 conversion in the reverse water-gas shift (RWGS) and methanol synthesis reactions over different Cu-MWW(x) catalysts with x = 0.01–1.00. As the Cu loading increases from 1.2 to 47.0 wt.%, the CO2 conversion exhibits a volcano-type trend in both reactions, reaching maximum values at a Cu loading of 21.9 wt.% (Cu-MWW(0.25)), with 47.1% conversion in the RWGS reaction and 17.4% in methanol synthesis. Hydrothermally synthesized Cu-MWW exhibits an enhanced external surface area and tunable Cu speciation, which together facilitate the effective dispersion and stabilization of Cu active sites. Among the different Cu species, highly dispersed extraframework Cu, predominantly in the Cu+ state after reduction, plays a dominant role in promoting CO2 conversion in both the RWGS reaction and methanol synthesis. These results highlight a clear structure–performance relationship, underscoring the importance of controlling Cu distribution within zeolitic frameworks for efficient CO2 conversion.

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2026 / SEOUL, KOREA

CDU0318

CO2 Methanation for Energy Transition: A Study on Flow Rate Variability, and on the role of Steam in Transient Operation

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: Carbon Capture and Utilization, CO2 Methanation, Power to Gas,Fuel Synthesis

Abstract Body.

Introduction. Carbon Capture and Utilization (CCU) techniques can be combined with green hydrogen to produce synthetic fuels, like Synthetic Natural Gas (SNG), in Power to Gas applications [1]. However, due to the known intermittency of renewable energy, the production of green hydrogen is highly unstable. In this work, we have investigated the effect of the flow rate variability and of the steam injection on the methanation performance.

Methods. To assess the impact of unstable conditions, experiments were carried out in a lab-scale fixed bed reactor by changing operating parameters such as Gas Hourly Space Velocity (GHSV), the ratio between the reactants, and the introduction of steam in the feed gas. The goal was to simulate the effect obtained in processes such as VESTA [2], using a commercial nickel catalyst, but in milder conditions compared to industrial applications (e.g. pressure was kept constant to 1 bar).

Results and discussion. The effect of actual GHSV and H2/CO2 were studied in the range [15000-25000 h-1] and [2-4], respectively. The results were compared to thermodynamic simulations carried out in Aspen+. The lower the residence time, the farther the system was from equilibrium, with an increasing presence of CO as intermediate and of solid carbon (Figure 1). Furthermore, in the lean-H2 scenarios the presence of undesired products was enhanced. The proposed solution for the transition periods was the introduction of steam in the feed, which can avoid the formation of solid carbon and significantly diminish the presence of CO. For example, with just 10% of steam the yield in CO for GHSV=25000h-1 and H2/CO2 =2 dropped from 3.75% to 1.82%. These preliminary results suggest that the recommended approach is worth of further investigation.

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CDU0338

Synthesis of sustainable polyurethanes using CO2 as a feedstock

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: CO_2, polyurethanes, CO_2-based polyol

Abstract Body.
Polyurethanes, widely used in various industries, are primarily derived from non-renewable fossil resources. The excessive dependence of the chemical industry on petroleum-based feedstocks contributes to the acceleration of global warming. To achieve net-zero emissions, there is a growing demand for sustainable materials that minimize the use of fossil resources, reduce CO_2 emissions, and enable the utilization of captured CO_2. In response to these demands, this study aims to replace one of the key components of polyurethanes with CO_2-based alternatives.

In this study, CO_2-based polyols were synthesized via Zn-gallate-catalyzed process. The synthesized CO_2-based polyols were subsequently used to prepare polyurethanes in combination with isocyanates and a chain extender. The effects of compositions and structures of CO2 polyols on the thermal and mechanical properties of the resulting polyurethanes were systematically investigated.

The properties of the prepared polyurethanes were evaluated using differential scanning calorimetry (DSC), thermogravimetric analysis (TGA), Shore hardness testing, and tensile strength measurements. The results demonstrate that the thermal and mechanical properties of polyurethanes can be effectively tuned by adjusting the PU composition.

This study confirms the feasibility of synthesizing polyurethanes based on CO_2-derived polyols, providing a practical pathway for converting captured CO_2 into high-value polymeric materials. The resulting CO_2-based polyurethanes offer a promising alternative for reducing fossil resource dependence while maintaining the required material properties, thereby contributing to the development of sustainable polyurethane materials and the large-scale utilization of CO_2.

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CDU0341

Zinc-gallate-catalyzed terpolymerization using CO2

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: CO2-polymer; Zn-gallate; terpolymerization; CO2 utilization.

Abstract Body.
Carbon dioxide (CO2) is unavoidably emitted from fossil fuel combustion and industrial activities and is regarded as a major contributor to global warming. To address the urgent need for CO2 utilization in climate change mitigation, this work presents a highly efficient Zngallate-catalyzed terpolymerization approach that incorporates CO2 into the polymer chains. By precisely controlling the monomer composition, we successfully synthesized polymers with distinct architectures, including random and block-type structures. Furthermore, variation of reaction pressure and the use of different chain transfer agents (CTAs), such as linear diols and branched polyols, enabled the formation of polymers with diverse architectures. The influence of polymer structure on adhesive performance was also systematically investigated. The properties of the synthesized polymers were characterized using DSC, TGA, GPC, 1H NMR, DOSY NMR, lap shear testing, and tensile testing.

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CDU0342

Effect of ZrO2 Phase on Ethanol Synthesis over Rh–Fe Catalysts from Syngas

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Abstract Category: Heterogeneous/Homogeneous Catalysis - Heterogeneous Catalysis - Thermal

Keywords: Ethanol, CO hydrogenation, Zirconia support, Crystal phase effect

Abstract Body.

Introduction. The selective production of ethanol from syngas remains challenging, although Rh/Fe-based catalysts have shown promising performances. However, catalysts without Rh/Fe exhibit low ethanol selectivity and STY [1]. When different types of supports were examined, zirconia (ZrO2)-supported catalysts achieved higher ethanol selectivity and space–time yield (STY) [2], highlighting the crucial role of the support. ZrO2 is particularly attractive because of its acid–base properties and high stability [3], and its different crystalline phases can further influence metal interactions and catalytic performance.

Methods. In this study, ZrO2 supports with different crystal phases and structures were prepared using various synthesis methods. Commercial ZrO2 (Sigma-Aldrich) was used as a benchmark, while tetragonal ZrO2 (t-ZrO2) was synthesized via sol–gel and precipitation methods. Amorphous ZrO2 was prepared using xerogel and aerogel methods. Rh–Fe-based catalysts were impregnated on as-prepared ZrO2 supports, and their crystal phases were identified by X-ray diffraction (XRD).

Results and discussion. XRD results showed that ZrO2 prepared by sol–gel and precipitation methods were predominantly in the tetragonal phase, whereas the commercial ZrO2 showed a monoclinic phase. The amorphous structures were observed for ZrO2 prepared by xerogel and aerogel methods. Among as-prepared catalysts, the best-performing catalyst was prepared by t-ZrO2, showing an ethanol selectivity of 30.76% and an ethanol STY of 102.6 mg·gcat-1·h-1. This enhancement can be attributed to the higher oxygen vacancy concentration and phase-dependent metal-support interactions of t-ZrO2, as reported for metal/ZrO2 systems [4]. Overall, this work demonstrates that precise control of the ZrO2 crystal phase can be a key factor in designing efficient Rh–Fe catalysts for selective ethanol synthesis from syngas.

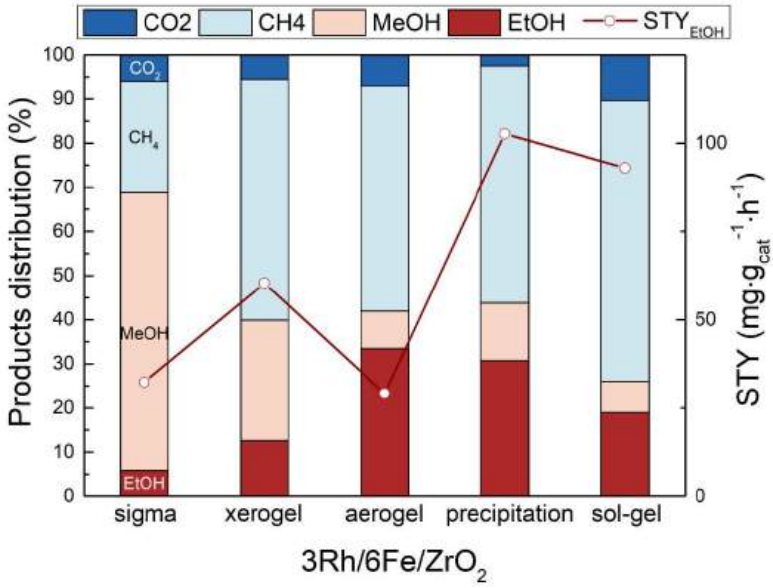

Figure 1. Product distribution and ethanol STY over Rh/Fe catalysts supported on different ZrO_2. (H2/CO = 3, 260 °C, 3 MPa, 9,000 mL·g −1·h−1)

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Impact of Reaction Conditions on the Synthesis of Methanol from a Combined CO and CO2 Feedstock

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: Methanol, CO2 utilization, Methanol synthesis, Catalyst

Abstract Body.
Methanol is a vital chemical commodity that acts as a precursor for numerous compounds, such as formaldehyde, methyl-tert-butyl ether (MTBE), dimethyl ether (DME), and acetic acid. Additionally, it plays an essential role in the manufacture of plastics, resins, paints, adhesives, and other materials commonly used in daily human activities [1-2]. Recently, there has been a concerted effort to develop a direct method for producing methanol without relying on fossil fuels. This method seeks to use carbon dioxide that is either already present in the environment or captured before its release, along with hydrogen generated from renewable energy sources [3], to produce methanol. In this study, the catalytic activity of a commercial catalyst was examined by altering the reaction conditions, including pressure, gas hourly space velocity (GHSV), and temperature.
The performance of the catalyst was assessed using a fixed-bed reactor, as depicted in Figure 1. Online gas chromatography (GC) was used to analyze the gas-phase products resulting from methanol synthesis. The reactivity of the catalyst was verified across a spectrum of reaction conditions, which led to the production of methanol. It was established that a decrease in the gas hourly space velocity (GHSV) enhances the catalyst reactivity, and the reaction only begins when the temperature surpasses a specific threshold. Additionally, it was confirmed that increasing the reaction pressure boosted the catalytic activity of the catalyst used in methanol synthesis.

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CDU0364

Reverse Water–Gas Shift over Reduced Spinel-Derived Cu-Al Oxide Catalysts

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: CCU. Reverse water–gas shift. Cu/Al2O3 catalyst

Abstract Body.

Introduction. The reverse water–gas shift (RWGS) reaction is a key CO2 utilization route that produces CO as a versatile carbon feedstock, and Cu-based catalysts are widely studied for selective CO formation [1]. For Cu-based RWGS catalysts, catalytically relevant active sites are generated during reduction; therefore, the oxidized precursor state prior to activation governs the nature of reduced Cu0 sites and Cu0–support interfacial structures formed under reaction-relevant conditions. In this study, we investigate how high-temperature calcination of impregnated Cu/Al2O3 alters the Cu-Al precursor state and the resulting reduced Cu0 sites relevant to RWGS. .

Methods. Cu/Al2O3 catalysts with Cu loadings of 5, 10, 15, and 20 wt% were prepared by incipient wetness impregnation. After drying, the catalysts were calcined in air at either 600oC or 950oC to obtain two sets of oxidized precursors. Phase information was examined by X-ray diffraction (XRD). Reducibility of the oxidized precursors was evaluated by H2 temperature-programmed reduction (H2-TPR). Specific surface area was measured by N2 physisorption (BET method). Catalytic performance was tested in the RWGS reaction at 500oC.

Results and discussion. XRD-based identification of CuAl2O4 in the high-temperaturecalcined samples is not straightforward because diffraction features assigned to CuAl2O4 substantially overlap with those of Al2O3, limiting unambiguous discrimination by XRD alone. H2-TPR profiles of the 950oC-calcined catalysts were shifted to higher reduction temperatures relative to the 600oC-calcined catalysts, indicating the formation of more strongly bound Cu-Al species in the high-temperature-calcined precursors. This change in reducibility is expected to influence the generation of metallic Cu (Cu0) during activation and the resulting Cu0–support interfacial configuration.

The catalytic consequence of precursor variation was evaluated in RWGS at 500oC. The catalyst calcined at 950oC exhibited higher activity than the counterpart calcined at 600oC. BET measurements showed a pronounced decrease in specific surface area after calcination at 950oC; nevertheless, RWGS activity increased, suggesting that performance

is not governed simply by textural factors but rather by modified Cu-Al precursor interactions and the resulting reduced Cu0 sites responsible for RWGS. These findings demonstrate that high-temperature calcination can serve as a precursor-engineering strategy for impregnated Cu/Al2O3 RWGS catalysts.

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CDU0372

Inducing Structural and Electronic Alterations of Ceria for Activating Low-Temperature Reverse Water-Gas Shift Reaction

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: CO2 conversion, RWGS, CeO2, Mg-modified

Abstract Body.
Introduction. The global reliance on traditional fossil fuels has significantly contributed to the escalation of greenhouse gas emissions, particularly carbon dioxide, aggravating climate change with evident temperature rises and unpredictable weather patterns. Addressing this pressing environmental challenge requires innovative approaches, with one promising strategy being the utilization of carbon dioxide to value-added chemicals [1]. The reverse water-gas shift reaction (RWGS), an endothermic CO2 conversion reaction that is crucial for carbon monoxide production and sustainable fuel synthesis with renewable hydrogen.
Methods. CeO2 is widely studied for RWGS catalysis due to its oxygen vacancies, redox properties, and strong metal–support interactions [2]. In this work, the catalytic performance of CeO2 was enhanced through Mg incorporation using a facile synthesis approach. A series of Mg-modified CeO2 catalysts with varying Mg contents was prepared, systematically characterized, and evaluated in a fixed-bed reactor.
Results and discussion. By leveraging Mg properties to promote activity, a CO2 conversion of 12.20% at a lower reaction temperature of 400°C was achieved. Characterization techniques confirmed that low Mg content ensured good dispersion, while excess Mg formed MgO phases on the surface. The possible substitution of Ce4+ by Mg2+ increased the electron density of oxygen atoms, promoting Lewis basic sites and oxygen vacancy formation. However, higher Mg content also increased the H2/CO ratio, suggesting potential retention of H2 and reduced catalytic efficiency. Overall, Mg incorporation strategically modifies CeO2 structure and surface chemistry, facilitating low-temperature activation and hence, contributing to the development of more efficient catalysts for sustainable chemical processes.
Acknowledgments
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CDU0376

Catalyst and Process Design Driven Facilitation of Commercial Single-Amine CO_2-to-Formic Acid Conversion

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: CO2 Conversion and Utilization, Reactive Capture and Conversion, CO_2 Hydrogenation, Process Design and Optimization

Abstract Body.

Amine-promoted CO_2 hydrogenation provides a thermodynamically favorable route to formate formation; however, purification challenges have led conventional process designs to rely on dual-amine schemes, as the limited reactivity of weak-base amines has long been perceived as a fundamental barrier to single-amine operation. While effective from a separation standpoint, dual-amine processes introduce an additional amine-exchange step, increasing process complexity and, critically, low-pressure steam demand. Herein, we demonstrate that this long-standing trade-off between reaction performance and separability can be overcome through a catalyst-to-process integrated strategy, enabling a unified singleamine CO_2-to-formic acid (FA) process using n-butylimidazole (NBIM) as both the reaction amine and the separation handle.

From a catalytic perspective, the weak basicity of NBIM inherently constrains reaction kinetics and equilibrium conversion, making catalyst selection a decisive design variable. Accordingly, catalyst systems were systematically screened under identical conditions, identifying Ru-MACHO-POMP as the most effective system, capable of simultaneously enhancing reaction rates and shifting the equilibrium toward high acid-to-amine ratios. At 80 °C and 80 bar in 1.0 M aqueous NBIM, Ru-MACHO-POMP achieved a formic acid productivity of 53,230 g_FA kg_cat^{-1} day^{-1} and approached an equilibrium acid-to-amine ratio (AAR) of approximately 0.9. This elevated AAR provides sufficient separation leverage while maintaining practical reaction rates, rendering single-amine operation viable despite the weak-base nature of NBIM.

From a process-design perspective, rigorous simulation and techno-economic analysis were conducted for a plant treating 100,000 t CO_2 yr^{-1}. The resulting NBIM-based single-amine flowsheet achieves a levelized production cost of \$0.583 kg^{-1} for 85 wt% FA, corresponding to an approximately 31% reduction relative to a conventional benchmark process at the same purity (\$0.84 kg^{-1}). Operating expenditures dominate the total cost, with low-pressure steam consumption for water removal identified as the primary economic bottleneck, indicating that separation energy—not reaction performance—ultimately governs commercial viability.

Life cycle assessment further confirms this process-level insight, revealing that steam demand similarly dominates environmental performance, yielding a baseline global warming impact of 4.87 kg CO_2-eq kg_FA^{-1}. Importantly, replacing steam-based evaporation with electricity-driven mechanical vapor recompression (MVR) reduces this impact to 0.63 kg CO_2-eq kg_FA^{-1}, underscoring that shifting separation energy demand from thermal to electrical inputs is a critical lever for both cost and emissions reduction. Collectively, this study demonstrates that catalyst-enabled recovery of reactivity in weak-base systems, combined with energy-aware separation design, can overturn the long-standing reliance on dual-amine processes and establishes NBIM-based single-amine CO_2-to-formic acid conversion as a viable and scalable platform for commercial deployment.

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CDU0380

Mn-Promoted Cu–Fe/MgAl2O4 Catalysts for LowTemperature RWGS Reaction: Role of Metal–Oxide Interfaces

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: Reverse water gas shift reaction, Mn promoted Cu–Fe/MgAl2O4, CO2 adsorption, Oxygen vacancy, Interfacial interaction

Abstract Body.

Carbon Capture and Utilization technologies have emerged as a key strategy for mitigating climate change by converting captured CO2 into value-added chemical feedstocks. Among these technologies, the reverse water–gas shift (RWGS) reaction, which converts CO2 and H2 into CO, is a critical step for downstream syngasbased processes such as Fischer–Tropsch synthesis. Although the endothermic RWGS reaction is thermodynamically favored at elevated temperatures, operation above 800 °C causes catalyst sintering, high energy demand, and limited compatibility with downstream processes operating at 300–450 °C. Therefore, developing catalysts that exhibit high activity and long-term stability at moderate temperatures is essential. Cu-based catalysts exhibit high CO selectivity in RWGS but suffer from severe sintering due to poor thermal stability. Although Fe promotion can improve thermal stability, iron carbide formation during RWGS may induce carbon deposition. As an alternative strategy, MnOx has attracted attention as a promoter capable of enhancing Cu and Fe dispersion while suppressing carbon deposition. Nevertheless, a systematic understanding of the effect of Mn content on low-temperature RWGS performance remains limited.

Herein, the influence of Mn loading on the low-temperature RWGS performance of Mn promoted Cu–Fe/MgAl2O4 catalysts was investigated. A series of catalysts with Mn contents ranging from 0 to 5 wt% were prepared via an ultrasonic-assisted method to achieve high metal dispersion. RWGS performance was evaluated at 300–450 °C, and the physicochemical properties were characterized using XRD, H2-TPR, N2O-pulse, and CO2TPD analyses.

The RWGS performance exhibited a non-linear dependence on Mn content. Compared to the Mn-free catalyst, the catalyst containing 1 wt% Mn resulted in lower activity, whereas the highest catalytic performance was achieved at a Mn loading of 2.5 wt%. However, further increasing the Mn loading to 5 wt% led to a decrease in activity. The optimal catalyst with 2.5 wt% Mn achieved a CO2 conversion of 41.0% at 400 °C under a gas hourly space velocity of 360,000 mL $gcat^{-1}$ min^{-1}. This behavior is attributed to enhanced metal dispersion and an

increased concentration of oxygen vacancy induced by MnOx, which promote CO2 activation at optimal Mn loadings. In contrast, excessive Mn incorporation alters the catalyst structure and weakens metal–support interactions.

In addition, compared to the Mn-free catalyst, the optimal catalyst maintained stable RWGS performance at 400 °C for 20 h. These results demonstrate that controlled Mn promotion is an effective strategy for designing Cu–Fe-based catalysts with enhanced activity and durability for low-temperature RWGS.

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CDU0388

Sorption-Enhanced Methanation with 3D printed NiCe/zeolite 13X catalyst

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: CO2 Utilization, Sorption enhanced methanation, 3D printed catalyst

Abstract Body.

The decarbonization of energy- and carbon-intensive sectors is pushing for the development of Power-to-Gas routes, in which renewable hydrogen is combined with carbon dioxide to produce synthetic natural gas (SNG). CO2 methanation is an attractive pathway for the wide availability of catalytic materials and the production of grid-compatible fuel. In particular, 3D printed monolithic materials allow to fine tune the geometry aiming to improve mass and heat transport, flow distribution, and catalyst lifetime. Since CO2 methanation is an exothermic reaction and thermodynamically limited, often affected by mass transfer limitations, 3D printed structured catalyst allow to adjust geometrical and material properties to better fit the reaction demands. Therefore, this work investigates an additivemanufacturing route to structured, bifunctional material by fabricating zeolite 13X–based ceramic monoliths via vat photopolymerization and subsequently introducing a Ni–Ce active phase. In particular, the zeolite 13X body provides CO_2 sorption capacity, exploiting LeChatelier principle pushing the equilibrium towards the products, while the Ni–Ce phase supplies the catalytic function for methanation. This allows the integration of product water removal and CO2 conversion within a single structured body. After printing and post-curing, the green bodies were subjected to iterative post-treatments to enhance structural integrity and manage dimensional changes while preserving access to the internal channel network. The catalytic functionality was then introduced by wet impregnation using Ni and Ce precursors. Initial deposition trials indicated that metal uptake and spatial uniformity across the monolith could be improved; therefore, a revised impregnation approach is being implemented alongside sectioning-based checks of distribution. A coordinated characterization campaign is being used to connect processing and deposition conditions to support properties, sorption behaviour, and active-phase dispersion. Planned characterization includes N_2 physisorption (BET), XRD, H_2-TPR, CO_2-TPD, SEM/TEM, and STEM-EDX. Methanation testing will be carried out to evaluate temperature, H_2/CO_2 ratio, and space velocity effects on the performance. Overall, the study establishes a practical framework for producing 3D-printed, zeolite-based structured bodies functionalized with Ni–Ce to realize bifunctional sorption–catalysis systems for CO_2 conversion to methane.

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CDU0406

Bi-Reforming of Methane over Ni/CeSiOx Catalyst: A Synergistic Effect of Oxygen Vacancy and Metal-Support Interaction

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: Bi-reforming, Ni/CeSiOx, Syngas, Oxygen storage capacity

Abstract Body.

Introduction. Metal-support interaction (MSI) is one of the most important factors determining the catalytic performance of supported metal catalysts. Among the various oxide materials, CeO2 has attracted considerable attention as a catalyst support due to its ability to generate oxygen vacancies (Ov) via the Ce3+/Ce4+ redox transition, providing high oxygen storage capacity (OSC) and enhanced MSI [1]. The incorporation of Si into CeO2 induces lattice distortion and increases Ov concentration, leading to the formation of CeSiOx mixed oxides that are favorable for stabilizing metal species and suppressing carbon deposition. In this study, Ni/CeSiOx catalysts with different Si contents were applied to the bi-reforming of methane (BRM) to elucidate the role of Ov and MSI on the catalytic performance. Methods. CeSiOx mixed oxides were prepared by hydrothermal treatment of tetraethyl orthosilicate (Si(OC2H5)4) and cerium nitrate (Ce(NO3)2) mixed solutions at 100 °C for 24 h, followed by washing, drying, and calcination. Ni/CeSiOx catalysts were prepared by deposition–precipitation (DP) and incipient wetness impregnation (IWI) methods using nickel nitrate aqueous solution and calcined at 500 °C for 6 h. The resulting catalysts were denoted as y-Ni-CS(x), where y and x represent the synthesis method (DP or IWI) and the Si/(Si+Ce) molar ratio in support, respectively.

Results and discussion. The influence of surface OSC on CH4 and CO2 conversions during BRM was compared over DP-Ni-CS(x) and IWI-Ni-CS(x) catalysts (Figure 1). It can be observed that the CH4 and CO2 conversions over DP-Ni-CS(x) catalysts are more strongly influenced by surface OSC than those over IWI-Ni-CS(x) catalysts. This can be explained by the stronger MSI between Ni and the support on DP-Ni-CS(x) catalysts, which arises from the smaller NiO particles, as confirmed by XRD analysis. As the Si content increased from 0.0 to 1.0, both CH4 and CO2 conversions exhibited a volcano-shaped trends with maxima

in at x = 0.2 over DP-Ni-CS(x) catalysts. The CH4 and CO2 conversions of DP-Ni-CS(0.2) was 98 and 76%, respectively, without coke formation. However, these increases in CH4 and CO2 conversions with the increase of Si content were less significant over IWI-Ni-CS(x) catalysts. These results demonstrate a synergistic effect between surface OSC and MSI of Ni/CeSiOx catalysts on the catalytic performance on BRM.

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CO2-derived Carbon Coated Si anode via Tandem process for Li-ion Battery

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: Carbon utilization, CO2 methanation, CH4 pyrolysis, Thermocatalyst, Lithiumion battery, Silicon anode

Abstract Body.
Conventional CO2 utilization has largely focused on fuels and commodity chemicals, whereas direct upcycling of greenhouse gases into battery anode materials remains comparatively underexplored. Meanwhile, Silicon (Si) anodes offer high theoretical capacity but suffer from severe volume expansion, motivating carbon-coating strategies. Here, we present a two-step continuous tandem process that couples CO2 methanation in Step 1 with CH4 pyrolysis in Step 2 to synthesize carbon-coated silicon (Si@C) as a Li-ion battery anode material. In Step 1, CO2 is converted to CH4 over a 30 wt.% Ni/SiO2 thermocatalyst, generating a CH4-rich effluent that directly feeds Step 2. In Step 2, Si is positioned within the CH4 pyrolysis environment to enable formation of solid carbon layer on the Si surface, thereby transforming a CO2-derived carbon pathway into a practical coating strategy for Si anodes. To achieve sufficient carbon deposition, the coating duration was varied (1, 3, and 5 h), producing (T)Si@C_1h, (T)Si@C_3h, and (T)Si@C_5h (T: Tandem). The tandem process was quantified by reporting Step 1 CO2 methanation metrics, including CO2 conversion of 91.2 %, CH4 selectivity of 93.7 %, and CH4 yield of 85.5 % which collectively characterize the effective feed composition delivered to the downstream Step 2 under prolonged operation. Under these conditions, the amount of solid carbon deposited on Si was quantified as a solid carbon yield of 14.9, 20.4, 35.5 % (g/g), demonstrating that the CO2 methanation-derived CH4 stream can serve as an integrated carbon source for Si surface coating. Also, longer deposition times led to rougher carbon layer morphology, with with (T)Si@C_5h showing the roughest surface and (T)Si@C_1h the smoothest. Electrochemical evaluation revealed distinct first-cycle behavior consistent with morphologydependent SEI formation, delivering initial discharge/charge capacities of 3177/2562 mAh g1 (ICE: 80.6 %) for (T)Si@C_1h, 3041/2399 mAh g-1 (ICE: 79.9 %) for (T)Si@C_3h, and 2741/2055 mAh g-1 (ICE: 75.0 %) for (T)Si@C_5h, respectively. Overall, this work demonstrates a process-to-material translation in which a continuous CO2→CH4→solid carbon route is validated for silicon carbon coating and initial electrochemical feasibility. The proposed tandem process provides a practical platform for connecting greenhouse gas conversion with value-added energy-storage materials manufacturing, while future optimization of effluent composition and deposition conditions is expected to further improve coating efficiency and electrochemical performance.

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CDU0420

Economic Feasibility of Power-to-Liquid e-Kerosene: Process and Policy Perspectives

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: CO2 hydrogenation, Modified Fischer-Tropsch, E-fuel, e-kerosene, TEA

Abstract Body.
Introduction.
The economic viability of Power-to-Liquid (PtL) fuels strongly depends on the cost of renewable hydrogen, electricity supply conditions, and regulatory frameworks. This work presents a comprehensive techno-economic assessment of e-kerosene production via CO2-modified Fischer-Tropsch (MFT) synthesis, comparing it with conventional Fischer-Tropsch (FT) and Alcohol-to-Jet (AtJ) pathways.

Methods.
Experimental data obtained with a Na-Fe3O4 catalyst [1] were used to develop and simulate multiple CO2-modified Fischer-Tropsch (MFT) process scenarios, including the effect of CO recirculation. Detailed heat and mass balances were integrated with a water electrolyzer (WE) economic model to construct a comprehensive techno-economic assessment (TEA) for e-fuel production. A composite pricing methodology, consistent with current EU mandates and policy mechanisms, was developed to estimate the potential market values of e-naphtha, e-diesel, and e-kerosene. MFT performance was benchmarked against conventional FT and Alcohol-to-Jet (AtJ) pathways [2]. Finally, sensitivity analyses identified the most influential cost drivers and were extended to explore how real market mechanisms could affect e-fuel adoption and the potential impact on end consumers.

Results and discussion.
MFT showed very high carbon efficiency (>99%) and competitive energy efficiency (up to 56%), with a product distribution more shifted towards kerosene and naphtha compared to conventional FT and AtJ routes. Break-even production costs for e-fuels were estimated at 4000–5000 €/t, in line with these benchmark pathways. Around half of the total cost was linked to electricity for hydrogen production, while roughly 20% was associated with capitalrelated expenses, a large share of which stemmed from the WE investment. Geographically resolved scenarios across EU countries highlighted how local electricity prices and availability can shift e-kerosene costs by several thousand euros per ton, confirming the decisive role of regional energy mixes. Market analysis further indicated that, under supportive policies, partial redistribution of the additional cost of e-kerosene across larger fossil fuel markets could significantly limit increases in jet fuel prices and airfares.

Overall, the large-scale deployment of e-fuels will depend not only on technological improvements but also on coordinated industrial strategies and strong energy and climate policy support.

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Effect of unconverted CO recirculation on CO2-modified Fischer-Tropsch Synthesis

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: Modified Fischer-Tropsch synthesis, CO2 and CO co-hydrogenation, E-fuels, Fe-based catalyst

Abstract Body.
Introduction. In recent years, CO2-modified Fischer-Tropsch Synthesis (FTS) has emerged as a promising route for producing synthetic liquid hydrocarbons (HCs), reducing dependence on fossil fuels. This work investigates the effect of recirculating unconverted CO during CO2-modified FTS over a 5 wt% Na-Fe3O4 catalyst offering important industrial insights on the optimal syngas mixture composition that maximizes conversion and yield to liquid HCs.
Methods. The Na-Fe3O4 catalyst was synthetized according to the protocol reported by Tauro et al. [1] and then pelletized in the range 200-500 µm. Prior to the tests, the catalyst was reduced (90% H2/N2, 450 °C, 2 bar, 16 h) and then carburized (50% CO/H2, 400 °C, 2 bar, 5 h) [1]. Catalytic tests were performed in a fixed bed reactor flowing 7 NL/h/gcat of reactant mixture at 360 °C and 23 bar. Starting from a stoichiometric mixture (H2/CO2 = 3), tests were subsequently carried out with an inlet CO composition of 5, 10 and 15 vol.%, maintaining a stoichiometric H2/(CO2 + CO) molar ratio between 2 and 3. The gas phase was analyzed using an in-line Gas Chromatograph, whereas the two oil phases, separated at 150 °C and 5 °C, were analyzed following ASTM D6352 and Detailed Hydrocarbon Analysis (DHA) according to ASTM D6730, respectively. Additionally, each catalyst was characterized by Mössbauer spectroscopy to identify iron species and relate them to the catalytic performance.
Results and discussion. Increasing the inlet molar fraction of CO up to 10% led to a marked decrease in CO2 conversion, which dropped from 41% to 13%; while, at the same time, CO conversion increased from 75% to 92%. In the experiment conducted with 5% CO test, a pronounced transient behavior was observed at the beginning of the test, followed by stabilization after approximately 40 hours on stream. Using DHA, more than 200 HCs were identified, and the results confirm that light oil (C6-C15) consists mainly of olefins and isoparaffins. Variations in the feed gas composition were found to significantly affect oil production, with the highest overall oil productivity achieved under the 10% CO condition, corresponding to a C6+ HC yield of 19%. Conversely, the 5% CO test favored the formation of heavier HCs, resulting in the maximum yield of heavy oil fractions (>C15).

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CDU0423

Effect of pre-treatment conditions on Fe-based catalyst for e-fuel production via modified Fischer-Tropsch synthesis

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: CO2 hydrogenation, Modified Fischer-Tropsch, E-fuel, Fe-based catalyst

Abstract Body. Introduction.

The rising demand for sustainable fuels has driven advancements in CO_2 conversion technologies, particularly in Fischer-Tropsch synthesis (FTS) for producing liquid hydrocarbons. This study examines the effects of various pre-treatment conditions on a Na-Fe3O4 catalyst in CO2-modified FTS, focusing on how iron carbide formation influences hydrocarbon yield and distribution

Methods.
The Na-Fe3O4 catalyst was synthesized via a precipitation method, followed by a series of pre-treatment conditions, including activation and carburization at varying temperatures and gas atmospheres, to promote specific iron carbide phases: H2 activation at 450°C (pretreatment A); H2 activation at 450°C followed by carburization (CO/ H2 1:1 P=2 bar) at 300°C (AC) and at 400°C (AC400). Characterization techniques such as XRD, Mössbauer spectroscopy, and Detailed Hydrocarbon Analysis (DHA), according to ASTM D6730, were employed to evaluate the catalyst's bulk composition, surface properties, and resulting hydrocarbon distributions. Principal Component Analysis (PCA) was applied to DHA data to examine correlations between the hydrocarbon product distribution and the iron carbide phases of the catalyst.

Results and discussion.
The results reveal that pre-treatment conditions significantly influence the formation of active iron carbides. Carburization at 400°C (AC400) proved optimal [1], promoting ε'-Fe2.2C formation while minimizing α-Fe content, an inactive site for the reaction. The hightemperature carburization (400°C) an improved yield of $C5^+$ hydrocarbons, ranging from 14% to 18%, comprising a balanced light-to-heavy oil ratio, while A and AC lead to a predominance of light oil (Tcond<150°C). Although the Hagg Carbide (χ-Fe5C2) is the main phase often associated with CO2 conversion activity, other carbides could play a role [2]: in this case, the presence of ε'-Fe2.2C enhanced the catalyst's selectivity for long-chain hydrocarbons, resulting in a diverse hydrocarbon distribution dominated by iso-paraffins, while shorter-chain olefins were predominant in other pre-treatment samples with lower or no ε'-Fe2.2C. The combined use of Mössbauer, DHA, and chemometric analysis proved instrumental in identifying active carbide phases and understanding their impact on reaction

pathways. These insights contribute to the development of tailored catalytic processes for CO2-to-fuel conversion, highlighting the potential of optimized Na-Fe3O4 catalysts for sustainable fuel production.

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CDU0450

Synthesis of Carbon Nanotube from CO2 via a Tandem System under Oxidative Conditions

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: Carbon dioxide (CO2); Carbon capture and utilization (CCU); Tandem process; Fe-Mo; Molybdenum carbide (Mo2C); Carbon nanotube (CNT)

Abstract Body.

The continuous accumulation of atmospheric CO2 represents a major challenge in addressing global climate change. Accordingly, the efficient conversion of CO2 into valueadded materials has become an important objective for carbon-neutral technologies. Among products, carbon nanotubes (CNTs) are particularly attractive due to their high economic value.

However, the direct synthesis of CNTs from CO2 is constrained by the oxidative nature of CO2. Under CO2-containing environments, conventional Fe catalysts used for CNT growth readily undergo oxidation, which suppresses carbon deposition and CNT formation. To overcome this limitation, tandem reaction systems have been proposed, in which CO2 is first converted into CH4 intermediates prior to CNT growth.

Despite this advantage, tandem processes inevitably introduce residual CO2 into the CNT growth environment. The presence of CO2 oxidize CNT growth catalysts, leading to catalyst deactivation. Therefore, the development of catalyst systems capable of maintaining activity under CO2-containing conditions remains a critical challenge for CNT synthesis via tandem CO2 conversion routes.

In this study, Fe-Mo bimetallic catalysts supported on MgO were investigated to overcome catalyst deactivation under oxidative conditions. The introduction of Mo significantly altered the catalyst behavior in the tandem system. While Fe-only catalysts failed to produce solid carbon due to oxidation by residual CO2, Mo-containing catalysts enabled CNT growth by preferentially reacting with CO2 to form molybdenum carbide species. This process stabilized the metallic Fe phase, which is essential for CNT nucleation and growth. X-ray photoelectron spectroscopy confirmed this stabilization effect, showing enhanced metallic Fe signals accompanied by the formation of Mo2C. These findings indicate that Mo plays a critical role in regulating the reactive atmosphere around Fe sites, thereby preserving their catalytic activity under CO2 containing conditions.

The effect of Mo content on CNT structure and selectivity was investigated by varying Fe:Mo ratios. The 0.1 wt. % Mo loading enabled the selective formation of single-walled CNTs, whereas excessive Mo favored multi-walled CNT growth, as confirmed by Raman spectroscopy and transmission electron microscopy. These results underscore the need to optimize catalyst composition and reaction conditions to achieve selective CNT growth under CO2-containing environments.

Overall, this study demonstrates an effective strategy for converting CO2 into high-value carbon nanomaterials through a tandem reaction system. The integration of CO2 conversion and CNT synthesis via catalyst design provides insights into catalyst stabilization in oxidative atmospheres and supports the development of sustainable CNT production pathways.

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CDU0471

Modulation of CO2 activation pathway by Ca promoter in PtSn/Al2O3 catalyst for CO2-assisted oxidative dehydrogenation of propane

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: CO2-assisted oxidative Propane dehydrogenation, CO2 reduction, Calcium, CO2 intermediates

Abstract Body.

CO2-assisted oxidative dehydrogenation of propane (ODPC, C3H8 + CO2 → C3H6 + CO + H2O) has attracted considerable attention as a promising route for propylene production while simultaneously enabling CO2 utilization. In this process, propane reacts with CO2, allowing CO2 to function as a soft oxidant. The involvement of CO2 promotes coupling between propane dehydrogenation(C3H8 → C3H6 + H2) and the reverse water–gas shift (RWGS, CO2 + H2 → CO + H2O) reaction, which effectively drives the reaction equilibrium toward the formation of desired products and improves overall catalytic performance. In this work, an alkaline earth metal was introduced as a promoter into a platinum–tin catalyst supported on Al2O3 (PtSn/Al2O3) to enhance catalytic activity further.

The PtSn/Al2O3 catalyst was prepared via the co-impregnation method, followed by sequential impregnation of calcium to obtain the Ca–PtSn/Al_2O_3 catalyst. The influence of calcium on CO2 adsorption behavior and the modification of reaction intermediates was investigated by CO2 temperature-programmed desorption (CO2-TPD) and in situ diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS).

Calcium incorporation significantly improves both CO2 and C3H8 conversions in the ODPC system by promoting efficient removal of hydrogen generated during propane dehydrogenation through the RWGS reaction, thereby overcoming the intrinsic thermodynamic equilibrium limitation associated with propane dehydrogenation. CO2-TPD results indicate that calcium addition significantly increases the amount of CO2 adsorbed on the catalyst surface, reflecting an enhanced CO2 adsorption capacity compared to the unmodified PtSn catalyst. In addition, in situ DRIFTS analysis shows that calcium modification changes the type of CO2-derived surface intermediates formed on the catalyst surface. The Ca-modified catalyst facilitates the formation of RWGS-active bicarbonate species, in contrast to the carbonate species mainly observed on the PtSn catalyst. In summary, Calcium modification of PtSn catalysts enhances CO2 adsorption and facilitates a reaction pathway that enables continuous CO2 activation and hydrogen consumption, thereby accelerating the RWGS reaction and improving ODPC performance. These findings

highlight calcium promotion as an effective strategy for coupling CO2 utilization with propane dehydrogenation.

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CDU0475

Spatial optimization of catalyst configuration for selective reverse water-gas shift in an electrified Joule-heated reactor

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: RWGS; Joule heating; Electrified reactor; CO2 conversion; Methanation

Abstract Body.

Introduction. The conversion of CO2 with H2 to synthesis gas via the reverse water-gas shift (RWGS) reaction is a key pathway for sustainable production of fuels and chemicals [1]. Electrified reactors based on Joule heating have recently emerged as an effective platform for endothermic reactions such as RWGS, because electrical energy is directly converted into heat through resistive materials, enabling high heating efficiency and rapid thermal response [2]. Direct electrical contact delivers heat locally to catalyst beds, which enables fast temperature modulation and selective control of reaction rates while minimizing bulk hot spots. In this study, we design a Joule heated reactor with spatially controlled catalyst packing to elucidate the relationship between catalyst reaction zone and overall reactor performance.

Methods. The RWGS reaction was evaluated at 5 bar using a resistively heated FeCrAl tube reactor, in which Ni catalysts were packed in different spatial configurations. Flow rate, current, and voltage were varied to control reaction conditions, and RWGS performance was evaluated while monitoring axial temperature profiles. The effluent was analyzed using online gas chromatography.

Results and discussion. Axial temperature gradients in Joule heated reactors cause different catalyst zones to participate unequally in the RWGS reaction, which directly influences overall activity and selectivity. When current in the range of 20A - 60A was applied to the FeCrAl tube packed with Ni catalysts under He flow, the reactor temperature increased from 140 °C to 767 °C. Along the 40 cm insulated zone, a maximum temperature of 767 °C was achieved at 60 A, and the temperature difference between the maximum and minimum values was 429.7 °C. Even at a high weight hourly space velocity of 189000mL gcat-1h-1, the catalytic reactor achieves a CO2 conversion of 68.1%, while maintaining a low methane selectivity. These results highlight the importance of tailoring temperature profiles, flow conditions, and catalyst distribution to efficiently convert CO2 to CO.

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CDU0477

An Integrated Electrochemical Power-to-Liquid Process for Sustainable Aviation Fuel Production from Captured CO_2

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: Global warming, Sustainable Aviation Fuel (SAF), Electrochemical power-toliquid (PtL)

Abstract Body.
The transition from fossil fuels to renewable energy sources is becoming increasingly important for mitigating global warming and achieving carbon neutrality. Electrification has emerged as a promising decarbonization strategy across various industrial sectors; however, its application in the aviation sector faces fundamental limitations due to the low volumetric energy density of batteries, the extremely high energy demand of aircraft, and the lack of realistic alternatives to turbine engines for high-altitude operation.

In this context, sustainable aviation fuel (SAF), produced from renewable feedstocks such as waste cooking oil, animal and vegetable fats, and municipal solid waste, has gained attention as a practical solution for decarbonizing the aviation industry. SAF can be produced via diverse feedstocks and process pathways, among which Power-to-Liquid (PtL) technology is particularly attractive due to its capability to convert renewable electricity into high-quality liquid fuels. Nevertheless, the commercialization of SAF still requires process designs that simultaneously satisfy economic feasibility, energy efficiency, and environmental performance.

In this study, we propose an integrated PtL process that converts captured carbon dioxide and water into syngas via electrochemical conversion, followed by the production of sustainable aviation fuel through the reverse water–gas shift (RWGS) and Fischer–Tropsch (FT) reactions. Conversion efficiency and economic analyses were conducted for the proposed process and benchmarked against previously reported SAF production pathways.

The results indicate that increasing pressure in the CO_2 electroreduction (CO_2RR) system enhances CO selectivity, whereas the RWGS reaction becomes thermodynamically unfavorable under high-pressure conditions. By accounting for these competing effects and optimizing the reaction conditions and process parameters, an overall carbon conversion efficiency of approximately 80% was achieved. Meanwhile, the economic assessment revealed that the levelized cost of the proposed process is somewhat higher than those reported for conventional PtL-based SAF pathways, primarily due to increased energy

demand associated with process integration and the cost burden of the electrochemical conversion steps.

These findings demonstrate that electrochemically driven CO_2-to-fuel synthesis can achieve high carbon conversion efficiency and represents a promising pathway for sustainable aviation fuel production. With further process optimization and reductions in electricity costs, this approach has the potential to contribute significantly to the long-term decarbonization of the aviation sector.

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CDU0491

Integrated CO2-Derived Sustainable Aviation Fuel Production via CO2 Electrolysis, Syngas Fermentation, and Alcohol-to-Jet Conversion

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: CO2 electrolysis, Sustainable aviation fuel (SAF), Alcohol-to-Jet (ATJ)

Abstract Body.
REFuelEU Aviation's sustainable aviation fuel (SAF) blending mandate necessitates the rapid scale-up of low-carbon aviation fuel supply in the near term. Moreover, SAF is widely regarded as a key option for mitigating the environmental impacts of the aviation sector. While various SAF production pathways are being explored, their large-scale commercialization remains challenging due to technical and economic barriers. Therefore, it is crucial to develop economically viable and environmentally sustainable processes, making process simulation-based design and comprehensive assessment studies increasingly essential. This study investigates an integrated SAF process that converts captured CO2 to syngas via electrolysis, converts syngas to alcohols via fermentation, and converts the resulting alcohols to SAF via Alcohol-to-Jet (ATJ). Fermentation is performed using Clostridium carboxidivorans P7, enabling the production of C2-C6 alcohols (e.g., ethanol, butanol, and hexanol). By producing longer-chain alcohols, this approach reduces the need for extensive recycling within the process compared to ethanol-oriented pathways, thereby enhancing overall process efficiency. The overall process is modeled in Aspen Plus, and techno-economic analysis (TEA) and life-cycle assessment (LCA) are conducted to quantitatively evaluate economic feasibility and environmental impacts. With feasibility as a central criterion, the process model is validated using experimental data to improve the credibility of the simulation results. By leveraging the carbon-chain elongation capabilities of C. carboxidivorans P7 and integrating efficient CO2-to-syngas electrolysis, this study proposes an optimized process design that overcomes the limitations of conventional SAF production pathways. This approach not only enhances process efficiency through reduced recycling but also establishes a viable pathway for high-carbon-chain fuel synthesis. Furthermore, a comprehensive sensitivity analysis was conducted to identify and quantify the key process variables that govern both the techno-economic viability and environmental performance of the system.

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CDU0588

Optimization of Ni Loading in Egg-shell-type Ni/Al_2O_3 Pellet Catalysts for Enhanced Performance and Coke Resistance in DRM

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: Dry reforming of methane, Egg-shell-type pellet catalyst, Carbon deposition, Nisupported alumina catalyst

Abstract Body.

Introduction.

Dry reforming of methane (DRM) is an attractive process for syngas production by simultaneously converting CH_4 and CO_2, contributing to carbon resource efficiency and greenhouse gas mitigation [1]. Because DRM is typically conducted at elevated temperatures, Ni-based catalysts, although widely employed owing to their high activity and cost-effectiveness, suffer from deactivation caused by carbon deposition and sintering [2]. Pellet-type catalysts offer advantages over powder catalysts in terms of mechanical strength and resistance to pressure drop, making them favorable for commercial applications. Eggshell-type pellet catalysts, in which active metal species are preferentially distributed near the outer surface of the support, allow reactions to proceed at locally high metal concentrations, thereby improving the utilization efficiency of active metals. In this study, egg-shell-type Ni/Al_2O_3 pellet catalysts with different Ni loadings were investigated to clarify the influence of Ni content on structural properties and catalytic performance in DRM.

Methods.

Pellet-type Ni/Al_2O_3 catalysts with Ni loadings of 2, 1, 0.5, and 0.1 wt.% were prepared using a developed wetness impregnation (DWI) method modified from conventional incipient wetness impregnation. This method enables simple yet precise control of metal distribution on pellet supports [3].

Results and discussion.

Based on averaged values obtained from repeated experiments, the initial CH_4 conversion followed the order: 1 wt.% Ni (~75%) > 0.5 wt.% Ni (~72%) > 2 wt.% Ni (~68%) > 0.1 wt.% Ni (~63%) at 800°C. Thermogravimetric analysis revealed that carbon deposition increased markedly with Ni loading, with substantial coke formation on the 2 wt.% and 1 wt.% Ni catalysts, whereas negligible carbon deposition was observed on the 0.5 wt.% and 0.1 wt.% Ni catalysts. H_2-TPR analysis showed that higher Ni loadings enhanced reduction peaks above 700 °C, indicating strengthened interactions between Ni species and the Al_2O_3 support, while lower Ni loadings exhibited dominant reduction features in the 400–600 °C range. NH_3-TPD and XRD analyses further demonstrated that both surface acidity and Ni particle characteristics varied systematically with Ni loading. Considering these results

collectively, the 0.5 wt.% Ni/Al_2O_3 pellet catalyst exhibited a favorable balance between catalytic activity and resistance to carbon deposition, highlighting the importance of optimized Ni loading in pellet-type DRM catalysts.

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CDU0606

Tandem Fe/Zeolite system for CO2 hydrogenation to e-SAF

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: CO2 utilization; Fischer-Tropsch; e-SAF

Abstract Body.

Introduction. CO2 conversion to long chain hydrocarbons via CO2 Fischer-Tropsch (FT) is a promising route for sustainable aviation fuels (SAF) production. CO_2-FT products are mainly linear, unsaturated hydrocarbons that require further upgrading for practical applications.

This work focuses on CO_2 hydrogenation to e-kerosene precursors via FT synthesis using Fe-based catalysts, coupled with bare or Pt-promoted zeolites to steer the product distribution.

Methods. Fe-Zn-Cu-K catalyst (100:10:1:4 mol ratio) [1] was tested for CO_2 hydrogenation, coupled with an equal mass of HY or HZSM5 zeolites, with or without Pt promotion (0.1 %wt). Tests were run at high-conversion conditions (30 barg, 6 L(STP)/h/gFe-Zn-Cu-K, 300–380 °C, H2/CO2 = 3) both as consecutive segregated bed and as mechanical mixture of the two samples. Full speciation of the gaseous and condensed products was obtained via online GC and offline GC-FID/MS.

Results and discussion. The Fe-based catalyst alone can convert 42% of the fed CO_2 at 350°C, with a proven stability of more than 300 h and with a condensed product distribution dominated by linear olefins (Fig 1A). The addition of the zeolite in mechanical mixture leads in all cases to a steady decline in hydrocarbon yield. Characterization of the spent materials indicated the migration of K from the Fe catalyst to the acidic zeolite, lowering the performance of both materials. At variance, when the zeolite is added after the Fe-based catalyst, hydrocarbon yield and distribution remains stable for several hundred hours on stream. The introduction of zeolites markedly modifies the hydrocarbon composition (Figure 1B-C): alcohol intermediates are completely converted on zeolitic acid sites, significantly simplifying downstream separation. Bare zeolites promote the isomerization of n-1-olefins to internal and branched olefins, whereas Pt-promoted zeolites favor extensive olefin hydrogenation to paraffins. As a result, the C8–C16 fraction contains nearly 40% isoparaffins, yielding a hydrocarbon mixture that is largely compliant with ASTM specifications for SAF [2], requiring only minor post-processing adjustments.

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Effect of activation on phase evolution and performance of Fe-based catalysts in CO2 hydrogenation to hydrocarbons

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: CO2 utilization; Fischer-Tropsch; iron carbides

Abstract Body.
Introduction. One-pot CO2 hydrogenation over Fe-based catalysts can enable renewable liquid fuel production, through the consecutive RWGS and Fischer–Tropsch (FT) reactions catalyzed by Fe3O4 and FexCy, respectively [1]. This study examines how the activation atmosphere influences iron phase evolution and structure–activity relationships under a complex reaction environment, where a thermodynamically controlled RWGS step is coupled to kinetically controlled FT chemistry and to the dynamic oxidation of the active carbide phase.
Methods. A Fe-Zn-Cu-K catalyst was prepared in-house [2]. Activation was performed under H2/CO (carburizing), H2/N2 (reducing), or N2 (inert) atmosphere, and catalysts were then tested at T=300 °C, P=10 barg and GHSV=2.4 L(STP)/h/gcat. The catalyst was loaded as 5 segregated catalytic beds to allow the spatially-resolved characterization of the spent samples after quenching the reaction at different time on stream (Fig. 1A-C at ToS = 120 h).
Results and discussion. After 120 h, all catalysts converge to ~33% CO2 conversion (Fig 1D) in the presence of a nearly equilibrated RWGS reaction (Kp/Keq = 0.8). The spatiallyresolved XRD and Mössbauer characterization of the activated and spent samples indicated that despite the different starting phase of the catalyst (carburized, reduced, oxide) the final composition of the catalyst is similar, with Fe5C2 at the inlet and Fe3O4 towards the outlet sections (Fig. 1A-C). The observed trends were rationalized by imposing the thermodynamic equilibrium constraints for RWGS and Fe5C2 oxidation when varying the extent of reaction of the FT. The two resulting equilibrium lines for the gas and solid phase converge over the stability point: the initial states of reduced and carburized catalysts deactivate evolving towards oxidation, while for the N2-activated sample both thermodynamic and kinetic driving forces enable progressive carbide formation until a common steady state is reached (Fig 1E).

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Mechanistic Modelling of the Local Electrode Environment in MEA CO2 Reduction: The Role of Cation Size and Steric Effects

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: Electrochemical CO2 reduction, Local reaction environment, Cation effect, Continuum Modelling, Bayesian optimisation

Abstract Body.
Scaling electrochemical CO2 reduction (CO2ER) to industrial relevance requires a rigorous optimization of the local reaction environment near the electrode surface. However, standard continuum models, such as the classical Poisson-Nernst-Planck (PNP) equations, often fail to describe high-potential behaviors, predicting unphysical ion accumulation and neglecting finite ion sizes. To address these limitations, this study presents a novel robust modelling approach: the Mass-Transport-Corrected-Tafel Size-Modified-Poisson-Nernst-Planck (MTCT-SMPNP) model.
The developed 1D full-scale continuum model integrates two critical frameworks to provide a physico-chemically plausible description of the electrode-electrolyte interface. First, the SMPNP framework enhances flux accuracy by modifying the excess chemical potential formulation to account for the finite size of hydrated ions and steric saturation effects. This explicitly defines the structure of the Electric Double Layer (EDL), including the Stern layer and Outer Helmholtz Plane, preventing unrealistic ion packing. Second, the MTCT formulation integrates the Tafel equation with Koutecky-Levich (KL) kinetics, explicitly incorporating mass transfer limitations to accurately determine limiting current densities at high overpotentials. Additionally, Bayesian optimization was utilized to estimate governing parameters (exchange current density, charge transfer coefficient) to elucidate the specific roles of different cation species.
Validated against experimental data for Ag-catalyzed CO production across a wide potential range (-2.5 V to -3.5 V vs. SHE), the MTCT-SMPNP model demonstrates superior fidelity compared to classical PNP and Reaction-Diffusion models. The simulation results highlight the profound impact of steric repulsion; as electrode potential becomes more negative, cations accumulate to form a condensed layer at the interface, acting as a physical barrier to neutral CO2 diffusion. Furthermore, the model successfully reproduces cation-dependent performance variations ($Li^+ < K^+ < Rb^+ < Cs^+$). The analysis reveals that these trends are not random fitting artifacts but are driven by systematic correlations between the optimized kinetic parameters and the hydration radii of the cations. Specifically, the model confirms that larger cations (e.g., Cs^+) lower the activation energy barrier more effectively than smaller ones (e.g., Li^+).

In conclusion, the MTCT-SMPNP model serves as a powerful tool for analyzing the local electrode environment. By rigorously accounting for ion size effects and EDL structure, it offers new mechanistic insights into how dense counter-ion packing modulates mass transport and reaction kinetics, providing a reliable platform for designing next-generation CO_2 reduction systems.

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CO2 Conversion into Lower Hydrocarbons using Catalytic Structures: Structure-Resolved CFD Simulations

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: Catalytic structures, Reaction modelling, Heat and mass transfer, Structureresolved CFD simulations

Abstract Body.

Introduction: Recently researchers have focused on the capture and conversion of CO2 from chemical and energy-generation processes into lower hydrocarbons (e.g., CH4, CH3OH, DME) as secondary energy sources. Among carbon utilization routes, CO2 hydrogenation to methanol, Dry Reforming of Methane has gained significant importance. Structured packings have emerged as promising alternatives to conventional catalytic pellets due to their higher surface-area-to-volume ratio, lower pressure drop, and enhanced transport characteristics. Advances in additive manufacturing have enabled the fabrication of complex catalytic structures, whose flow and heat-transfer performance require systematic evaluation. CFD simulations provide detailed insight into flow characteristics, heat transfer, and reaction performance. Therefore, the present work investigates the reactive performance of various complex catalytic structures and their influence on CO2 conversion to methanol and syngas under reactive flow conditions using structure-resolved CFD simulations.

Methodology: A rectangular computational domain with a 48x48 mm² cross-section [Figure1(a)] is used to evaluate the reaction performance of structured packings (simple hexagonal opening, TPMS, and Lattice based structures). The Reynolds-averaged continuity, momentum, energy, and species transport equations are solved to simulate flow, heat, and species transport, respectively using Ansys CFX.

Results: CFD simulations were performed to investigate the reaction performance of catalytic structures for CO2 conversion to methanol and syn gas. The velocity distribution is relatively uniform for MBCC structure compared to hexagon and primitive strut structures, however, significant differences in ΔP were found. The pressure drops for the hexagonal, primitive strut and MBCC structures are 48, 800 and 1945 Pa, respectively, owing to their shape features.

A qualitative analysis of temperature and concentration distribution shows that the MBCC exhibits lower temperature and methanol concentrations in solid domain compared to the hexagonal structure [Figure1(i)-(ii)]. Further, the quantitative comparison of the volumeaveraged temperature <Tv> indicated that the hexagon, primitive strut and MBCC have <Tv> values of 582, 569 and 542 K, respectively. However, significantly higher conversion of CO2 was found in the MBCC (4.84%) followed by strut (3.58%) and Hexagon (2.28%). A detailed discussion of reaction performance for different catalytic structures will be presented at the conference.

Conclusions: The present study suggests that the reaction performance of catalytic structures is significantly influenced by the structure geometry, flow and mixing pattern within the reactor. The complex structures showed significantly higher conversion of CO2 for methanol and syngas production owing to their geometric features. Therefore, it is important to optimize the design of catalytic structures depending on the reaction conditions (kinetics and operating conditions).

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Role of reverse Water-Gas Shift Reaction for CO_2 Utilization in Molten Carbonate Electrolysis Cells

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: reverse Water-Gas shift, CO2 utilization, Molten Carbonate Electrolysis Cell

Abstract Body.

Purpose

Molten Carbonate Electrolysis Cells (MCECs) are emerging as promising technologies for high-temperature CO2 utilization and conversion and hydrogen production. Under typical operating conditions for water and CO2 co-electrolysis, chemical reactions such as the reverse water gas shift (rWGS) may significantly affect gas composition and apparent CO2 conversion. This work aims to isolate and quantify the purely chemical contribution of rWGS reaction under conditions representative of MCEC operation, with the objective of improving the understanding and optimization of CO2 utilization pathways in molten carbonate systems. Methods

An experimental campaign was carried out on a laboratory-scale single molten carbonate cell operated at three high temperature (620-650-680 °C), without applying any electrical load. To decouple chemical effects from electrochemical phenomena, synthetic gas mixtures were fed to the cell to simulate inlet compositions corresponding to different water and CO2 co-electrolysis operating points. A systematic parametric analysis was performed by varying steam and CO2 concentrations over a wide range representative of MCEC conditions. The outlet gas composition was continuously monitored using an N-DIR infrared gas analyzer, allowing quantitative evaluation of CO, CO2, H2 concentrations and direct assessment of rWGS reaction extent.

Results

The experimental results demonstrate that rWGS reaction contribute to gas composition changes under molten carbonate conditions. Reaction extents were found to slightly depend on temperature over the the investigated range. Quantifiable deviations between inlet and outlet CO2 concentrations confirm the active role of chemical reactions in CO2 consumption in MCEC environment. Was found that rWGS can lead to an increase of utilization of CO2 up to 50% in simulated high current condition while producing up to 20% surplus of CO2 in other conditions. This can significantly affect MCECs co-electrolysis efficiency, depleting or increasing reactants availability. Based on the experimental data, effective reaction rates and thermodynamic parameters were derived for conditions representative of hightemperature co-electrolysis operation.

Conclusions

By isolating the chemical contribution of rWGS reactions, this study provides essential experimental insight into CO2 utilization mechanisms in molten carbonate electrochemical

cells. The results highlight the need to explicitly account for chemical kinetics when evaluating CO2 conversion efficiency in MCECs and related technologies. The derived kinetic information supports improved modeling and operational strategies aimed at maximizing CO2 utilization, contributing to the development of high-temperature electrochemical systems within net-zero CO2 emission and carbon capture and utilization frameworks.

$$H_2 + CO_2 \rightleftharpoons H_2O + CO$$

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CDU0699

Dynamic operation of reverse water-gas shift via rapid pulsed Joule heating

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: Electrified reactor, Joule heating, rapid pulsed heating, dynamic operation, reverse water gas shift reaction

Abstract Body.
Electrified reactors powered by renewable electricity have attracted increasing attention as an alternative to conventional combustion-based chemical processes, which often suffer from a trade-off between energy efficiency and productivity. In particular, dynamic operation enables transient control of reaction environments beyond steady-state conditions, offering new opportunities to improve reaction performance. In this study, an electrified reactor operated under rapid pulsed Joule heating (RPJH) is investigated for the reverse water–gas shift (RWGS) reaction.

A carbon felt electrode selectively impregnated with nickel nitrate was prepared via dipcoating and installed between copper electrodes inside a quartz reactor. RPJH was implemented by applying periodic millisecond-scale on–off current cycles to the electrode, and RWGS performance was evaluated under different current amplitudes and operation modes.

Compared with continuous Joule heating (CJH), RPJH limits prolonged high-temperature exposure through rapid heating and cooling cycles. As a result, RPJH achieves comparable RWGS performance at significantly lower electrical power input. In addition, nickel particle sintering is effectively suppressed, leading to enhanced catalyst stability. The RWGS activity and stability strongly depend on nickel loading, and an optimal loading maximizes both properties. Under optimized conditions, a 3 wt% Ni/carbon felt electrode achieved a CO_2 conversion of 44% with a CO selectivity of 93%. These results demonstrate that dynamic operation enables temporal control of local reaction environments in electrified reactors and extends reactor operation beyond conventional steady-state limitations.

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Gas-Velocity-based operating window for thermal runaway prevention in a CO2 Fischer-Tropsch fluidized-bed reactor

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: CO2 Fischer-Tropsch synthesis, Fluidized-bed reactor, Computational Particle Fluid Dynamics, Thermal runaway, Heat removal (cooling coils), Na-promoted Fe catalyst

Abstract Body.
Purpose : Direct CO2 Fischer-Tropsch synthesis (CO2-FTS) can provide higher thermal efficiency than the indirect route of reverse water-gas shift(RWGS) followed by FTS for liquid-fuel production, but its strong exothermicity makes heat removal and thermal runaway prevention a primary design constraint. Here we quantify the thermal constraints that govern stable operation in CO2-FTS fluidized-bed reactors.

Methods : We performed three-dimensional Computational Particle Fluid Dynamics (CPFD) simulations coupled with an experimentally derived kinetic model. Kinetic parameters were obtained from fixed-bed experiments using Na-promoted Fe catalysts at 553-603K and 3.5 MPa, accounting for direct CO2 hydrogenation and RWGS pathways, and were implemented in a cylindrical CPFD reactor (height 1.0 m, diameter 0.05 m) equipped with internal cooling coils.

Results: The simulations indicate that achieving near-uniform temperature requires a superficial gas velocity (u) of at least 0.055 m/s, corresponding to approximately twice the minimum fluidization velocity (umf) of 0.027 m/s, identified from pressure-drop analysis. At velocities near minimum fluidization (u/umf 1.0), the lower-bed temperature near the gas distributor rises rapidly and does not converge over the analysis time window (thermal runaway), leading to kinetic extrapolation beyond the experimentally validated range and nonphysical conversion behavior with apparent conversions approaching 100%. At u of 0.040 to 0.055 m/s, (u/umf 1.5-2.0), temperature non-uniformity is reduced and CO2 conversion of 31-38% are achieved; at the same velocity, CO2 conversion varies only slightly (within ~3%) as the cooling coils temperature decreases from 573K to 473K and 373K. Lowering the cooling coils temperature constrains temperatures in the middle and upper bed but does not suppress runaway near minimum fluidization without sufficiently high gas velocity. Bubble statics further indicate that operating at u/umf of 1.5-2.0 yields bubble distributions that enhance gas-solid contact while limiting temperature non-uniformity.

Conclusions : Overall, fluidization design for CO2-FTS should be guided by thermal stability metrics (particularly the critical gas velocity required to avoid thermal runaway and the required heat-removal duty) rather than hydrodynamic criteria alone, and the coupled kineticCPFD framework provides a quantitative basis to guide the design of thermally stable CO2FTS fluidized-bed reactors.

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Sustainable Integrated Process for Methyl Formate via CO_2 hydrogenation over Ru-Based Heterogeneous Catalysts with Reactive Distillation

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: CCU, Methyl Formate, Heterogeneous catalyst, TEA, LCA

Abstract Body.

Purpose

CO_2 hydrogenation-based CCU is a promising route to produce value-added C1 chemicals such as methyl formate (MF), but scale-up is limited by reaction–separation integration.

Methods

Ru-MACHO-POMP was applied for CO_2 hydrogenation in methanol using tripropylamine (TPA). Products were quantified by quantitative NMR. Reactive distillation and Aspen Plus modeling were used for downstream separation design.

Results

The catalyst showed stable activity over multiple recycling cycles. Reactive distillation enabled MF-rich distillate recovery while retaining the TPA-containing bottom phase for reuse. Aspen modeling supported integrated process feasibility. Conclusions

This work demonstrates an integrated CO_2-to-MF pathway combining recyclable heterogeneous catalysis, separation design, and preliminary TEA/LCA toward sustainable MF production.

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CDU0731

Catalytic CO2 Hydrogenation for Sustainable Fuel Production

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: CO2 hydrogenation; Fe-based catalysts; Sustainable aviation fuel (SAF); Solid oxide

Abstract Body.
Introduction. As a chemical conversion technology for carbon neutrality, catalytic CO2 hydrogenation is one of the most realistic and promising CCU (Carbon Capture & Utilization) technologies. Fe-based catalysts are most commonly used for CO2 hydrogenation and are capable of both reverse water-gas shift reaction and Fischer-Tropsch reaction. This presentation shows our research progress of using various promotors to control the catalytically active species of Fe-based catalysts and the corresponding hydrocarbon chain length of the products. We will also demonstrate a strategy to further control the structure of long-chain hydrocarbons using a dual-bed reactor with an additional catalyst layer. If the catalyst is designed rationally, the products of the CO2 hydrogenation can be selectively adjusted to olefins, paraffins, aromatic compounds, etc. and can also be applied as sustainable aviation fuel (SAF) in the future.

Results and discussion. Within the context of Fe3O4-based CO2 hydrogenation, zeolites, featuring robust acid sites within their micropores, induce the cracking of extended hydrocarbon chains, thereby impeding the production of hydrocarbons exceeding 12 carbon atoms. Zeolites, such as ZSM-5, effectively facilitate the conversion of light olefins and hydrocarbons into aromatic compounds in the C6–C11 range [1].
This paper introduces novel solid oxides including Pt/WO3-ZrO2 and Pt/Al2O3, specifically designed for the production of liquid isoparaffins, aligning with the requirements of sustainable fuel characteristics. For example, the precise adjustment of Pt and W contents in Pt/WO3-ZrO2 enhances the hydrogenation and isomerization of linear olefins, amplifying the yield of paraffins, with a particular emphasis on isoparaffins. A dual-bed reactor integrating 0.01 wt% Pt supported WO3-ZrO2 with Fe3O4 catalyst achieved a CO2 conversion rate of 40% and a CO selectivity of 10%, while maximizing isomerization performance, attaining 42% isoparaffinic selectivity within liquid hydrocarbons at operating conditions of 340 °C, 20 bar, WHSV = 4,500 mL·h−1·gcat−1. In contrast to zeolite catalysts prone to coke deposition during the reaction, the Pt/WO3-ZrO2 catalyst exhibited remarkable stability, sustained activity without discernible deterioration, and negligible coke deposition, even after continuous operation for more than 100 h
This outcome delineates an optimized catalyst technology for the sustainable production of fuel from CO2, offering a viable alternative to the prevailing dependence on fossil fuels.

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CDU0742

Enhanced Performance of Cu-Zn-Mg-Al Catalysts for Methanol Synthesis via CO_2 Hydrogenation: Impact of Sequential Precipitation on Active Phase Dispersion

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: CO2 hydrogenation, Methanol synthesis, Sequential precipitation, Cu-based catalysts

Abstract Body.

In this study, an optimized precipitation strategy was investigated to improve the activity, stability, and selectivity of catalysts for methanol synthesis via CO2 hydrogenation, a critical carbon capture and utilization (CCU) technology. The sequential precipitation method was employed to overcome component imbalances often encountered in large-scale production due to the varying pH requirements of different metal ions in Cu-Zn-Mg-Al systems. By sequentially precipitating precursors, we aimed to ensure high dispersion of the active copper (Cu) phase. Given that Cu tends to lose activity through crystal growth during conventional precipitation, this study prioritized a sequence where the Cu component is precipitated last.

Four distinct precipitation sequences were evaluated: MZAC (co-precipitation), MZA-C, MZA-C, and M-ZA-C. While XRF analysis confirmed consistent metal loading across all samples, catalytic performance under reaction conditions (250°C, 50 bar) varied significantly. The conventional co-precipitated MZAC catalyst yielded a CO2 conversion of 25.3% and methanol selectivity of 67.3%. In contrast, the MZ-A-C catalyst—prepared by first co-precipitating Mg and Zn, followed by Al, and finally Cu—demonstrated superior performance with a CO_2 conversion of 30.9% and selectivity of 76.6%.

N_2 physisorption analysis revealed that the MZ-A-C catalyst possessed a 25% larger surface area and a 55% higher total pore volume compared to other sequential variants. Furthermore, XRD and SEM analyses confirmed that while the MZAC catalyst suffered from Cu crystal growth, the MZ-A-C catalyst maintained highly dispersed Cu species within a unique hierarchical structure, where Cu was uniformly distributed over an Al-rich layer. These results demonstrate that the catalyst's microstructure and active site dispersion can be optimized through precise control of the precursor precipitation sequence, offering a robust methodology for the design of high-performance CO2 hydrogenation catalysts.

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CDU0743

Investigating the Role of Mg in Ni-Mg/Al_2O_3 Catalysts for Syngas Production via Dry Reforming of Methane: Experimental Validation of DFT-Proposed Mechanisms

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: Dry reforming of methane (DRM), Ni-Mg/Al2O3 catalyst, Carbon deposition (Coking), Reaction mechanism validation

Abstract Body.
This study experimentally validates a computational reaction mechanism for synthesis gas production via methane decomposition and CO2 dissociation over Ni-Mg/Al2O3 catalysts. The catalysts were synthesized by sequential impregnation of Mg and Ni precursors onto an alumina support. Previous DFT studies have proposed a mechanism where methane undergoes stepwise dehydrogenation on Ni sites (CH4 → CH3 → CH2 → CH → C), while CO2 dissociates at the support's active sites to generate CO and surface-adsorbed oxygen (Oads). This Oads species subsequently oxidizes CHx intermediates to form CHxO, which decomposes into CO and H2, thereby preventing coking. To verify this, Ni/Al2O3 catalysts (10 – 40 wt% Ni) were tested, revealing that higher Ni loading significantly accelerated deactivation due to carbon deposition—a phenomenon typically associated with Ni crystallites exceeding 10 nm. While Mg addition was found to reduce Ni particle size, this study focused on its chemical role in CO2 activation. XPS analysis confirmed a significant increase in surface-adsorbed oxygen on the Ni-Mg/Al2O3 catalyst following the reaction. Comparative studies on Mg/Al2O3 and Al2O3 further demonstrated that Mg promotes CO2 dissociation, increasing CO production even in the absence of Ni. Our results suggest that the suppression of carbon deposition in Mg-promoted Ni catalysts is not merely a physical effect of particle size control. Instead, the formation of MgAl2O4 enhances the CO2 dissociation rate, providing sufficient surface oxygen to effectively remove carbon precursors. These findings provide experimental evidence for DFT-based mechanistic models and offer strategic insights for designing highly stable catalysts for CO2 reforming.

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Development of Sn-Partially Substituted SrFeO3-δ Oxygen Carriers for Chemical Looping Oxidative Dehydrogenation of Ethane with CO2 Splitting

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Abstract Category: Net-zero CO2 Technologies - Net-zero CO2 Technologies - CO2 Utilization

Keywords: Oxygen carrier, Chemical Looping Oxidative Dehydrogenation (CL-ODH), Redox catalyst, Metal oxide, Perovskite structure

Abstract Body.
Chemical looping oxidative dehydrogenation (CL-ODH) has attracted considerable attention as an energy-efficient alternative to conventional steam cracking for ethylene production, owing to its ability to achieve selective dehydrogenation through lattice oxygen while mitigating CO2 emissions. The replacement of air with CO2 as the oxidant further extends the CL-ODH concept toward carbon utilization, but simultaneously imposes stringent requirements on the redox stability and oxygen transfer behavior of oxygen carriers. In this context, perovskite-type oxides based on SrFeO3-δ are promising candidates due to their reversible lattice oxygen exchange and structural robustness under cyclic redox conditions. In this study, SrFeO3-δ and Sn-partially substituted SrFe0.9Sn0.1O3-δ oxygen carriers were investigated for the CL-ODH of ethane using CO2 as the oxidant. The materials were synthesized by a solid state method and evaluated in a fixed-bed reactor under cyclic reduction and oxidation conditions. Ethane was selectively dehydrogenated by lattice oxygen during the reduction step, while CO2 was employed to regenerate the reduced oxygen carriers. The catalytic performance was assessed over multiple redox cycles in terms of ethane conversion, ethylene selectivity, and cyclic stability.

Under CO_2 oxidation conditions, both oxygen carriers exhibited a gradual decrease in ethane conversion accompanied by an increase in ethylene selectivity with increasing cycle number, indicating a transition from highly reactive to more controlled lattice oxygen participation. While SrFeO3-δ showed higher initial conversion, it suffered from enhanced hydrogen formation and progressive performance degradation during cycling. In contrast, SrFe0.9Sn0.1O3-δ maintained lower conversion but consistently higher ethylene selectivity and superior redox stability. The improved performance is attributed to Sn substitution at the B-site, which stabilizes the perovskite framework and moderates Fe redox behavior, thereby suppressing excessive oxidation and enabling controlled oxygen release under CO2-based CL-ODH conditions.
These results demonstrate that partial Sn substitution in SrFeO3-δ is an effective strategy for developing selective and durable oxygen carriers for CL-ODH, providing a viable pathway for ethylene production coupled with CO2 utilization.

Poster Presentation

Environmentally-friendly and sustainable Chemicals

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SCM0054

PFAS-Free Microporous Ionomer Enabling High-Performance CO_2 Electrolysis for New Era Energy Technologies

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Materials (Zeolite, MOF etc)

Keywords: PFAS-free materials, CO_2 electrolysis, Low-carbon energy systems, Ionomeric binder

Abstract Body.
The global expansion of renewable energy sources such as wind and solar power has intensified the demand for efficient and sustainable energy storage and conversion technologies [1]. In this context, CO_2 electrochemical reduction represents a strategic pathway to close the carbon loop while producing valuable chemicals. However, the performance of CO_2 electrolyzers remains strongly dependent on the properties of the binder, which govern ion transport, reactant accessibility, product removal, and the mechanical stability of catalyst layers. Conventional ionomers based on perfluorinated chemistries provide excellent conductivity and durability, but their environmental persistence has raised significant concerns, culminating in recent European regulations targeting the phase-out of PFAS-class materials [2]. This motivates the urgent development of alternative binders that are both environmentally benign and capable of matching or surpassing the electrochemical performance of state-of-the-art ionomers. Here, we present a newly functionalized Polymer of Intrinsic Microporosity (PIM) engineered as an ionomeric binder for electrochemical CO_2 reduction. PIM structural microporosity arises from its contorted, non-planar backbone, which prevents efficient chain packing and generates interconnected micropores with an intrinsic surface area approaching 1000 $m^2 g^{-1}$. Through targeted molecular design, ion-conducting groups were introduced into the PIM framework to ensure efficient charge transport while preserving the advantageous microporosity. This architecture enhances ionic and molecular transport within catalyst layers. When implemented in CO_2 RR cells targeting C_2 products, the PIM binder enabled high efficiency, achieving C_2 conversion and selectivities equal to or superior to those obtained using commercial ionomers. The improved performance is attributed to enhanced catalyst–binder interactions and optimized mass transport within the porous binder matrix. In CO_2 electrolyzers, the PIM achieved over 32.5% C_2 Faradaic efficiency, whereas commercial ionomers remained below 28% under identical conditions. The PIM also exhibited a significantly suppressed H_2 generation, remaining below 10%, compared to nearly 20% for commercial binders—further confirming its selectivity profile and demonstrating performances matching state-of-the-art materials. In addition, devices incorporating the PIM binder showed stable operation over extended durations, with negligible degradation of electrochemical performance. These results confirm that the designed PIM binder constitutes a fluorine-free, high-performance

alternative for next-generation CO_2 electrochemical conversion systems, supporting sustainable, circular-carbon technologies.

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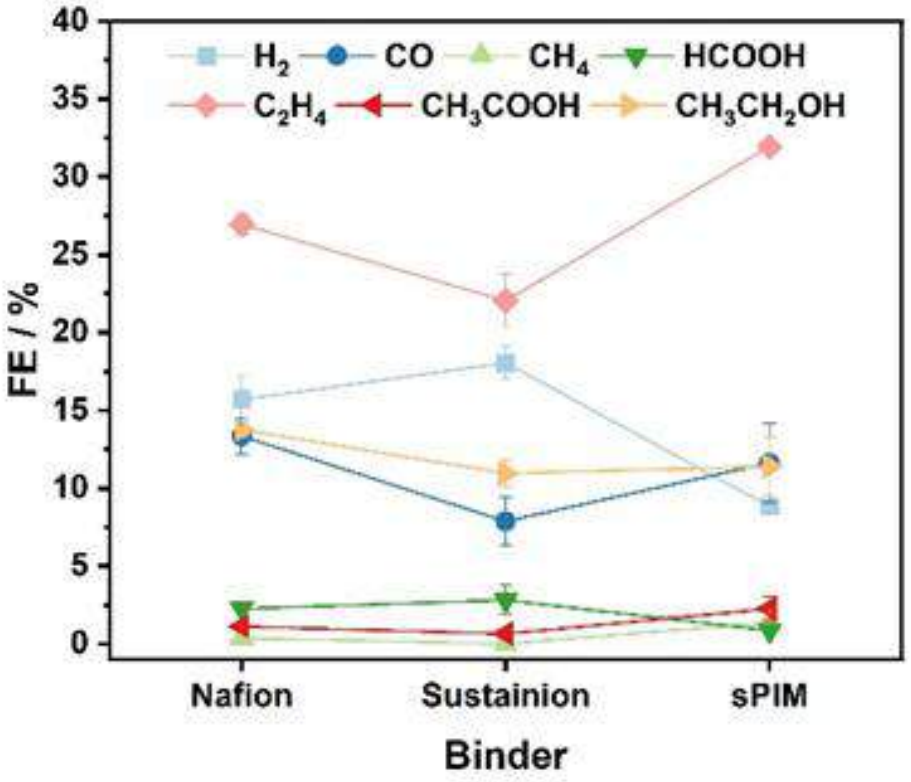

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

SCM0126

Asymmetric Gradient Porous Fabric with Dynamically Tunable Thermal Management and Electromagnetic Interference Shielding via Delayed Phase Separation

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Materials (Zeolite, MOF etc)

Keywords: asymmetric gradient porous, delayed phase separation, dynamically tunable, electromagnetic interference shielding, thermal management

Abstract Body.
The rapid pace of global urbanization has exacerbated urban heat island effects and electromagnetic radiation pollution. Urban infrastructure, including buildings, roads, and other structures, absorbs and re-emits heat, leading to more frequent and intense heatwaves. This phenomenon poses a significant threat to human well-being, increasing energy consumption, reducing productivity, and disrupting urban ecosystems. Concurrently, the proliferation of wireless communication base stations , coupled with the growing number of vehicles and household appliances, has led to a continuous rise in electromagnetic radiation density in urban environments. Prolonged exposure to electromagnetic waves is associated with potential health risks, including increased cancer incidence, sleep disorders, and neurological diseases. Consequently, there is an urgent need to develop advanced fabrics capable of managing personal thermal comfort while providing electromagnetic radiation protection, effectively mitigating the challenges posed by urban heat islands and electromagnetic pollution.

AGPF was fabricated via a delayed evaporation–induced phase separation strategy, producing a gradient porous polystyrene-block-poly(ethylene-ran-butylene)-block-polystyrene (SEBS) matrix with fully sedimented liquid metal (LM) networks at the bottom. The gradient pore architecture broadens light scattering across the solar spectrum and enhances mid-infrared absorption through a progressive refractive-index transition, while the transversely oriented LM forms conductive pathways activated by pre-stretching.

The gradient porous structure of AGPF broadens the scattering spectrum with a wider micro-nano pore size distribution and enhances air-medium interface absorption in the mid-infrared region due to the progressive refractive index transition, achieving 93.9% solar reflectivity and 94.7% infrared emissivity. The gradient porous SEBS provides conditions for the stretch activation of the LM networks and reduces the percolation threshold. The fully sedimented LM at the bottom is activated by pre-stretching, forming a transversely oriented structure with vertical wrinkles, which significantly improves both mechanical and electrical properties. AGPF demonstrates exceptional EMI SE of 80.6 dB and superior electrical heating performance. Moreover, AGPF exhibits dynamically tunable thermal management and EMI shielding performance across a strain range of 0% to 200%, adapting to complex outdoor environments. The design of AGPF provides an advanced solution to protect individuals

from the dual threats posed by urban heat island effects and electromagnetic pollution.

In conclusion, we have developed an AGPF composed of gradient porous SEBS and transversely oriented LM networks with vertical wrinkles at the bottom, achieved through a delayed evaporation-induced phase separation strategy. This work presents an advanced solution to address the dual challenges of urban heat island effects and electromagnetic pollution arising from urbanization.

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SCM0221

Impact of Short-Range Order on Lattice Thermal Conductivity in High-Entropy Thermoelectric Chalcogenides

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Materials (Zeolite, MOF etc)

Keywords: High-entropy chalcogenides, Short-range order, Lattice thermal conductivity, Machine-learning interatomic potential

Abstract Body.
High-entropy thermoelectric chalcogenides are emerging as a promising class of functional materials for waste-heat recovery and energy-efficient operation of chemical processes. Their intrinsically low lattice thermal conductivity, arising from strong mass and strain disorder, makes them attractive for environmentally-friendly and sustainable chemical technologies. However, the role of chemical short-range order (SRO) in controlling phonon transport in these multi-component alloys remains largely unexplored, despite its potential importance for rational thermoelectric materials design.
In this work, we develop a machine-learning interatomic potential based on the Moment Tensor Potential (MTP) formalism to investigate the impact of SRO on the lattice thermal conductivity of rocksalt-type high-entropy chalcogenides composed of Pb, Ge, Sn, Cu, Ag, Sb, Bi, Se and Te. The potential is trained on a large density-functional-theory (DFT) dataset of 64-atom supercells spanning diverse compositions and local environments, and is coupled to a hybrid atom-swap Monte Carlo and molecular dynamics (MC/MD) sampling scheme. The resulting finite-temperature configurations are analyzed using Warren–Cowley SRO parameters to quantify the degree and pattern of chemical ordering.
Using the trained MTP, we will compute the lattice thermal conductivity via the Green–Kubo formalism and systematically compare (i) special quasi-random structures that mimic ideal random solid solutions and (ii) SRO-stabilized configurations for selected high- and low-performance thermoelectric compositions. Based on these comparisons, we aim to clarify how composition and chemical SRO jointly govern lattice thermal conductivity in high-entropy chalcogenides. The implications of this structure–property relationship for designing next-generation thermoelectric materials to recover low-grade waste heat and enhance the energy efficiency of sustainable chemical processes will be discussed.

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SCM0370

Selective Recovery of Cesium Ions Using Zeolite-Modified Nafion Membranes for Sustainable FDCA Production

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Materials (Zeolite, MOF etc)

Keywords: bipolar membrane electrodialysis, cesium ion recovery, cation exchange membrane, composite membrane, zeolites, molten salt catalyst recycling, FDCA production

Abstract Body.
2,5-Furandicarboxylic acid (FDCA) is a promising bio-based monomer for sustainable production. Recent research has shown that cesium-based molten salt catalysts can effectively produce FDCA from carbon dioxide, offering a route to carbon circularity. However, the high cost of cesium necessitates efficient recovery and reuse for economic feasibility. Despite its importance, the selective recovery of cesium remains a challenging task. Conventional separation techniques, such as precipitation and adsorption, exhibit limited recovery capacity and recyclability.
In this study, we developed cesium-selective cation exchange membranes by fabricating thin film composite membranes with additives. For the sustainable separation of high-concentration cesium ions, the bipolar membrane electrodialysis system was utilized at different operating conditions (e.g., current density and feed concentration). The different chemical structures of commercially available cation exchange membranes (CEMs) were screened to find a suitable backbone structure for cesium selective recovery. The commercial membranes were investigated to optimize operating conditions, resulting in more than five times enhancement in cesium/sodium selectivity. Furthermore, zeolite-based composite CEMs were developed to further enhance separation performance, demonstrating a 16-fold higher cesium selectivity compared to the pristine membrane. It was demonstrated that can be reused. The energy consumption was also calculated to confirm the economic feasibility. The detailed information will be discussed in the presentation.
Acknowledgments
This research was supported by the to the National Research Council of Science & Technology (NST) grant by the Korea government (MSIT) (No. GTL25021-000).
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SCM0472

Silanol-assisted pathway over alkali-modified ZSM-5 for selective dehydration of lactic acid to acrylic acid

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Materials (Zeolite, MOF etc)

Keywords: Zeolite, Acid/Base, Defected site, Silanol group

Abstract Body.
Alkali-exchanged zeolites such as K–ZSM–5 have emerged as promising catalysts for the selective dehydration of lactic acid (LA) to acrylic acid (AA). However, the formation of Brønsted acid sites via ion exchange between LA's carboxyl group and alkali cations promotes undesired decarbonylation, yielding acetaldehyde as a byproduct. Herein, we elucidate the pivotal role of framework-associated silanol defects in promoting AA selectivity over K–ZSM–5 catalysts. Using a combination of defect-controlled syntheses (via OSDA removal, HF treatment, and desilication), solid-state NMR, FT-IR, and DFT calculations, we demonstrate that intra-pore silanol groups adjacent to extra-framework K+ cations modulate their acidity and facilitate efficient AA formation. Specifically, silanol-rich K–ZSM–5 (Si/Al = 15) achieved over 81% AA selectivity, a substantial enhancement compared to ~11% for defect-free K–ZSM–5. In situ DRIFTS analysis further confirmed that silanol-assisted dehydration occurs at significantly lower temperatures (~150 °C) without relying on lactate intermediates or Brønsted acid formation. Tuning KOH concentration enabled control over silanol density, which strongly correlated with ion-exchange degree, acid site distribution (Brønsted vs Lewis acids), and product selectivity. These findings establish a clear structure–activity relationship, revealing that silanol defects are not merely passive but actively direct reaction pathways in alkali zeolite catalysis.

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SCM0572

Hierarchically Porous MFI Zeolite Nanosponge Catalyst for Efficient Glucose-to-HMF Conversion

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Materials (Zeolite, MOF etc)

Keywords: MFI Zeolite Nanosponge; Mesoporous; Glucose; HMF; Acid sites

Abstract Body.
Introduction.
The catalytic conversion of glucose into 5-hydroxymethylfurfural is a key step in biomass valorization, yet it remains challenging due to diffusion limitations and catalyst deactivation. MFI zeolites are promising solid acid catalysts for glucose isomerization and subsequent dehydration reactions; however, their narrow micropores often restrict molecular transport and accelerate deactivation under hydrothermal conditions. In this study, we report a hierarchical MFI zeolite nanosponge designed to overcome these limitations and systematically investigate its catalytic advantages over bulk MFI zeolites.
Methods.
The MFI zeolite nanosponge was synthesized via a seed-assisted hydrothermal synthesis method, using a [C18H37-N+(CH3)2-C6H12-N+(CH3)2-C4H9(Br-)2] surfactant molecule as a structure-directing agent [1]. For comparison, bulk MFI zeolite was also synthesized using tetrapropylammonium hydroxide. Glucose conversion reactions were conducted in a batch-type reactor at 473 K using a biphasic H2O/THF system under vigorous stirring. After the reaction, glucose conversion and product selectivity were quantitatively analyzed by high-performance liquid chromatography equipped with refractive index and ultraviolet detectors.
Results and discussion.
The MFI zeolite nanosponge consists of nanolayered MFI building units assembled into a three-dimensional disordered network, giving rise to a well-developed hierarchical pore system. In contrast to solely microporous bulk MFI, the nanosponge catalyst exhibits uniformly distributed mesopores in addition to intrinsic micropores, resulting in a substantially increased BET surface area and total pore volume. Acid site analysis revealed that, while maintaining sufficient framework Brønsted acidity, approximately 30% of the total acid sites are located on the external and mesopore surfaces, where reactant accessibility is significantly enhanced.
These structural and acidic features directly translated into superior catalytic behavior during glucose conversion. The bulk MFI zeolite showed an initial increase in glucose conversion but rapidly deactivated in batch operation, which can be attributed to severe diffusion constraints and the accumulation of reaction intermediates and byproducts within the narrow micropores. As a result, catalytic activity was not recovered after the early reaction stage. In contrast, the MFI nanosponge catalyst exhibited a rapid increase in glucose conversion and sustained high activity without pronounced deactivation throughout the reaction period. The

open mesoporous network effectively alleviated mass transport limitations, while the strong acid sites exposed on the mesopore surfaces actively promoted isomerization and dehydration reactions under hydrothermal conditions. Furthermore, process parameter studies revealed that the nanosponge structure mitigates sensitivity to reactant concentration, salt addition, and particle size, highlighting its superior robustness and prolonged catalyst lifetime.

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2026 / SEOUL, KOREA

SCM0650

Mapping the CVD Growth-Rate Window of (101)-Oriented Bismuth Perovskite Thin Films

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Keywords: Lead-free perovskite solar cells, chemical vapor deposition, thin-film growth, bismuth oxide precursor.

Bismuth-based perovskite solar cells are attractive lead-free candidates. However, most reported bismuth perovskite thin films show strong c-axis texture, and charge transport along the c-axis is intrinsically poor [1]. We previously developed a surface-reaction model for chemical vapor deposition (CVD) growth of $(CH_3NH_3)_3Bi_2I_9$ (MABI) [2]. In this work we mapped the processing window that enables (101)-oriented MABI thin films.

MABI films were deposited in a horizontal stainless-steel CVD reactor using Bi_2O_3 solid as the Bismuth source. Hydrogen iodide diluted in He was fed to an upstream zone, where it reacted with Bi_2O_3 to form BiI_3 vapor. The resulting BiI_3/He/residual HI stream was then mixed with a methylamine/He stream just upstream of the substrate zone to form MAI in situ and followed with MABI thin film deposition. Phase purity and out-of-plane orientation were evaluated by X-ray diffraction.

The texture was quantified by the Lotgering factor using twelve reflections from the reference powder pattern and summarized in an orientation map as a function of BiI_3- and MAI-related surface reactivity parameters. The map shows a distinct (101)-oriented window at high BiI_3 reactivity, where the deposition rate is up to almost one order of magnitude higher than in the MAI-rich region; for example, strongly (006)-oriented films at 160 °C grow at about 0.03 μg cm^{-2} s^{-1}, whereas weakly (006)-oriented films under higher BiI_3 supply reach over 0.2 μg cm^{-2} s^{-1}. Data at 160 and 180 °C fall on the same trend, which supports the surface-reaction framework. The high-rate regime with weak c-axis texture lies well outside the rate range used previously to fit the kinetic parameters of our surface-reaction model, which suggests a change in the dominant growth mode. We propose that roughening of (101)-type surfaces, which have more step and kink sites than the relatively flat c-axis facets, promotes fast secondary nucleation and can explain the strong increase in deposition rate and the improved control of film orientation.

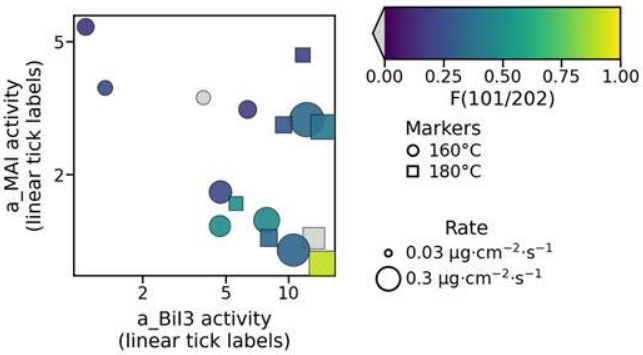

Figure 1. Orientation map of MABI thin films versus BiI_3 and MAI surface reactivity parameters ($\log(K_i p_i)$).

Acknowledgments

This work was supported by JST SPRING, Grant Number JPMJSP2110.

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2026 / SEOUL, KOREA

SCM0690

Selective ring hydrogenation of aromatic amines over Ru-Loaded A520 aluminum MOF

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Materials (Zeolite, MOF etc)

Keywords: Cyclohexanamine, Metal-organic-framework, Cyclohexylamine-N-cyclohexyl

Abstract Body.
Introduction. Hydrogenation is a key catalytic process widely used in the chemical, pharmaceutical, and polymer industries due to its high atom economy and efficiency [1]. While conventional carbon-supported noble metal catalysts enable aromatic ring hydrogenation, their performance is often limited by structural and surface constraints, motivating the development of advanced supports. Metal-organic frameworks (MOFs), particularly aluminum-based MOFs, offer tunable porosity, surface acidity, and strong metal–support interactions that enhance hydrogenation activity and selectivity [2]. In this context, an aluminum-fumarate MOF (A520) supported Ru catalyst demonstrates superior performance for the selective ring hydrogenation of aniline and related aromatics, highlighting its potential for efficient and scalable catalytic applications.
Methods. MOF A520 was synthesized via a modified aqueous precipitation method using fumaric acid and aluminum sulfate under mild conditions, yielding a highly stable and porous framework after activation. A Ru/A520 catalyst (3 wt% Ru) was prepared by incipient-wetness impregnation followed by hydrogen reduction to form metallic Ru nanoparticles. For comparison, Ru/γ-Al_2O_3 and Ru/Activated Carbon catalysts with identical metal loadings were prepared using the same impregnation procedure. Aromatic amine ring hydrogenation was performed in a high-pressure batch reactor at 100 °C and 15 bar H_2, and reaction products were analyzed by GC-MS.
Results and discussion. Achieving high selectivity toward ring hydrogenation remains challenging, as it requires precise control over metal dispersion, pore structure, and MOF demonstrated outstanding catalytic performance compared with conventional Ru/AC and Ru/Al_2O_3 catalysts. Under mild hydrogenation conditions (15 bar H_2, 120 °C, 1 h), Ru/A520 achieved nearly complete aniline conversion with a high cyclohexanamine selectivity of 91.1% (Fig.1). This superior performance is attributed to the high porosity of the A520 framework and the uniform dispersion of Ru nanoparticles, which together enhance reactant accessibility and promote efficient aromatic ring hydrogenation. Beyond aniline, the Ru/A520 catalyst exhibited promising activity for the hydrogenation of various substituted aromatic amines, yielding high amounts of the corresponding saturated products. Mechanistic investigations revealed that cyclohexanamine can further transform into cyclohexylamine-N-cyclohexyl via imine intermediates over the Ru/A520 catalyst.
Acknowledgments This work was supported by National Research Foundation of Korea (RS-2024-00341143)...
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SCB0067

Can Reductive Catalytic Fractionation Biorefinery Be a Pathway for Paper-Making Pulp?

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Biomass

Keywords: Reductive Catalytic Fractionation (RCF), Lignin-first biorefinery, Fibers; Pulp, Paper-making, Sustainable Materials

Abstract Body.
Reductive Catalytic Fractionation (RCF) has emerged as a leading lignin-first strategy for the sustainable refining and valorization of lignocellulosic biomass, traditionally optimized for the production of high-quality lignin-derived phenolic compounds. However, its potential to simultaneously generate pulp suitable for papermaking remains largely underexplored. This study evaluates the feasibility of employing RCF as an integrated pathway for pulp production from spruce chips, while maintaining the superior quality of the recovered lignin. Experiments were carried out in polar solvents using a Metal catalyst under hydrogen pressure. The pH was increased to assess the effect on delignification, fiber morphology, and paper properties. The resulting pulps were comprehensively characterized in terms of chemical composition, fiber deformation, and mechanical performance, and benchmarked against industrial unbleached kraft pulp (UKP). At higher pH, RCF achieved efficient delignification (Kappa number below 30) while preserving fiber integrity, yielding pulps with long fibers (> 2500 µm), low fines content (< 20%), and enhanced brightness. The corresponding papers exhibited tensile and tear indexes comparable to Kraft pulp. These findings demonstrate that properly tuned RCF conditions can produce high-quality papermaking pulp alongside valuable lignin oil, thereby extending the scope of lignin-first biorefineries toward integrated pulp and paper production.

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SCB0132

Catalytic Transformation of Lignin into Low Molecular Weight Oil Rich in Active Groups Using a Vanadium-Based Catalyst

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Biomass

Keywords: oxidative depolymerization, vanadium-based catalyst, phenolic hydroxyl group, carboxyl group

Abstract Body.

Introduction

Lignin is the most abundant renewable aromatic compound in nature. However, its complex three-dimensional network structure, chemical bonding patterns, and hydrogen bonding interactions make it difficult to degrade efficiently into phenolic monomers or chemicals. As a result, most lignin is often discarded or directly burned for heat and power generation. Among various depolymerization methods, such as pyrolysis, acid/base-catalyzed depolymerization, oxidative depolymerization, and reductive depolymerization, oxidative degradation is particularly attractive due to its relatively mild reaction temperature and pressure. While catalysts including homogeneous catalysts (e.g., copper salts), heterogeneous catalysts (e.g., transition metal oxides, polyoxometalates, perovskites), and enzymatic catalysts (e.g., laccase) have been studied for lignin oxidative depolymerization, vanadium-based catalysts have rarely been explored. This study aims to investigate vanadium-based catalysts for the oxidative depolymerization of lignin, a process that offers a promising route for converting lignin into valuable phenolic monomers or chemicals under relatively mild conditions.

Method

Catalysts including V_2O_5, $VO(acac)_2$, V_2O_5/WO_3, V_2O_5/diatomite, and V_2O_5/SiO_2 were synthesized via calcination, impregnation, and pH-regulated co-precipitation methods. The prepared catalysts were characterized using scanning electron microscopy (SEM) and X-ray diffraction (XRD). Their catalytic performance was evaluated under different reaction conditions, including temperature, catalyst dosage, and reaction time. The depolymerized lignin oil was analyzed by potentiometric titration to determine phenolic hydroxyl and carboxyl group contents, Fourier-transform infrared spectroscopy (FT-IR) for structural and bonding information, and gel permeation chromatography (GPC) for molecular weight distribution.

Results

Among all tested catalysts, V_2O_5/diatomite exhibited the best catalytic performance. Under optimized conditions (60°C, 0.075 g of V_2O_5/diatomite, 4 h reaction time), the highest lignin oil yield reached 42.63%. Potentiometric titration results showed that the phenolic hydroxyl content increased from 1.158 mmol·g-1 to 2.079 mmol·g-1, and the carboxyl content increased from 0.801 mmol·g-1 to 6.650 mmol·g-1, indicating that prolonged reaction time promoted both lignin oil formation and the enrichment of active functional groups. FT-IR analysis further confirmed the structural changes, consistent with the titration results. GPC

analysis revealed that the enzymatic hydrolysis lignin was efficiently depolymerized into low-molecular-weight fragments.

Conclusion

This study developed a solid vanadium oxide catalyst supported on natural diatomite for the alkaline oxidative depolymerization of lignin. Under mild reaction conditions, a lignin oil yield of 42.63% was achieved. The obtained lignin oil possesses abundant phenolic hydroxyl and carboxyl groups, along with a low molecular weight, indicating high potential for applications such as lignin-based natural polymers or natural emulsifiers.

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SCB0228

Hydrotreating of Used Cooking Oil over γ-Al_2O_3 : Impact of Heavy Impurities on Mass Transfer and Catalyst Deactivation

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Biomass

Keywords: Used cooking oil, Triglyceride, Hydrotreating, Egg-shell, Mass transfer limitation

Abstract Body.
Deoxygenation of triglyceride feedstocks via hydrotreating is a key pathway for producing renewable hydrocarbon fuels. Among various triglyceride sources, used cooking oil (UCO) has emerged as a promising biomass feedstock due to its economic and environmental advantages. However, unlike fresh sources such as vegetable oils, UCO contains a range of impurities that can significantly affect catalytic conversion—a factor that is often overlooked. In this study, we rigorously analyzed the chemical composition of UCO and investigated its impact on hydrotreating performance. While soybean oil (SBO, a representative fresh vegetable oil) consists primarily of triglycerides, UCO contains various degradation products generated during cooking, including free fatty acids, mono- and diglycerides, and heavy species such as dimerized triglycerides and aromatic compounds. During hydrotreating over Pt/γ-Al2O3 catalysts, both SBO and UCO experience significant mass transfer limitations due to the large molecular size of triglycerides. However, the conversion of UCO is more severely constrained owing to the presence of heavy organic impurities. Notably, the use of large-pore γ-Al2O3 as a support and an egg-shell Pt distribution effectively alleviated mass transfer limitations, enhancing catalytic activity and mitigating deactivation. Furthermore, implementing a pre-hydrogenation step to remove unsaturated fatty acids and aromatic impurities prior to deoxygenation further reduced catalyst deactivation caused by coke formation.

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SCB0245

Sustainable Biomass-Derived Liquid Crystal Films with Intelligent Magnetic Reconfiguration for Programmable Microwave Absorption

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Biomass

Keywords: sustainable biomass; cellulose liquid crystal; tunable microwave absorption; magnetic reconfiguration

Abstract Body.
Developing sustainable and adaptive materials is crucial for next-generation green electronics. The static nature of conventional microwave absorbers limits their adaptability in dynamic electromagnetic environments. Stimuli-responsive absorbers, particularly magnetic tunable systems, offer a promising solution but face challenges in achieving reversible structural reconfiguration. While tunable microwave absorbers are in demand, most rely on synthetic or non-renewable components. This work presents a fully biomass-derived, magnetically responsive liquid crystal film as an environmentally friendly platform for programmable electromagnetic absorption. A reconfigurable microwave absorption film was fabricated using renewable hydroxypropyl cellulose (HPC) as the cholesteric liquid crystal matrix. Magnetic Ni@CNT chains (NCC) were incorporated into the HPC phase. A unique solid-shell/fluid-core structure was formed via UV-induced surface polymerization, preserving the fluidity of the biomass-derived core while ensuring mechanical stability. The film was magnetically aligned into distinct orientations (horizontal, random, vertical) to study structure-dependent performance. The fluid HPC core enabled reversible magnetic reorientation of NCC, which in turn guided the alignment of the sustainable cellulose matrix through hydrogen bonding. This dynamic reconfiguration allowed real-time tuning of conductive and magnetic networks, leading to programmable microwave absorption directly controlled by magnetic fields. Magnetic tuning reshapes extended magnetic coupling, conductive pathways and dissipation interfaces, creating anisotropic, orientation-dependent microwave absorption. The horizontally aligned film exhibited excellent performance: a minimum reflection loss of −42 dB at 12 GHz and a broad effective absorption bandwidth of 9.8 GHz across the X–Ku bands. The system demonstrates fully reversible and stable tuning, highlighting the synergy between sustainable biomass materials and adaptive functionality.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

SCB0261

Enhancing Pyrolysis with Ultrasound Treatment at High Temperatures as a Novel Process

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Keywords: pyrolysis; biochar; ultrasounds; sonochemistry; Raman spectroscopy

Introduction. Biochar has gained increased attention because of the potential use in various sustainability applications, such as in batteries, supercapacitors, and as a soil amendment [1]. To obtain biochar with desired properties, simple ultrasonic activation of biochar in water has been proposed, but the process requires an energy-intensive step of drying. Here, the previously considered infeasible application of ultrasounds during pyrolysis [2] is demonstrated and proposed as a novel process in biochar production.

Methods. Pellets of Sargassum algae powder were placed in a hollow metal cylinder attached to an ultrasonic cleaner, forming a pyrolysis reactor. A copper rod wrapped in heating tape was placed on top of the pellet to conduct heat for pyrolysis. The reactor was fitted with a cover, and an inert atmosphere was created by flowing 4 L min^{-1} N_2 (at 20°C, 1 bar) through the setup. The pellet was heated to ca. 450°C during a heating stage of 27 min, with ultrasounds applied via the ultrasonic cleaner over 20 min during heating. Raman spectra were taken from the resulting biochar and processed by smoothing, subtracting the fluorescence background, and applying principal component analysis (PCA). The biochar was additionally analysed in a thermogravimetric analyser (TGA), applying a heating rate of 10°C min^{-1} with air and N_2 as reactive gas, respectively.

Results and discussion. The results from PCA of the Raman spectra collected on the produced char pellets show a distinction between samples with and without the ultrasound treatment (Fig. 1). No such distinction was observed for samples heated to 300°C, indicating the ultrasounds affected the pyrolytic decomposition between 300 and 450°C, potentially because of the interaction with denser tar-type components, released at higher temperatures. The results from the TGA showed no difference between samples with and without ultrasound treatment, suggesting the ultrasounds did not affect the reactivity of the sample. Further analysis will determine the physical effect of the ultrasounds and examine possible underlying mechanisms, such as a distinction between samples with and without acoustic cavitation in liquid tars of the sample. The proposed process of applying ultrasounds at elevated temperatures might be translatable to other applications and serve as the first step towards new chemical processes.

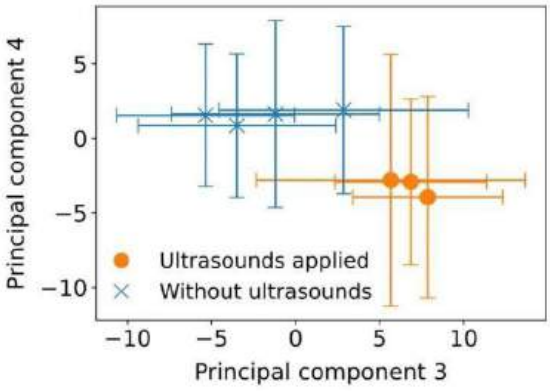

Figure 1: Principal components 3 and 4 of Raman spectra of Sargassum pellets, showing ultrasound treatment (no distinction visible for principal components 1 and 2). Each point represents the mean of all Raman spectra collected on a sample; error bars show the standard deviation.

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SCB0272

Electronic-structure control of source-dependent hydrogen utilization in selective C–O bond cleavage in furfural conversion

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Biomass

Keywords: electronic-structure effect; hydrogen utilization; C-O bond cleavage; furfural hydrogenation, 1,5-pentanediol

Abstract Body.
Selective conversion of furfural (FFA) to 1,5-pentanediol (1,5-PDO) requires precise control over hydrogen activation [1], and charge redistribution in the catalyst surface [2]. Here, we demonstrate that modified electronic structures of Co-Zr mixed oxides regulate hydrogen partitioning and reaction selectivity in the on FFA to 1,5-PDO productions.
Two distinct methods were used to modify the surface electronically of Co-Zr mixed oxide: the first approach is a chemical reduction method with 1 M NaBH4, named the catalyst as Co2.5Zr1-CR, and the second approach with in-situ reduction process named Co2.5Zr1-IR. By systematic comparison of in-situ reduced and chemically reduced Co–Zr mixed oxides, we show that as Co2.5Zr1-CR achieves a markedly higher 1,5-pentanediol yield (70.5%) than its named Co2.5Zr1-IR catalyst (55.4%).
Based on spectroscopy analysis, ZrOx nanoclusters act as interfacial electron reservoirs that capable of stabilizing Co2+ centers rich in unpaired electrons within Ov-Co3O4, which generating electronically asymmetric and spin-polarized catalytic environments capable of heterolytic hydrogen activation and C−O cleavage of furan ring. Isotope labelling and kinetic isotope effect uncover unique hydrogen chemical potential on the catalyst surface, where ethanol-derived hydrogen preferentially participates in the rate-determining C2−O bond cleavage, while H2-derived hydride do selective hydrogenation of FFA carbon backbone. Density functional theory calculations further confirm that C2−O bond scission is the rate-limiting step and show that rich Ov-Co3O4 in the Co-Zr mixed oxide system lowers the activation barrier by inducing charge depletion at the reaction carbon and charge accumulation in the furan ring. These findings signify that electronic asymmetry, spin polarization (unpaired electron of Co2+ in Co3O4), and hydrogen partitioning are the key descriptors for selective biomass-derived FFA hydrogenation and C−O bond activation in mixed oxide catalysts.

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CDU0274

Pyrolysis and in-line catalytic cracking of olive stone-derived volatiles

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Biomass

Keywords: fast pyrolysis, olive stone, catalytic cracking, spouted-bed reactor

Abstract Body.
Introduction. The transition toward a less fossil-dependent circular economy requires efficient technologies for producing fuels and chemicals from renewable resources. Olive stone is an abundant Mediterranean residue, generated at roughly 0.2 ton per ton of raw olives [1]. Ex-situ catalytic fast pyrolysis offers a promising valorization pathway for such lignocellulosic waste.
Methods. In this work, olive-stone pyrolysis vapours were upgraded using a dual spouted-bed/fixed-bed bench-scale unit. Spouted-bed reactors are well established for biomass and plastic conversion, offering intense solid–gas circulation, rapid particle heating, and effective mitigation of agglomeration issues common in bubbling beds [2]. The study examines the influence of pyrolysis temperature, cracking temperature, and catalyst space-time on product yields, quality, and catalyst deactivation. Preliminary insights into the effect of catalyst type on product distribution are also reported.
Results and discussion. Increasing catalyst space-time and cracking temperature enhanced water and gas formation at the expense of organics. Char yield remained insensitive to catalytic conditions but decreased with higher pyrolysis temperatures. Micro-GC analysis showed that HZSM-5 (zeolite used as catalyst) favoured decarbonylation and dehydration as primary deoxygenation routes. The catalyst significantly reduced light oxygenates in bio-oil and promoted the production of aromatic hydrocarbons, but its strong Brønsted acidity also drove secondary condensation to PAHs. Spent-catalyst analysis indicated rapid deactivation, with ~10 wt% coke deposition and substantial losses in surface area and porosity within 45 min. Type I coke—poorly ordered deposits in meso- and macropores—was more abundant than type II, and acidic sites (measured by NH3-TPD) were progressively masked by coke and condensed hydrocarbons. A screening of different catalysts demonstrated that the functionality must be tailored to the targeted upgrading outcome. HZSM-5 remained the most effective for aromatization and for suppressing light oxygenates, whereas calcined dolomite showed exceptional deacidification performance. In contrast, γ-Al2O3-based catalysts and Fe/dolomite exhibited limited improvements, indicating the need for further research.

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SCB0286

Selective Production of C4-C12 Alcohols from Bio-derived Aldehydes

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Biomass

Keywords: Biomass; Aldehyde; Aldol condensation; Hydrogenation; Mixed-oxide

Abstract Body.
The conversion of bio-derived aldehydes to plasticizer alcohols (>C8) via the one-pot aldol condensation and hydrogenation reactions has attracted increasing attention in the plastic industry[1,2]. In this study, the synthesis of C4-C12 alcohols from the one-pot reaction of n-butanal and n-hexanal has been studied over bi-functional catalysts, yNi/CaxAl-mixed oxide prepared by the urea hydrothermal method and impregnation method. The characterization, including BET, H2-TPR, TPD, XRD, XPS, and TEM, and the catalytic performance were investigated in detail for the catalysts. The result showed C8 alcohol (2-ethylhexanol), C10 alcohols (2-butylhexanol, 2-ethyloctanol) with different branching, and C12 alcohol (2-butyloctanol) as major products. For the catalysts, the strength of Brønsted basic sites were controlled by tuning the Ca/Al molar ratio, and the hydrogenation sites were tuned by varying the Ni loading. Ni(10wt%)/Ca4Al-mixed oxide (10NCA) exhibited excellent catalytic performance with a 85.0% total alcohol yield.

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SCB0303

Techno-economic Analysis, Sustainability Assessment and Mechanistic Kinetic Modeling of Furfural Transfer Hydrogenation to 2-Methylfuran

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Biomass

Keywords: Catalytic transfer hydrogenation, Furfural upgrading, Process simulation, Techno-economic analysis, Life cycle analysis, Kinetic modeling

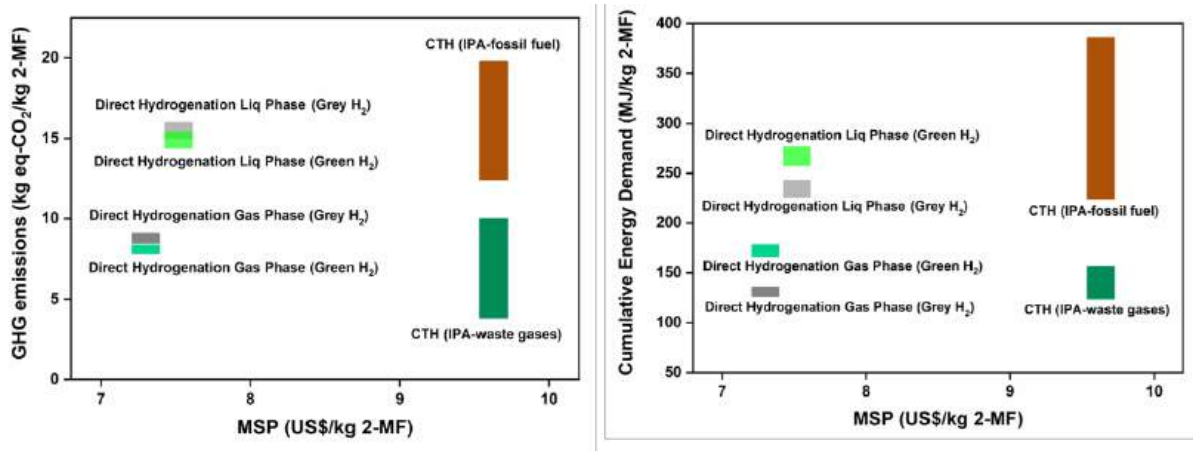
Abstract Body.
Introduction: Catalytic transfer hydrogenation (CTH) of biomass-derived furfural to 2-methylfuran (2-MF) using alcohol hydrogen donors provides a hydrogen-free upgrading route, yet its process-level competitiveness with direct hydrogenation remains uncertain. This work integrates process modeling, techno-economic analysis (TEA), life cycle assessment (LCA), and mechanistic kinetic modeling to evaluate furfural CTH over Cu–Re/SiO_2 catalysts and benchmark it against literature hydrogenation processes.

Methods: Power-law kinetics were obtained from liquid-phase batch experiments at 210–240 °C using isopropanol as hydrogen donor, achieving complete furfural conversion and up to ~81% 2-MF yield. The kinetics were implemented in Aspen Plus RCSTR model to simulate continuous operation with solvent recovery and recycle. Comparative process models were developed for reported gas and liquid-phase hydrogenation routes under consistent economic assumptions. TEA estimated capital expenditure (CAPEX), operating expenditure (OPEX), minimum selling price (MSP), and sensitivity of MSP to feedstock, solvent, and utility costs. Cradle-to-gate LCA evaluated global warming potential (GWP) and cumulative energy demand (CED) using both economic allocation and system expansion, with Monte Carlo simulations to assess uncertainty. Mechanistic Langmuir–Hinshelwood–Hougen–Watson (LHHW) models were fitted to discriminate among possible surface reaction pathways on Cu–SiO_2 and Cu–Re/SiO_2 catalysts.

Results: Process simulation shows that solvent recovery strongly affects both economics and environmental impact, with isopropanol makeup contributing over half of variable operating costs in the base case. TEA indicates that CTH achieves MSP values comparable to liquid-phase hydrogenation but remains higher than optimized gas-phase routes, with MSP most sensitive to furfural price, solvent loss fraction, and catalyst productivity. A ±20% change in solvent recovery efficiency leads to ~10% variation in MSP. LCA results show that GWP and CED differ substantially by allocation method, with system expansion yielding lower net impacts due to hydrogen displacement credits, while economic allocation reflects higher burdens dominated by solvent production and energy utilities. Monte Carlo analysis reveals wide uncertainty bands, primarily driven by upstream solvent and electricity datasets. Mechanistic modeling indicates that Cu–Re/SiO_2 follows a dual-site stepwise pathway

involving ReOx-mediated O–H activation and Cu-mediated hydride transfer, whereas Cu–SiO_2 is better described by a single-site concerted mechanism.

Conclusions: While CTH of furfural to 2-methylfuran remains economically less favorable than conventional gas-phase hydrogenation, integration of hydrogen donor production from waste refinery gases enables substantially lower GWP, highlighting a trade-off between economic performance and environmental sustainability.



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SCB0304

Comparative Techno-Economic and Life Cycle Assessment of Bioplastic Precursor Production Routes

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Biomass

Keywords: FDCA production, Process simulation, Techno-economic analysis, Life cycle assessment, Biomass valorization

Abstract Body.
Purpose: 2,5-Furandicarboxylic acid (FDCA) is a key bio-based monomer for polyethylene furanoate (PEF) and a potential substitute for terephthalic acid. Several biomass-derived production pathways have been proposed, yet their relative economic and environmental performance remains uncertain. This study presents a comparative techno-economic analysis (TEA) and life cycle assessment (LCA) of three FDCA synthesis routes: (i) oxidation of 5-hydroxymethylfurfural (HMF), (ii) furfural-based Henkel-type disproportionation, and (iii) furfural carboxylation-based pathways.

Methods: Process flowsheets for all routes were developed in Aspen Plus using literature-reported conversions and selectivities, assuming identical plant capacities and downstream purification targets. For the HMF oxidation route, FDCA yields above 90% were assumed, while furfural-based routes were modeled with overall FDCA yields in the range of 60–75% due to additional rearrangement and carboxylation steps. Capital and operating costs were estimated to determine minimum selling price (MSP) of FDCA. Sensitivity analysis evaluated the effects of feedstock price, catalyst replacement, and separation energy. Cradle-to-gate LCA quantified global warming potential (GWP) and cumulative energy demand (CED) using both economic allocation and system expansion. Monte Carlo simulations (10,000 runs) were performed to quantify uncertainty in environmental indicators.

Results: The HMF oxidation route exhibits the highest yield but also the highest operating cost, primarily due to HMF price and oxidant consumption, resulting in an MSP in the range of ~2.0–2.5 USD/kg FDCA. Furfural-based Henkel and carboxylation routes show lower feedstock costs but higher capital intensity, leading to MSP values of ~1.6–2.1 USD/kg depending on conversion efficiency and separation energy. A ±20% change in platform chemical price results in ~15–25% variation in MSP across all routes, identifying feedstock cost as the dominant economic driver. LCA results indicate GWP values of ~2.5–4.0 kg CO_2 -eq/kg FDCA for the HMF route, compared to ~1.8–3.0 kg CO_2 -eq/kg FDCA for furfural-based routes under system expansion assumptions. CED follows similar trends, with utility generation and upstream biomass processing contributing more than 60% of total energy demand. Monte Carlo analysis reveals wide uncertainty intervals (up to ±30% for GWP), largely driven by variability in biomass conversion yields and regional electricity mixes.

Conclusions: Although HMF oxidation offers superior reaction yields, its economic and environmental performance is strongly constrained by feedstock and oxidant requirements. Furfural-based pathways can achieve comparable or lower production costs and reduced carbon footprint when low-cost biomass-derived furfural and integrated carboxylation strategies are applied. The results highlight that feedstock sourcing and process integration, rather than reaction yield alone, determine the sustainability of FDCA production routes.

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SCB0344

Controlling the hydrogenation of furfuryl alcohol by modulating the local environment of Ru species in Ru/Zeolite catalysts

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Biomass

Keywords: Biomass Valorization, Ruthenium, Heterogeneous catalysis

Abstract Body.
The selective hydrogenation of furfuryl alcohol to valuable chemicals remains a challenging catalytic reaction due to the involvement of multiple hydrogenation and ring-rearrangement pathways. Achieving high selectivity toward cyclopentanol (CPOL), a key intermediate for cyclopentadiene (CPD) production, therefore requires not only efficient hydrogenation but also the suppression of side reactions leading to 1,4 pentanediol (1,4-Diol) and tetrahydrofurfuryl alcohol (THFA), which originate from ring opening of furfuryl alcohol. Therefore, precise control over the metallic sites on support is crucial.

Ru/zeolite catalysts were prepared by wet impregnation and grafting approach with organometallic Ru compound. For wet impregnation, an aqueous RuCl3·xH2O solution was added to a zeolite suspension, followed by solvent removal, drying, and calcination under N_2 . In contrast, grafted Ru catalysts were synthesized by grafting a Ru precursor onto surface hydroxyl groups of the zeolite under inert conditions, with Ru loading controlled by the hydroxyl density of the support, followed by washing and calcination steps.

In this study, we demonstrate that the hydrogenation selectivity toward CPOL over Ru catalysts supported on zeolite Y is governed not solely by Ru loading, but by the local chemical environment of activated Ru sites on the zeolite support. Under optimized conditions, the grafted Ru/zeolite catalyst achieved a CPOL yield of 70% at a Ru loading of 0.9 wt%. In contrast, a catalyst prepared by a conventional impregnation method with a comparable Ru loading exhibited lower CPOL yield of 54%. Notably, both catalysts contained similar amounts of Ru, indicating that differences in hydrogenation selectivity cannot be attributed solely to metal loading. The difference in CPOL selectivity between the grafted catalyst and impregnated catalyst highlights the critical role of the local chemical environment of Ru sites at the zeolite interface.

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SCB0379

A Calibration-Free Approach for Online Estimation of Metabolite Concentrations in Hyaluronic Acid Production using NIR-Spectroscopy

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Biomass

Keywords: Near-Infrared (NIR) spectroscopy; Parameter estimation; Process monitoring; Calibration-free method; Hyaluronic acid (HA).

Abstract Body.
Introduction: Access to metabolite concentrations is essential for online optimization and control of bioprocesses. Although spectroscopy-based multivariate calibration is widely used [1], it is time- and resource-intensive and requires frequent recalibration following instrument or process changes. To address this, a calibration-free approach that integrates mechanistic kinetic models with spectral information is employed. Here, we demonstrate the approach using HA production, where glucose concentration strongly influences HA molecular weight, necessitating effective real-time glucose regulation. Accordingly, NIR spectroscopy is used to monitor glucose, and other metabolite concentrations during batch HA production.
Methods: HA production was performed in batch using the recombinant Lactococcus lactis MKG6 strain [2]. Metabolite concentrations were predicted from inline NIR spectral data using a calibration-free framework (Fig. 1a), which projects spectra onto the concentration space defined by a dynamic model and estimates kinetic parameters by minimizing the squared Frobenius norm between measured and projected spectra [3]. To enhance robustness, parameters were constrained to be insensitive to minor data variations [4]. Accordingly, data from seven batch fermentations with different initial glucose concentrations (20 & 30 g/L) were augmented for parameter estimation, and the optimized parameters were subsequently used for online metabolite predictions.
Results and discussion: Figure 1b shows metabolite concentration predictions obtained using single and augmented multi-batch models, validated against offline measurements. Augmented multi-batch predictions resulted in lower RMSE values for glucose and HA (1.26 and 0.54) than single-batch models (1.55 and 0.73), with similar improvements for by-products, while biomass was slightly better predicted using individual batch data. These results demonstrate that multi-batch data augmentation with varying initial conditions improves parameter robustness and prediction accuracy for key metabolites. In future, the framework will be extended to support real-time monitoring and control of bioprocesses.

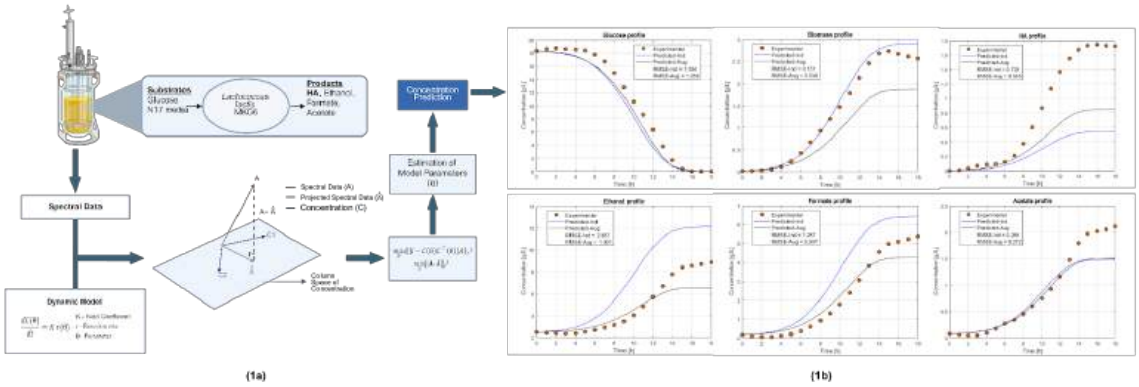

Figure 1: (1a) Schematic of the framework. (1b) Metabolites (Glucose, HA, Ethanol, Acetate, and Formate) and Biomass predictions using single and multi-batch augmented spectral data.

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SCB0394

Navigating the complexity in the valorization of microalgae HTC wastewater via aqueous phase reforming

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Biomass

Keywords: Aqueous phase reforming, Hydrogen production, Wastewater valorization

Abstract Body.
Introduction. Hydrothermal carbonization (HTC) converts wet biomass into a carbon-rich solid (hydrochar) with high fuel value. However, the process also generates a significant aqueous by-product (HTC-AP), which contains a complex mix of organic and inorganic compounds, and poses both environmental and economic challenges due to disposal costs. To address this issue, we explored the aqueous phase reforming (APR) process to convert biomass-derived compounds dissolved in water into hydrogen and alkanes at moderate temperatures (230-270 °C) and pressures. Despite its potential, APR of HTC-AP from microalgae remains unexplored: herein, we present the first study on this challenging feedstock with three main objectives: i) performing a comprehensive characterization of the organic and inorganic content of the wastewater; ii) identifying APR conditions that maximize H2 production and minimize residual organics in the liquid; iii) reducing catalyst deactivation by developing a series of physical pretreatments.
Methods. The HTC-AP was kindly provided by CEA Cadarache. It was characterized by complementary techniques for identifying and quantifying organic and inorganic compounds (e.g., GC-MS, HPLC, TOC, ion chromatography). APR tests were carried out in a batch reactor, and different reaction conditions were evaluated. A commercial 5% Ru/Al2O3 was used as reference catalyst, while glycolic acid was used as probe molecule in reuse tests.
Results and discussion. The figure below shows two representative outcomes. On the left, increasing the reaction temperature boosted both hydrogen productivity and selectivity, which was correlated with the higher glycerol conversion (within the organics pool). On the right, we demonstrated that diluting HTC-AP (from 1:3 to 1:18) mitigated catalyst fouling, as confirmed by reuse tests with glycolic acid, a model compound (namely fresh, in the figure). The implementation of ion-exchange adsorption to remove sulphate and phosphate further increased the H2 productivity and reduced the deactivation with respect to the base case (with adsorption, in the figures). These results support the integration of HTC and APR in a circular economy framework, enabling the conversion of solid and liquid outputs into energy carriers.

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SCB0480

The collaborative mechanism between adhered and planktonic microorganisms in anaerobic digestion of corn stalk and the performance enhancement of pretreatment

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Biomass

Keywords: Corn stalk, Anaerobic digestion, Adhered microorganisms, Planktonic microorganisms, Pretreatment

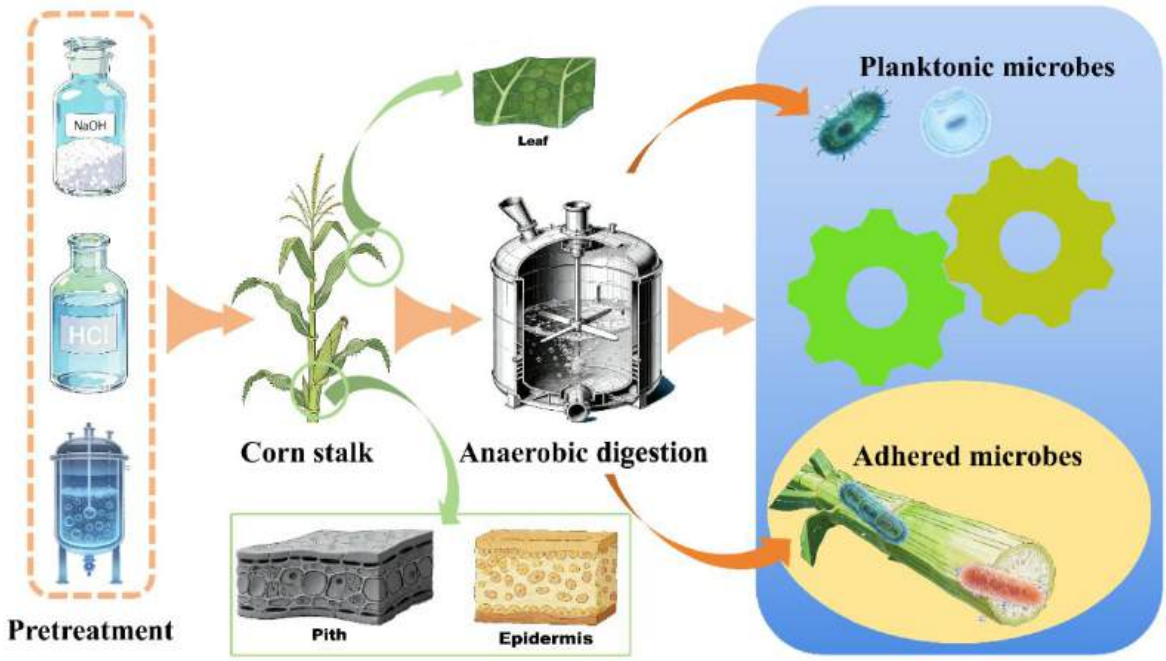
Abstract Body.
Purpose:
The mass transfer efficiency of corn stalk is limited in traditional anaerobic digestion. The study aims to reveal the spatial distribution of microbes and their synergistic role in intensifying transfer and reaction processes. Guidance for reactor design and process enhancement was provided by optimizing multiphase interface performance through pretreatment.

Methods:
(1) Linking substrate properties to reactor performance: Corn stalk was separated into epidermis, leaf, and pith for batch reactor tests, establishing a quantitative link between substrate chemical characteristics and methane yield. (2) Elucidating the phase behavior and functional zoning of microbes for process intensification: adhered and planktonic microbes were sampled and analyzed separately. The dynamic distribution and functional pathways of the two phases were elucidated. (3) Reaction process optimization: Systematic evaluation of the effects of chemical (acid/alkali) and micro aerobic pretreatment on the microstructure of stalk, microorganisms in the reactor, and final methane production.

Results:
(1) Substrate properties affected the reactor performance. Reactors fed with leaf and pith achieved significantly higher cumulative methane yields (275.3 and 263.7 mL/gVS) than fed with epidermis (187.8 mL/gVS). Differences in cellulose crystallinity and lignin encapsulation among the stalk parts, which directly determine mass transfer efficiency and reaction rate. (2) The dual-phase microbial system optimized the mass transfer and reaction processes. A spatial and functional zoning of microorganisms was established. Hydrolytic and fermentative bacteria enriched and attached to surface, forming biofilm. Acidogenic bacteria and methanogenic archaea predominantly exist in liquid phase. The biofilm acts as a "primary reactor" for hydrolyzing recalcitrant solids, while the planktonic microbial is a "secondary reactor" efficiently converting soluble intermediates. The phenomena mitigated potential product inhibition and enhanced mass transfer and overall reaction kinetics. (3) Pretreatment reshaped the reaction environment and enhanced mass transfer processes. The 2% NaOH treatment disrupted the crystalline regions of lignocellulose through saponification and swelling effects, greatly increasing the substrate specific surface area and

porosity, which raised the cumulative methane yield to 380.9 mL/gVS. Micro-aerobic pretreatment (4 mL/gVS O_2) modified surface properties via mild oxidation, increasing the yield to 319.5 mL/gVS. This optimization enhanced solid-liquid mass transfer efficiency and provided more favorable attachment sites for microbes within the main reactor by altering the physicochemical properties of substrate.

Conclusions:
The mechanism of microorganisms' spatial distribution and enhancement study provided new strategies for regulating multiphase mass transfer and reaction processes in lignocellulosic substrates anaerobic digestion reactors.



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SCB0499

Improving hydrothermal liquefaction of OFMSW through low-temperature pretreatment

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Biomass

Keywords: Hydrothermal liquefaction, pretreatment, two-stage, biocrude, waste valorization

Abstract Body.
Introduction. Hydrothermal liquefaction (HTL) is increasingly explored for energy recovery from the organic fraction of municipal solid waste (OFMSW). HTL performance strongly depends on biochemical composition, with biocrude yields typically following lipids > proteins > carbohydrates. Regional and seasonal variability in OFMSW can affect biocrude quality and process stability, while a low-temperature pretreatment may help homogenize feedstock and reduce biocrude nitrogen content [1].
Methods. This study presents a preliminary analysis of seasonal variations in the biochemical composition of OFMSW and food waste. Based on this variability, three representative feedstocks (carbohydrate-, protein-, and lipid-rich) were selected to investigate the effects of temperature (100–200 °C), residence time (5–120 min), and additive use (H2SO4, none, KOH) during a low-temperature pretreatment stage, using a Design of Experiments (DoE) approach.
Results and discussion. Figure 1 illustrates representative experimental carbon and nitrogen balances with pretreatment. Compared to direct HTL, the carbon yield in the biocrude remained unchanged (49% vs 50%), whereas the nitrogen yield was substantially reduced (8% vs 27%). Despite differences among feedstocks, temperature was the dominant factor affecting performance. Higher pretreatment temperatures reduced solid yields and promoted nitrogen transfer to the aqueous phase, especially under basic conditions. Subsequent HTL of the pretreated solids generated apolar compounds that, along with the lipidic content of the feedstock, contributed to the overall biocrude production. Accordingly, the biocrude N/C ratio decreased with increasing pretreatment temperature, especially for nitrogen-rich, more challenging feedstocks. This effect was attributed to effective nitrogen removal during pretreatment, which limited nitrogen availability during HTL and reduced its incorporation into the biocrude, thereby improving biocrude quality without excessively sacrificing yield.

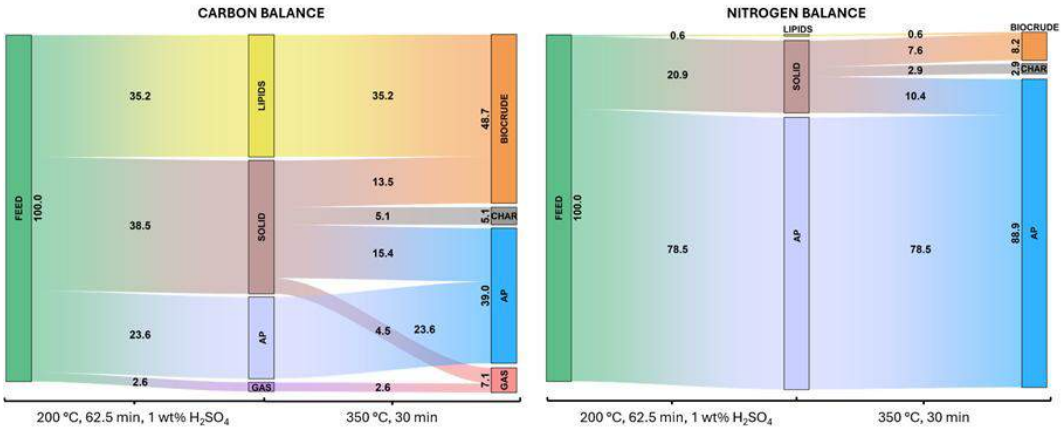

Figure 1: Overall carbon and nitrogen balance of a protein-rich feedstock after pretreatment at 200 °C, 62.5 min, 1 wt% H2SO4.

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SCB0777

Electronic Signatures of Size-Dependent Catalytic Activity in Lignin Depolymerization

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Keywords: Lignin depolymerization, β–O–4 bond cleavage, Density functional theory (DFT), Electronic delocalization, Pd, Ni, and Ru catalysts, d-band center modulation

The catalytic conversion of complex lignin structures into high-energy biofuels and value-added chemicals remains a central challenge in biomass valorization. Noble metal catalysts, particularly Pd-based systems, have demonstrated promising activity toward lignin-derived intermediates. In this work, density functional theory (DFT) calculations were performed to elucidate the reaction pathways involved in lignin depolymerization, with emphasis on the β–O–4 C–O bond cleavage step, a key elementary process in lignin breakdown.

Pd-, Ni-, and Ru-based catalysts in the form of single atoms, nanoclusters, and nanoparticles supported on nitrogen-doped carbon were systematically investigated. For Pd catalysts, the calculated activation barriers for β–O–4 bond cleavage were 1.80 eV on Pd(111), 0.58 eV on Pd nanoclusters, and 1.16 eV on Pd single atoms, indicating consistently favorable activity across different catalyst sizes. In contrast, Ni catalysts exhibited barriers of 0.60 eV, 2.75 eV, and 2.47 eV on Ni(111), nanoclusters, and single atoms, respectively. Ru-based systems showed barriers of 1.85 eV on Ru(001), 2.52 eV on nanoclusters, and 2.94 eV on single atoms. The significantly higher barriers for low-loading Ni and Ru configurations suggest limited effectiveness compared to their nanoparticle counterparts.

Electronic structure analysis in both real and reciprocal space reveals that metal–nitrogen interactions induce distinct charge redistribution patterns, which modulate adsorbate polarization and ultimately govern catalytic performance. These findings provide mechanistic insight into structure–activity relationships in lignin depolymerization and offer guidance for the rational design of efficient biomass conversion catalysts.

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SCB0642

Acrylamide-Tuned Tobacco Biochar–Hydrogel Controlled Release Fertilizer for Alkaline Red Mud: Swelling, Water-Holding Capacity, and Medium-Dependent N–P Release

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Biomass

Keywords: Red mud, Biochar–hydrogel composite, Controlled-release fertilizer, Water-holding capacity

Abstract Body.
Red mud (bauxite residue) is a highly alkaline industrial waste whose low organic matter, limited water retention, and constrained nutrient bioavailability hinder revegetation. This study engineers a red-mud-compatible controlled-release fertilizer (CRF) by integrating NPK-impregnated tobacco-stem biochar with an acrylamide-tuned hydrogel network to jointly enhance moisture storage and regulate macronutrient delivery under alkaline conditions. Tobacco-stem biochar was produced via pyrolysis at 600 °C, loaded with NPK, and subsequently immobilized within a polymer network formed using acrylamide (2.5–15% w/w) to systematically tune composite architecture. Increasing acrylamide content improved product formation and nutrient immobilization, reaching the highest composite yield (96.03%) and nutrient retention at 15% acrylamide (N: 28.61%, P: 13.37%, K: 7.05%). In contrast, hydration performance in alkaline media exhibited a clear structure–property trade-off: the 10% acrylamide formulation delivered the most favorable physicochemical response, achieving a swelling index of 1606.91% at pH > 7 and a water-holding capacity up to 92.25%. The enhanced alkaline swelling is attributed to increased ionization of acidic functionalities within the composite matrix, promoting osmotic-driven water uptake and electrostatic expansion of the network. Nutrient release depended strongly on the testing medium, highlighting the importance of evaluating CRF behavior beyond aqueous systems. Nitrogen release was substantially higher in water (95.56%) than in red mud (40.53%), indicating stronger retention and/or reduced mobility in the highly alkaline, ion-rich red mud matrix. Conversely, phosphorus release was enhanced in red mud (89.66%) relative to water (58.35%), demonstrating substrate-selective release behavior. Overall, acrylamide network tuning provides a practical route to biochar–hydrogel CRFs that combine high water retention with medium-dependent nutrient partitioning, offering a promising amendment to support early-stage plant establishment and accelerate revegetation of red mud disposal sites.

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SCB0691

SiO_2 modified Al_2O_3 supports with tunable acidity for efficient Bio-Oil hydrodeoxygenation

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Biomass

Keywords: Hydrodeoxygenation, Hydrocarbons dissociation, SiO_2 -Al_2O_3 Catalyst

Abstract Body.
Introduction. Hydrodeoxygenation (HDO) is a catalytic hydrotreating process in which oxygen-containing functional groups in bio-derived oils are selectively removed as water in the presence of hydrogen, yielding hydrocarbon fuels compatible with existing petroleum infrastructure. In Ni-based catalysts, surface Ni atoms promote C–O bond cleavage and hydrogenation steps necessary for converting oxygen-rich triglycerides into hydrocarbons. The effectiveness of these reactions is strongly influenced by the catalyst support. While γ-Al_2O_3 offers good activity, strong metal–support interactions can lead to the formation of inactive phases such as $NiAl_2O_4$. Incorporating SiO_2 into alumina mitigates this drawback by enhancing Ni dispersion, increasing oxygen-vacancy density, and tuning the balance of Lewis and Brønsted acidity. Together, these modifications improve hydrogen spillover, oxygenate activation, and resistance to coking, resulting in enhanced activity, stability, and selectivity of Ni-based catalysts for renewable fuel production via HDO.
Methods. A mixed aluminum precursor solution ($Al(NO_3)_3$ /$AlCl_3$ = 1:8) was hydrolyzed with aqueous ammonia (pH 5–10) to form an aluminum hydroxide gel, which was filtered, washed, and modified with sodium silicate to obtain Al_2O_3–SiO_2 supports. After drying (120 °C) and calcination (600 °C), 10 wt% Ni catalysts were prepared. Hydrodeoxygenation was conducted in a high-pressure batch reactor (35 bar H_2, 350 °C, 4 h), and products were analyzed by GC–MS.
Results and discussion. The catalytic performance of Ni-based catalysts was assessed through HDO of soybean oil using a conventional 10 wt% Ni/Al_2O_3 catalyst and a series of SiO_2-modified Ni/Al_2O_3 formulations. The unmodified 10%Ni/Al_2O_3 catalyst showed limited deoxygenation efficiency, yielding a high oxygenated compound content of 19.6%. In contrast, incorporation of SiO_2 into the alumina support markedly improved HDO performance, reducing the oxygenate content to 1.7–6.5% depending on the silica loading. Among the modified catalysts, 10%Ni/90%Al_2O_3–10%SiO_2 exhibited the best performance, achieving the lowest oxygenated compound content of 1.7%. Increasing the SiO_2 content to 20% and 30% led to higher residual oxygenates of 4.3% and 6.5%, respectively, indicating a decline in deoxygenation efficiency at excessive silica loadings. This performance improvement is attributed to favorable modifications in the physicochemical properties of the support. Incorporation of SiO_2 generates Si–O–Al linkages and bridging hydroxyl groups, increasing Brønsted acid site density and facilitating key reactions such as dehydration and hydrogenolysis.
Acknowledgments
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SCB0718

NMR-Guided Surrogate Mixtures for Fast Pyrolysis Bio-Oil and Pyrolignin: Composition and Property Estimation Using Synthetic Lignin Oligomers

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Keywords: FPBO fractionation, Pyrolignin (PL), synthetic lignin oligomers, Surrogate mixture modelling.

Introduction. Fast pyrolysis (FP) of lignocellulosic biomass and lignin yields up to 75% liquid products, known as fast pyrolysis bio-oil (FPBO). However, the chemical complexity of FPBO—especially its heavy organic fraction, pyrolignin (PL)—limits its full characterization and, therefore, the design of fractionation and valorization routes. PL contains highmolecularweight oligomers that remain poorly understood; elucidation is hindered by the absence of suitable reference libraries for these compounds and by the scarcity of ligninoligomer– specific standards.

Methods. In this work, we explore the use of synthetic lignin oligomers (SLOs) as a practical approach to improve the molecular interpretation of NMR spectra of FPBO, PL, and selected subfractions separated by column chromatography (CC). SLOs and their individual NMR signals serve as the basis for constructing chemically consistent surrogate mixtures. To achieve this goal, structures and experimental NMR data were first digitized and standardized from a public database (University of Wisconsin/USDA). For each entry, predicted ^{1}H and ^{13}C spectra and chemical shift lists were generated using ACD/Labs NMR Predictor (v2024.2.3) and systematically compared with the experimental values. The approach was further validated using the commercial standard pinoresinol (β–β linkage) and an in-house β-O-4 oligomer by evaluating spectral consistency across different NMR solvents and by creating a new NMR library.

Using this initial library, a linear additive model in Python was developed to simulate NMR mixture spectra by combining individual reference spectra and constraining the model with the composition derived from ultrahigh-resolution mass spectrometry (UHRMS) of the fractions (see Fig. 1).

Results. The algorithm estimates plausible surrogate compositions for FPBO, PL, and PL subfractions separated by column chromatography, minimizing the deviation between simulated and experimental spectra. Preliminary results indicate that the method reproduces key spectral features and proposes chemically reasonable compositions for each analyzed fraction. In parallel, thermophysical properties for the same set of molecules in the estimated composition were calculated using Aspen Plus v14, providing a thermophysical property dataset to support subsequent modeling. This approach enables liquid–liquid equilibrium modeling and a more mechanistic understanding of fractionation strategies aimed at sustainable valorization.

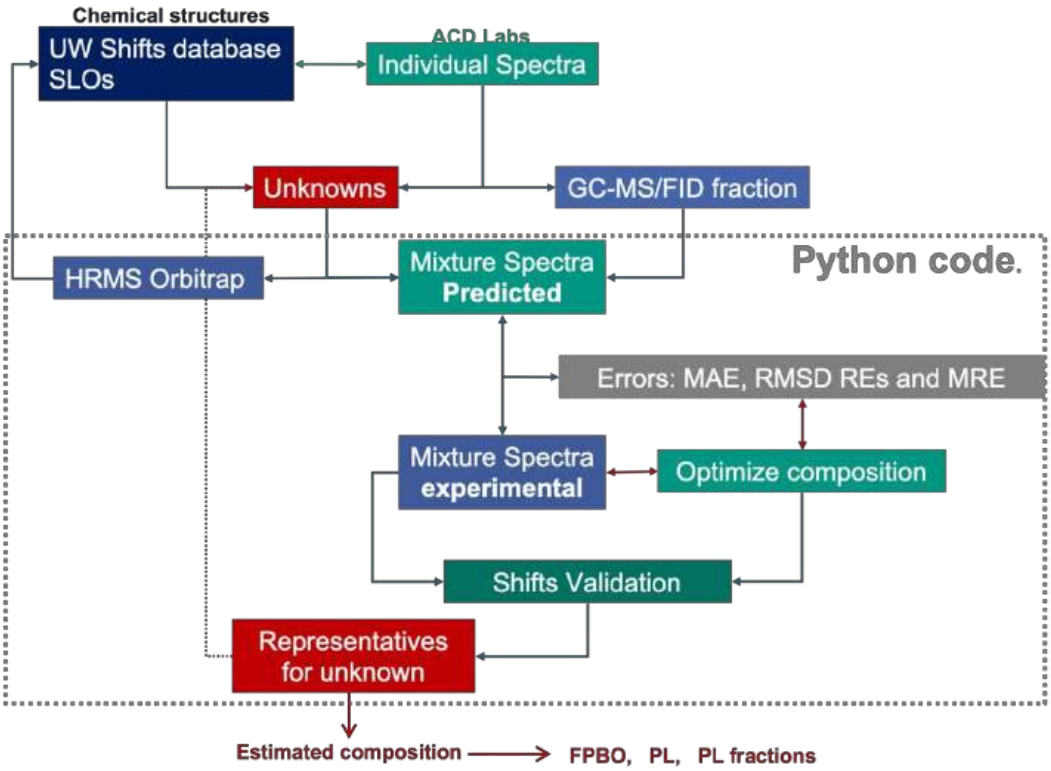

Fig 1. Data processing and modeling diagram for mixture simulation based on NMR data

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SCB0765

Designing NIR AIEgens for lysosomes targeting and efficient photodynamic therapy of tumors

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Biomass

Keywords: Aggregate-induced emission, Photodynamic therapy, NIR emission, ROS

Abstract Body.

Cancer is the most severe health problem facing most people today. Photodynamic therapy (PDT) for tumors has attracted attention because of its non-invasive nature, negligible adverse reactions, and high spatiotemporal selectivity. Developing biocompatible photosensitizers that can target, guide, and efficiently kill cancer cells is desirable in PDT. Here, two amphiphilic organic compounds, PS-I and PSS-II, were synthesized based on the D-π-A structure with a positive charge. The two AIEgens exhibited near-infrared emission, large Stokes shift, high $^1O_2$ and $O_2^{-\cdot}$ generation efficiency, good biocompatibility, and photostability. They were co-incubated with cancer cells and eventually accumulated to lysosomes by cell imaging experiments. In vitro and in vivo experiments demonstrated that PS-I and PSS-II could effectively kill cancer cells and sufficiently inhibit tumor growth under light irradiation. PS-I had a higher fluorescence quantum yield in the aggregated state, which made it better for bio-imaging in imaging-guided photodynamic therapy. In contrast, PSS-II with a longer conjugated structure had more ROS generation to kill tumor cells under illumination, and the tumor growth inhibition of mice reached 71.95% during the treatment. No observable injury or undesirable outcomes were detected in the vital organs of the mice within the treatment group, suggesting that PSS-II/PS-I had a promising future in efficient imaging-guided PDT for cancer.

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SCB0773

Mechanistic Insights into the Deoxygenation of Biomass-derived 6-amyl-α-pyrone: Experimental and DFT Insights

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Biomass

Keywords: Hydrodeoxygenation, Ir-ReOx/SiO2 catalyst, 6-amyl-α-pyrone

Abstract Body.
Advances in metabolic engineering have enabled the production of various platform molecules with varying carbon chain lengths directly from the fermentation of biomass-derived aqueous sugars. Catalytic conversion of these has received attention to producing value-added chemicals like n-alkanes [1], which were principally derived from crude oil. Therefore, a novel strategy is proposed in which 6-amyl-α-pyrone (6-PP), obtained from solid-state fermentation of biomass, is directly converted to n-decane, a fuel additive, in a single step using a bifunctional catalyst without the loss of any carbon atoms. Ir-ReOx/SiO2 catalyst (Re/Ir = 0.5) exhibited maximum conversion of 6-PP (99.8%) and n-decane selectivity of 81.8% at 473 K and 7 MPa in 14 hours. DFT simulations showed that on Ir (111) surface, the activation barrier for C2-O1 cleavage of 6-PP was 79.9 kJ/mol, which reduced to 50.9 kJ/mol on the Re3O6H2/Ir interface (Figure 1, (i)), explaining the relevance of Ir-ReOx interphase in enabling efficient C-O bond cleavage. Further, to reduce the cost of the catalyst, ReOx was replaced with cheaper promoters like WOx, VOx, NbOx and MoOx in which Ir-MoOx/SiO2 (Mo/Ir=0.25) catalyst exhibited maximum n-decane selectivity of 88.1 % and conversion of 96.4 %. Overall, this integration pathway enabled the production of long-chain alkane (n-decane) from 6-PP however, the presence of biogenic impurities in the fermentation broth along with 6-PP may lead to catalyst deactivation. Therefore, HDO of 6-PP on Ir-ReOx/SiO2 catalyst was carried in presence of impurities like Alanine, Arginine, Methionine, and Cysteine. Interestingly, 100 ppm of sulfur-containing impurities cysteine and methionine caused a significant decrease in 6-PP conversion (Table1, entries 4 & 5). This decrease in 6-PP conversion can be attributed to much stronger adsorption of impurities on the catalyst surface(Figure 1, (ii)). Alanine showed no effect, whereas Arginine was observed to cause only a moderate reduction in conversion (Table1, entries 2&3). Together, these studies establish how rational catalyst design critically governs deoxygenation pathways, providing valuable guidance for biomass valorization.

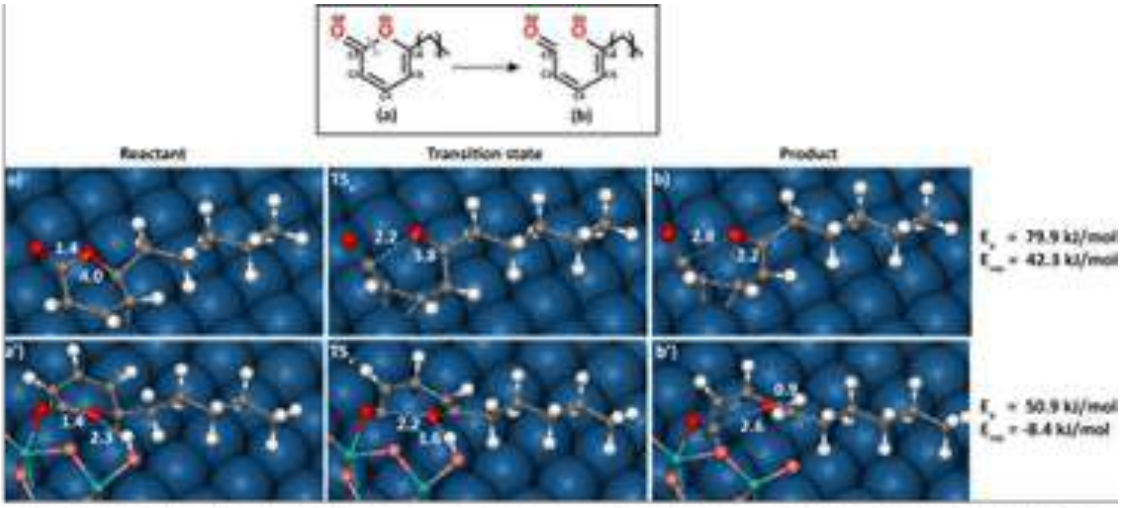
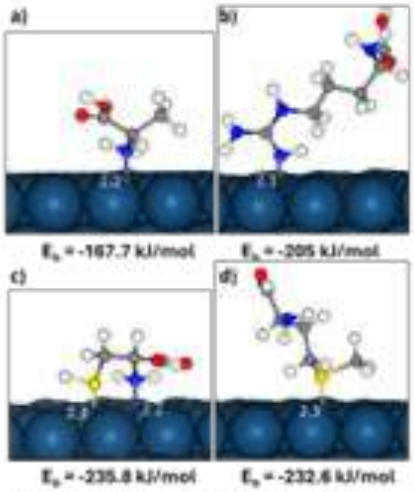


Figure 1. (i) Reactant, transition state and product structures for C2-O1 cleavage of 6-PP on (a to b) Ir (111) surface and (a' to b') $Re_2O_xH_y$/Ir (111) surface. Colour code: Ir (blue), Re (cyan), Cluster O (peach), C (grey), substrate O (red), H (white). All distances are marked in Å



(i)Adsorption configurations of (a) Ala, (b) Arg, (c) Cys and (d) Met on Ir (111) surface. Colour code: Ir (blue), N (royal blue), S (yellow), C (grey), O (red), H (white). All distances are marked in Å.

Table 1. The effect of biogenic impurities on HDO of 6-PP

S. No	Catalyst	Impurity	%Conversion
1	Ir-ReO_x/SiO_2	-	99.8
2	Ir-ReO_x/SiO_2	Alanine	97.6
3	Ir-ReO_x/SiO_2	Arginine	77.8
4	Ir-ReO_x/SiO_2	Cysteine	73.3
5	Ir-ReO_x/SiO_2	Methionine	37.6

Substrate: 5 wt% of solvent, Impurity: 100 ppm, Volume of the solvent: 10 ml, Temperature: 473 K, Pressure: 7 MPa, Time: 14 hours, Re/Ir: 0.5

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SCB9703

Online NIR-calibration Model Maintenance using Delayed Measurements for Sustainable Bioprocess Monitoring and Control

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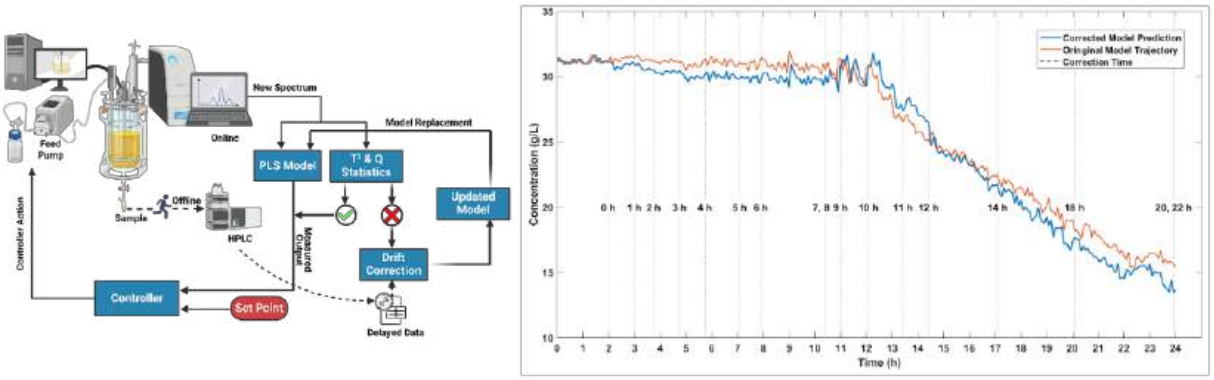
Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Biomass

Keywords: Near Infrared (NIR) Spectroscopy, Drift Correction, Calibration model maintenance, Online monitoring, Online control

Abstract Body.
Introduction: Sustainable bioprocess operation requires robust monitoring and control, yet intrinsic process variability and instrumental drift limit the reliability of static chemometric models, leading to inaccurate predictions and suboptimal control. This work presents an online model performance-monitoring strategy based on T^2 and Q statistics, combined with model correction using delayed, infrequent offline measurements. The approach is demonstrated for NIR-PLS-based glucose monitoring and control in Lactococcus lactis MKG6 fermentation for hyaluronic acid production, enabling timely detection and correction of model degradation and improving process robustness, efficiency, and batch reliability.
Methods: Figure 1a illustrates the proposed framework. NIR spectra acquired every 5 min are used to predict glucose using a PLS model, while T^2 [1] and Q [2] statistics concurrently monitor anomalies until delayed concentration measurements become available. Thresholds for T^2 and Q, derived from synthetic mixtures and experimental batch data, define acceptable operating limits. When delayed measurements are available, the prediction error is evaluated, and recalibration is triggered if it exceeds 4%. Drift correction is implemented via an implicit correction method (ICM) [3], which appends delayed measurements and corresponding NIR spectra to the calibration set to update the model. The updated model replaces the existing one without interrupting fermentation.
Results and discussion: Figure 1b compares glucose predictions obtained using the original and corrected models. Multiple model corrections were required to align online predictions with delayed offline measurements. Following the correction, the RMSE decreased from 2.567 to 1.975, and the glucose was maintained at 29.93±1.578 g/L. Controller performance, quantified using integral absolute error (IAE) and integral square error (ISE), was 3.286 and 2.100, respectively.



(1a) (1b)

Figure 1. (1a) Schematic of the experimental setup. (1b) Glucose prediction trajectories from the drift-corrected (blue) and original (red) models. The vertical dotted line indicates the model-correction time, with numbered points denoting the sampling hours used for correction.

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SCW0064

Understanding the Speciation Equilibria and Reaction Mechanism Between Bauxite Residue and Black Aluminum Dross for Co-valorization

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Waste Valorization

Keywords: Aluminum dross, bauxite residue, hydrogen, hydrometallurgy, speciation equilibria, kinetic modelling

Abstract Body.
Aluminum dross and bauxite residue (red mud) are two major waste streams from the aluminum industry, creating severe environmental and economic challenges. Black dross, rich in oxides and salts but low in metallic aluminum, is difficult to process and can release hazardous gases and leach harmful compounds. Similarly, bauxite residue from the Bayer process is produced in large volumes and contains highly alkaline mixtures of Fe, Al, Si, Ca, Na, and Ti oxides. Its storage in large dams poses long-term risks, including caustic leachates and potential structural failures. Despite decades of research, large-scale valorization remains limited, leaving most residues landfilled or mismanaged.
This work focused on elucidating the reaction mechanism and speciation of a novel hydrometallurgical process capable of treating both waste streams simultaneously. The reaction enables co-neutralization while producing hydrogen and recoverable heat. Aqueous speciation equilibria were modeled using PHREEQC V.3.8.6 and validated experimentally by preparing multiple bauxite residue suspensions across a wide pH range. Species in solution were quantified via ICP-OES and MP-AES. The hydrolysis reaction between red mud and black dross was studied in a batch stirred reactor, monitored by on-line µ-GC for hydrogen quantification. Solid phases before and after treatment were characterized using XRD, PSD, and SEM-EDX.
The model accurately represented bauxite residue equilibria across a broad pH range, including complex zeolite-type solids such as cancrinite, sodalite, and kaolinite. Combined reaction tests achieved hydrogen yields up to 99% with complete elimination of harmful secondary compounds from black dross. Kinetic analysis and speciation modeling identified the main limiting steps of the hydrolysis reaction, providing insights into parameters that could enhance hydrogen yield and reaction rate.
These results are highly encouraging and suggest optimization strategies for improving both hydrogen production and reaction speed. This integrated process represents a promising pathway for cleaner, safer, and more economical waste management, while simultaneously enabling hydrogen co-production and thermal energy recovery.
This work is funded by Novacium and the French National Association for Research and Technology (ANRT) under a CIFRE agreement.

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SCW0098

Aluminum in metallized plastic packaging waste enhances polymer pre-cracking and steam-cracker precursor formation over zeolite catalysts

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Waste Valorization

Keywords: Metallized plastic packaging waste, Catalytic pyrolysis, Hydrogenation, Naphtha, Al recovery, Kinetics.

Abstract Body.
Metallized plastic packaging waste (MPPW), composed of multilayer polymer–aluminum (Al) structures, poses a major recycling challenge due to its complex composition and resistance to conventional separation technologies. This study presents an integrated catalytic pyrolysis–hydrogenation strategy to valorize MPPW into steam cracker-compatible naphtha while enabling efficient recovery of metallic Al. Systematic experiments were conducted using model feedstocks (virgin LDPE, LDPE–Al, and PolyAl) and real post-consumer MPPW over microporous CBV-901 and mesoporous SIRAL 20 HPV catalysts. The presence of inherent Al in feedstocks enhanced heat transfer and promoted polymer pre-cracking, particularly over diffusion-limited microporous catalysts, resulting in improved conversion to naphtha-range hydrocarbons. Based on the pyrolysis of 1 kg of synthetic PolyAl composite, the overall product distribution comprised 0.62 kg of liquid oil, 0.13 kg of gas, 0.05 kg of solid residue, and 0.20 kg of recoverable Al. Post-pyrolysis wet gravity separation achieved over 92% Al recovery with purity exceeding 96%. Subsequent hydrogenation of the olefin-rich pyrolysis oil over Ni/SiO2–Al2O3 yielded highly saturated naphtha-like products (>95% n-paraffins and iso-paraffins), with H/C ratios and PIONA compositions closely matching those of fossil naphtha. Detailed energy balance calculations for the integrated PolyAl-to-naphtha process revealed a modestly endothermic net energy requirement (Qnet ≈ −2.07 MJ kg-1), while retaining substantial recoverable thermal and chemical energy. Overall, this work demonstrates a circular and industrially relevant route for converting MPPW into high-quality naphtha while recovering high-purity Al, highlighting the synergistic roles of catalyst pore structure, acidity, and inherent Al in enabling efficient polymer–metal recycling.

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SCW0162

Characterization of Carbon captured by High-Temperature Plastic Pyrolysis

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Waste Valorization

Keywords: Carbon capture, Circular economy, Plastic waste valorization, Pyrolysis

Abstract Body.

Characterization of Carbon captured by High-Temperature Plastic Pyrolysis
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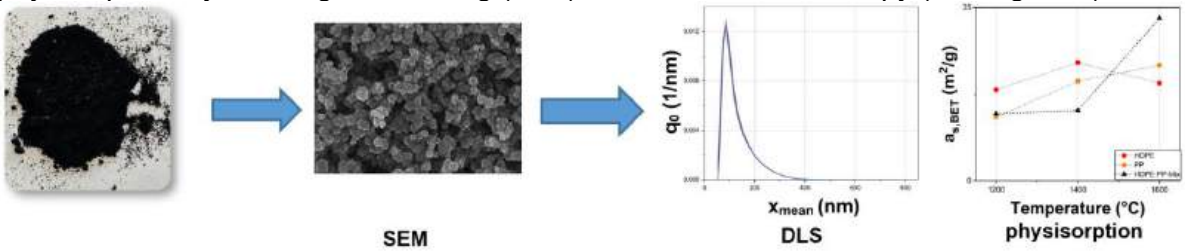
Keywords: Carbon capture; Circular economy; Plastic waste valorization; Pyrolysis

Introduction. The growing global production of plastics calls for effective strategies to manage and valorize plastic waste (PW). Most PW is landfilled or incinerated, causing environmental pollution, greenhouse gas emissions, and persistent microplastics. Polyolefins like high-density polyethylene (HDPE) and polypropylene (PP) are widely used for their chemical stability, but this complicates recycling and end-of-life treatment [1]. High-temperature pyrolysis offers a sustainable alternative valorization option, converting mixed PW into carbonaceous solids and hydrogen-rich gases, hereby reducing reliance on conventional hydrogen production. Understanding the effects of polymer composition, temperature, and pressure on reaction pathways is crucial for controlling product distributions.

Methods. The high-temperature pyrolysis of HDPE, PP, and a 1:1 (w/w) mixture was investigated in a high-temperature lab-scale setup [2,3] at temperatures ranging from 1200 to 1600 °C. Gaseous and liquid products were analyzed using gas chromatography, solid fractions were characterized by Raman spectroscopy, X-ray diffraction (XRD), N2-physisorption, dynamic light scattering (DLS), and electron microscopy (see Figure 1).



Results and discussion. The experiments yielded carbon materials whose particle size,

surface area, and pore volume were strongly influenced by reactor temperature and polymer composition. Generally, higher temperatures led to smaller particle diameters; however, while HDPE showed maximum surface area and pore volume at intermediate temperatures, PP exhibited a steady increase. The mixed polymer displayed a pronounced rise in surface area and pore volume at 1600 °C, indicating synergistic effects between degradation intermediates. Scanning electron microscopy (SEM) and DLS confirmed the formation of spherical, homogeneous carbon particles. Overall, the results demonstrate the critical role of temperature and polymer type in determining carbon textural properties.

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ISCRE29 & APCRE11
2026 / SEOUL, KOREA

SCW0230

Enhancing Long-Term Stability of Lewis Acidic Alumina Support in Hydrodechlorination Reaction for Plastic Chemical Recycling through Two-Step Processes

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Waste Valorization

Keywords: hydrodechlorination, plastic chemical recycling, pyrolysis, pre-hydrogenation, coke

Abstract Body.
Chlorine in pyrolysis oil must be reduced in pyrolysis-based plastic chemical recycling to prevent catalyst deactivation and reactor corrosion during downstream upgrading. γ-Al2O3 is an effective support for hydrodechlorination (HDC) because its penta-coordinated Al sites strongly adsorb and activate chlorinated species, but real pyrolysis oils contain olefins and aromatics that competitively adsorb and form coke, blocking the sites. In this study, we introduced a hydrogenation pre-treatment to suppress coking on γ-Al2O3, preserve access to penta-coordinated Al sites, and sustain HDC performance under realistic conditions. In this work, deactivation mechanisms in HDC were systematically investigated, and effective strategies were developed to enhance the long-term stability of γ-Al2O3 supported catalysts. Under realistic pyrolysis oil feeds, abundant olefins and aromatics competitively adsorb on these Lewis acidic penta-coordinated Al sites and subsequently grow into coke, leading to catalyst deactivation. As the reaction proceeds, heavy coke progressively accumulates, eliminating penta-coordinated Al sites and causing a continuous decline in activity. To suppress this deactivation pathway, the introduction of a pre-hydrogenation step prior to HDC enables hydrogenation of olefins and aromatics; despite identical overall Pt loading relative to the one-step process, the two-step configuration prevents active-site blockage and delivers both higher activity and markedly improved long-term stability. This approach provides a practical route to enhance the durability and performance of γ-Al2O3 supported HDC catalysts, addressing key challenges in the chemical recycling of mixed plastic waste.

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SCW0276

From Formation Pathways to Pretreatment: Mitigating Chlorine Contamination in Complex Plastic Waste Pyrolysis

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Waste Valorization

Keywords: PVC Pyrolysis, Pretreatment, Organochlorides, Two-dimensional gas chromatography, Chemical recycling, Plastic waste

Abstract Body.

Purpose

As pyrolysis scales to accommodate complex plastic waste streams, chlorine content in pyrolysis oil remains a critical bottleneck (1). Although PVC is the primary chlorine source, direct decomposition accounts for only a fraction of the organochlorides. Instead, the majority of chlorinated hydrocarbons arise from complex interactions between PVC, inherent additives, and other polymers in the waste matrix (2, 3). Therefore, resolving the chlorine challenge requires more than just PVC removal; it demands a fundamental understanding of these formation pathways. This study aims to address this gap by characterizing these specific interactions and leveraging that insight to design and evaluate targeted pretreatment strategies for post-consumer plastic waste.

Methods

Binary mixtures of PVC, common PVC additives, and typical polymers in plastic waste are pyrolyzed in two stages in a semi-batch configuration. The products collected in serial condensers and chilled organic solvent scrubbers are analyzed using GC×GC-AED for high-level speciation and chlorine content determination. Pretreatments targeting PVC waste matrix, including solvent washes and alkaline/acidic hydrolysis, are applied to real PVC waste streams, and the organochlorides in the oil were analyzed and compared.

Results

Additives and heteroatom-containing polymers led to substantial increases (50×) in oil chlorine content relative to PVC pyrolysis oil. An ether wash of post-consumer flooring targeting the plasticizer additives reduced the chlorine content in pyrolysis products by eliminating organochlorides derived from plasticizers. Furthermore, an alkaline wash of the feed targeting ester bonds achieved comparable success in reducing chlorine content.

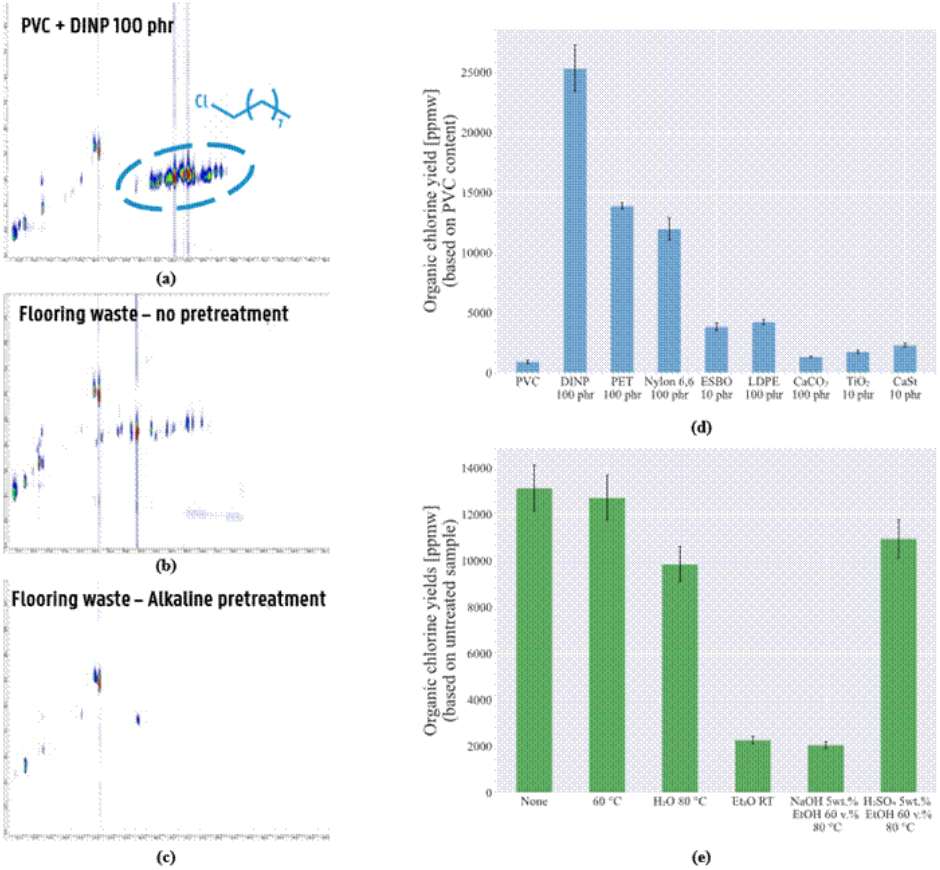

Figure 1 – (a): GC×GC-AED chromatogram at 481 nm showing the chlorinated species in virgin PVC oil with 100 phr DINP plasticizer; (b) GC×GC-AED chromatogram at 481 nm showing the chlorinated species in flooring waste with no pretreatment; (c) GC×GC-AED chromatogram at 481 nm showing the chlorinated species in flooring waste with alkaline (NaOH) pretreatment; (d) Total organochloride yield in samples with virgin PVC and additives/polymers; (e) Total organochloride yield in oil produced from flooring waste with different pretreatments.

Conclusions

The results show a pattern in organochloride production through pyrolysis and emphasize the role of non-PVC components in the chlorine problem. Chemical and physical pretreatments effectively reduced the oil chlorine content. Further optimizations can improve these technologies and enable a broader range of pyrolysis feedstocks.

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SCW0284

Catalytic Conversion of Waste Plastic Pyrolysis Oil to Light Olefins in a Micro-Activity Test Unit and a Circulating Fluidized Bed Reactor

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Waste Valorization

Keywords: plastic recycling; pyrolysis oil; catalytic cracking; light olefin; micro-activity test unit; circulating fluidized bed reactor.

Abstract Body.
Introduction. The rapid growth of global plastic production has led to a continuous increase in plastic waste, particularly polyolefins such as polyethylene (PE) and polypropylene (PP). Current routes for converting polyolefin-derived waste plastic pyrolysis oil (WPPO) into olefins mainly rely on energy-intensive thermal steam cracking. Moreover, this approach imposes stringent feedstock requirements regarding olefin content (< 2 wt%) and low impurity content. Therefore, post-treatment with hydrogen-demanding is necessary for removing impurities and converting olefins into paraffins to adapt to the specific requirements of steam crackers. Such constraints significantly limit the large-scale implementation of plastic waste valorization as a sustainable feedstock for producing light olefins. This study addressed these challenges by developing a scalable and environmentally benign catalytic strategy for the direct conversion of crude WPPO into light olefins.
Methods. Catalytic cracking of crude WPPO over a microspherical phosphorus-modified steam-treated ZSM-5 catalyst was systematically investigated in a fully automated micro-activity test unit (MAT) and a pilot-scale circulating fluidized bed reactor (CFBR). The catalyst was specifically designed to exhibit high hydrothermal stability and to withstand repeated reaction-regeneration cycles. In the MAT unit, the effects of catalyst type, reaction temperature, and space velocity on product distribution were investigated to determine the optimal operating conditions. The process was subsequently scaled up to a CFBR with a throughput of 1000 $g \cdot h^{-1}$, where the catalyst-to-oil ratio, feed rate, and the catalyst circulation rate were systematically examined. The catalyst durability was also assessed under continuous 24 h
operation with in situ regeneration.

Results and discussion. In the MAT unit, catalytic WPPO cracking achieved a high C2–C4 olefin yield of 56.6 wt%, markedly exceeding those obtained from thermal WPPO cracking (36.1 wt%) and catalytic naphtha cracking (29.7 wt%). In the pilot-scale CFBR, a significantly high C2–C4 olefin yield of 46.2 wt% was achieved through the catalytic WPPO cracking compared to conventional naphtha cracking (34.6 wt%). Stable light olefin production was maintained over 24 h of continuous operation, supported by effective coke removal and

regeneration. Overall, the proposed catalytic cracking process enables direct utilization of crude WPPO, offering higher olefin productivity, lower energy demand, and elimination of hydrogen consumption, and represents a promising pathway for sustainable plastic waste valorization.

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SCW0301

Pretreatment strategies for valorization of crude glycerol in synthesis of acetins via acetylation of glycerol

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Waste Valorization

Keywords: Glycerol utilization, Pretreatment, Heterogeneous catalyst, Acetins, Acetylation

Abstract Body.
By-product valorization of crude glycerol (CG) can enhance the economic viability of the biodiesel industry. This study focuses on the pretreatment methods of CG to produce acetins (monoacetin (MA), diacetin (DA), and triacetin (TA)). These valuable products have a wide range of industrial applications and are environmentally friendly. The catalytic performance in the acetylation of CG was benchmarked against that of commercial pure glycerol (PG). Graphene oxide (GO) was synthesized by Tour's method, followed by wet impregnation to load 20 wt.% of TPA on GO support to obtain the TPA/GO catalyst, and its performance for acetylation of CG and PG was compared to the commercial ion-exchange resin Indion 225H. The CG feedstock derived from the biodiesel industry, containing 83.6 wt.% glycerol, 10.7 wt.% moisture, and 4.8 wt.% salts, was pretreated prior to the reaction using 2 strategies: 1) evaporation at 120 °C (CG-EVAP) and 2) a sequential process including ion exchange, activated carbon, and evaporation (CG-RESIN). Acetins products were obtained at 110 °C for 2 h using a 6:1 molar ratio of acetic acid to glycerol and 5 wt.% catalyst loading, as illustrated in Figure 1. Under these conditions, CG-RESIN gave a higher glycerol conversion than CG-EVAP for both catalysts which can be attributed to the effective removal of inorganic salts and ionic impurities 74.96 and 70.86% were achieved using the TPA/GO catalyst, and 81.95 and 76.99% were obtained with Indion 225H catalyst, respectively. The highest MA selectivity was observed for both catalysts when using CG. However, the TA yield remained low when CG was utilized. Only 2.93 and 3.31% for TPA/GO and Indion 225H catalysts were obtained for CG-EVAP, while CG-RESIN gave only 3.27 and 3.93%, respectively. In contrast to using PG, the TPA/GO catalyst achieved the complete glycerol

conversion and highest TA yield of 27.2% after 2 h while Indion 225H catalyst provided lower catalytic activity in terms of glycerol conversion and TA yield. The TPA/GO catalyst was less active compared to Indion 225H in CG, which could be due to the different active sites. The SO3H functional group was substantial for Indion 225H while the combination of Keggin structure and SO3H were found for TPA/GO. In addition, the presence of salts in CG probably inhibits the active sites of the catalysts. Therefore, salt removal is an important step in CG pretreatment to improve catalytic performance.

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SCW0359

Thermally treated polyvinyl chloride (PVC)-derived highly microporous carbon support

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Waste Valorization

Keywords: PVC, Microporous carbon, KOH activation, Ruthenium catlalyst

Abstract Body.
Chemical recycling of polyvinyl chloride (PVC) via depolymerization is more challenging than that of polyolefins due to the formation of hydrogen chloride during thermal degradation. Thermal degradation of PVC produces a solid residue after dehydrochlorination, which can serve as a potential resource for carbon materials. In this study, highly microporous carbon materials were prepared by KOH activation of PVC-derived solid residues treated at 250–350 °C. The resulting carbons exhibited a maximum BET surface area of 3273 $m^2 g^{-1}$. A ruthenium catalyst supported on the PVC-derived carbon showed high catalytic activity for the hydrodeoxygenation of guaiacol. These highly microporous carbons demonstrate strong potential as upcycled materials for a wide range of applications.

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SCW0390

Maximizing light olefin production through catalytic cracking of crude waste plastic pyrolysis wax into light olefins

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Waste Valorization

Keywords: plastic recycling, waste plastic, pyrolysis wax, catalytic cracking, light olefin

Abstract Body.
Introduction. Energy-efficient technologies for light olefin production from polyolefin-rich waste are critical to reduce the dependence on fossil hydrocarbons and promote closed-loop plastic recycling. In this study, the physicochemical properties of crude waste plastic pyrolysis wax (WPPW), commonly considered a low-value pyrolysis byproduct, were comprehensively studied, and its potential application for light olefin production was evaluated. The catalytic cracking of WPPW offers an effective pathway for improving plastic recycling efficiency and light olefin recovery.
Methods. WPPW derived from virgin polyolefins, waste polyolefins, and their blends with waste PVC, was catalytically cracked over microspherical phosphorus modified steam-treated ZSM-5 (ms-P-HZSM5-S) without any feed purification. The catalytic tests were performed at 680 oC and a WHSV of 16 h-1 using a fully automated micro-activity test unit. Each run was carried out for 90 seconds under a helium flow. The highly viscous WPPW was diluted with toluene at a 1:3 mass ratio to facilitate the injection into the reactor. The gaseous and liquid products were subsequently analyzed by gas chromatography, and catalyst stability was evaluated under repeated reaction-regeneration cycles over 810s at identical conditions.
Results and discussion. Catalytic cracking of virgin-PE waxes yielded 62.1 – 63.8 wt% light olefins, while that for virgin-PP waxes was 58.6 wt%. Advantageously, despite containing significant nitrogen-, oxygen-, and chlorine-based heteroatoms, waste-polyolefin (PO) waxes produced only slightly lower light olefin yields (59.8 – 59.9 wt% for WPE, and 56.3 – 58.2 wt% for WPP). Interestingly, PP-derived feeds produced a much higher propylene-to-ethylene ratio but a relatively lower light olefin yield than PE-derived feeds. Thus, comparable C2 – C4 olefin yields of 60.1 – 60.8 wt% could be obtained from mixed waste-PO-derived feeds and PVC-containing feeds. Finally, the deactivation test demonstrated the stable performance of the ms-P-ZSM-5-S catalyst, with only minor activity loss as C2 – C3 yields dropped from 50.7 to 49.3 wt% after 9 consecutive cracking cycles. Nevertheless, the catalyst activity was completely recovered after regeneration in air at 700 oC, thereby confirming the feasibility of continuous operation with successive reaction-regeneration

cycles. The research results revealed the great potential of crude WPPW as an intermediate for a sustainable waste-to-chemicals pathway, with the monomer recovery exceeding 50 wt% via integrated pyrolysis- catalytic cracking process.

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SCW0395

Removal of inorganics in HTL/HTC-derived wastewater: a study on the competitive adsorption challenge

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Waste Valorization

Keywords: Adsorption, Inorganics removal, Wastewater valorization

Abstract Body.
Introduction. Wastewater derived from biomass hydrothermal processing contains inorganic compounds which can affect its further valorization by irreversible adsorption on the catalyst. For this reason, ion exchange is often proposed as a necessary pretreatment to preserve the catalyst lifetime. In this regard, despite its importance, the competitive adsorption between different inorganic species and between inorganics and organic molecules is scarcely investigated. In the present work, we have conducted a systematic work using Amberlite IRA-67 anion exchange to study the adsorption of anions in the case of synthetic solutions and real wastewater derived from hydrothermal processing of different feedstocks (e.g., microalgae, sewage sludge, etc.).
Methods. Batch experiments were carried out on synthetic solutions containing sulphate (SO42-), phosphate (PO43-) and chloride (Cl-), to derive both kinetic and thermodynamic information. Multiple-component tests were employed to study the competitive adsorption, using also representative organic molecules (acetic acid and glycerol). In addition, batch experiments were performed using real wastewater. Continuous experiments were carried out to derive breakthrough curves to propose a scale-up.
Results and discussion. The figure below shows two representative outcomes highlighting the resin's selectivity and the impact of competition. On the left, ion chromatography indicates that, at the lowest resin dosage, SO42- was preferentially adsorbed. Increasing the resin loading did not immediately promote PO43- uptake; instead, organic species were removed first, suggesting that organic components could also occupy sites and delay PO43- binding. Its removal became evident only at the highest resin dosage, implying that a larger availability of free sites was required once more competitive solutes have been depleted. On the right, the continuous competitive test confirmed that SO42- strongly suppressed PO43- capture under dynamic conditions. Consistent with the batch-derived capacities (ca. 100 mgPO4/g and 130 mgSO4/g), the equimolar breakthrough curve showed PO43- overshoot, indicating weaker retention and partial displacement as SO42- progressively occupied adsorption sites. Notably, the final phosphate capacity decreased to 15 mgPO4/g. Overall, the results quantify strong competitive effects, guiding and process design for robust inorganics removal/recovery.

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2026 / SEOUL, KOREA

SCW0437

Design Of Experiment optimization of Hazelnut Press Cake Protein extraction with Deep Eutectic Solvents: characterization and application in cell agriculture.

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Waste Valorization

Keywords: Keywords. DOE; side streams; circular economy; cell agriculture; plant protein

Abstract Body.
Introduction. The rate of the global population has risen with demographic forecast predicting global numbers to peak at roughly 10.3 billion by the mid-2080s [1]. Meanwhile, approximately one-third of food is lost or wasted throughout the supply chain from beginning to end [2].
This research valorizes hazelnut press cake, the industrial by-product from hazelnut oil production to replace fetal bovine serum (FBS) in cultivated meat/fish production.
Methods. The study optimized Deep Eutectic Extraction (DES) extraction of hazelnut press cake protein via Design of Experiment (DOE). Specifically mass yield and protein extraction rate. The extracted proteins were characterized through gel permeation chromatography/size exclusion chromatography (GPC/SEC) to determine the protein molecular weight distribution. Later, the ability of hazelnut press cake proteins to support cell proliferation was evaluated in porcine stromal cells.
Results. The results showed that the best conditions – in terms of extraction rate (ER) – were identified as: solid/liquid (S/L) ratio of 1:10, for 70 min at 90°C obtaining ER (%) = 40.1%. The GPC/SEC showed different molecular weight distributions at different temperatures as shown in Figure 1.

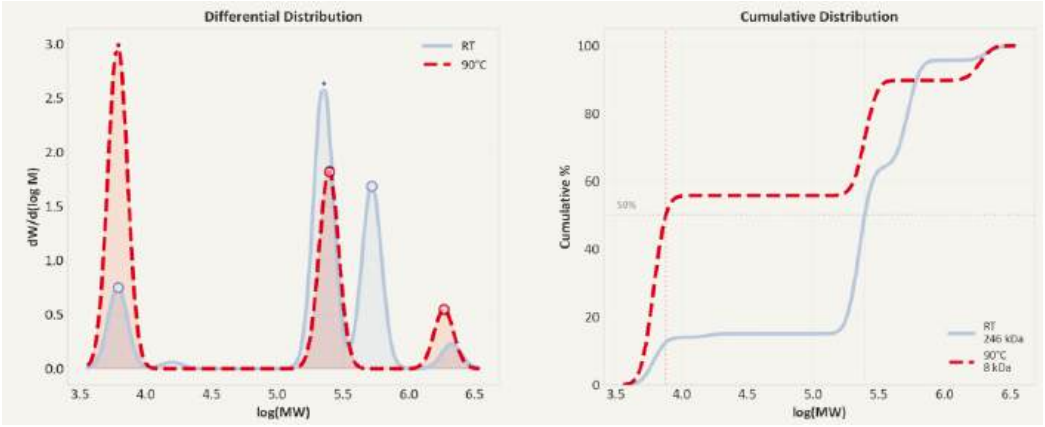

Figure 1. Differential and cumulative distribution of molecular weights at different temperatures.

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SCW0481

Sustainable Upcycling of Polyolefin Plastic Waste Using Spent FCC Catalysts

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Waste Valorization

Keywords: Polyolefin, Upcycling, Plastic waste, FCC Catalyst, Chemical recycling

Abstract Body.
Introduction. Despite advances in catalytic upcycling technologies, the global recycling rate of plastic waste remains 11% [1]. Compared to mechanical recycling, chemical recycling has contributed only marginally to plastic waste management, and most existing chemical recycling approaches rely on pyrolysis-based routes [2, 3]. A major impediment to broader implementation is that numerous high-performing catalytic systems depend on noble metals or require large-scale catalyst production, which raises concerns regarding economic feasibility, material availability, and process scalability. In this study, we propose a potentially economically and environmentally viable upcycling strategy that employs a spent fluid catalytic cracking (FCC) catalyst, a widely available industrial byproduct generated through decades of the petrochemical industry [4]. By utilizing an industrially mature and readily accessible waste catalyst, this study aims to advance the practical deployment of chemical recycling technologies and emphasizes the importance of integrating catalytic performance metrics with considerations of process maturity and material supply.
Methods. Reactions were performed in a 50 mL batch reactor using PP (1.0 g) and a catalyst (0.2-0.5 g). After purging with Ar, the reactor was pressurized to 2 bar and heated to 350 °C. Products were analyzed by gas chromatography equipped with FID and TCD detectors.
Results and discussion. The catalytic upcycling of waste PP (Fig. 1a) was investigated over HY(60) and a spent FCC catalyst. HY(60) achieved 60.4% conversion with a 52.6% naphtha yield (Fig. 1b). In contrast, the spent FCC catalyst exhibited lower activity, showing a conversion of 20.4% and a naphtha yield of 14.2%. NH3-TPD analysis indicated a lower total acid density for the spent FCC catalyst (0.337 mmol/g) compared with HY(60) (1.053 mmol/g) (Fig. 1c), suggesting that insufficient acid sites limit its performance. To address this limitation, the catalyst loading was increased, resulting in an increase in conversion to 63.3% and naphtha yield to 55.8% (Fig. 1d). These results demonstrate that, given a sufficient number of acid sites, the spent FCC catalyst can achieve catalytic performance comparable to that of a zeolite, supporting the feasibility of incorporating spent catalysts into plastic upcycling processes.
Acknowledgments
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SCW0533

Alcohol-Mediated Recycling of PLA/PGA via Oligomer Molecular Weight Control and Spontaneous Monomer Separation

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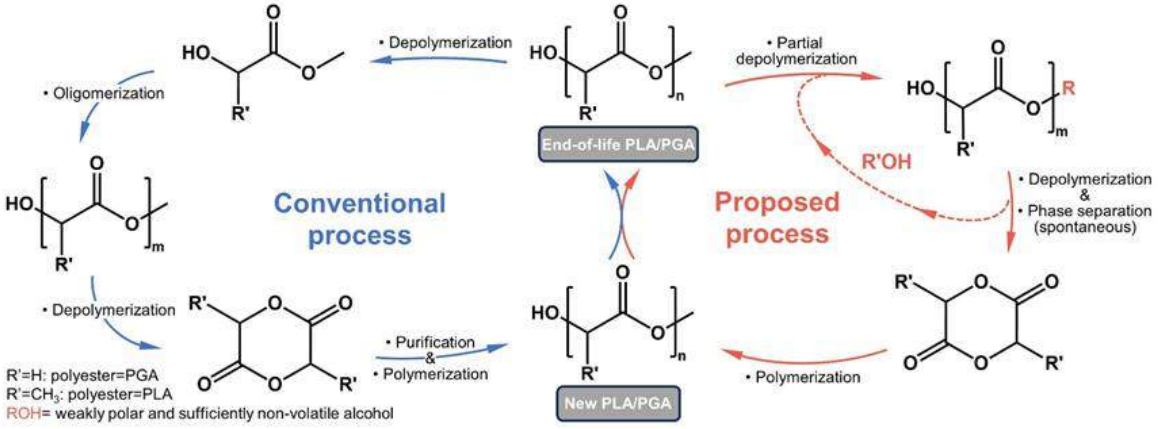
Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Waste Valorization

Keywords: Chemical recycling, Polylactic acid, Phase separation, Cyclic esters

Abstract Body.

Polylactide (PLA) and polyglycolide (PGA) face challenges in end-of-life management despite their degradability. Chemical recycling via depolymerization to recover monomers offers a viable route for the recycling of PLA/PGA.[1] Nevertheless, conventional depolymerization typically involves alcoholysis to the corresponding alkyl esters (e.g., methyl lactate or methyl glycolate), followed by purification, re-cyclization to cyclic monomers, and repolymerization to regenerate the polymer (blue arrow, Scheme 1).[2] Based on our prior compatibility studies of cyclic ester monomers (glycolide and lactide) and alcohols, weakly polar alcohols were found to be largely immiscible with these cyclic esters.[3] Leveraging this polarity mismatch, an alcohol-mediated recycling strategy for PLA/PGA was established that integrates oligomer molecular weight control with spontaneous monomer phase separation for direct cyclic ester recovery (red arrow, Scheme 1).



Scheme 1. Schematic comparison of conventional (blue) and proposed (red) recycling routes for PLA/PGA.

In this process, Behenyl alcohol (ROH), a weakly polar alcohol, was employed as the depolymerization alcohol and chain-end capping agent. PLA was first reacted with ROH at ~190 °C to form ROH-capped oligomers with controlled chain length and reduced viscosity.

The resulting oligomers were subsequently subjected to depolymerization at 200 °C under reduced pressure (<1 kPa), generating ROH and cyclic ester monomers. Due to their immiscibility, the ROH/monomer mixture spontaneously separated into ROH-rich and monomer-rich phases, and the ROH phase was collected and reused in subsequent cycles. Under the selected conditions, PLA depolymerization provided a one-pass cyclic ester yield of approximately 92% with a purity above 98%, while PGA showed a comparable yield of 88%. The alcohol-rich phase was directly reused for four consecutive cycles without noticeable loss of yield or purity. Kinetic analysis further indicated a reduced apparent activation barrier for depolymerization in the presence of ROH. Together, these results support the feasibility of the alcohol-mediated recycling process for both PLA and PGA. Overall, this alcohol-mediated strategy enables the direct and efficient recovery of cyclic monomers from PLA and PGA. These process design principles may be broadly applicable to other polyester systems.

Acknowledgments
This work was financially supported by the National Innovation Center par Excellence (NICE) and the National Natural Science Foundation of China (22478106).

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ISCRE29 & APCRE11
2026 / SEOUL, KOREA

SCW0539

From Post-Consumer Textiles to Biobased Polymers: Step-Wise Conversion and Life Cycle Impact

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Waste Valorization

Keywords: Textile waste valorisation, Building Blocks, Polyhydroxyalkanoates, LCA

Abstract Body.

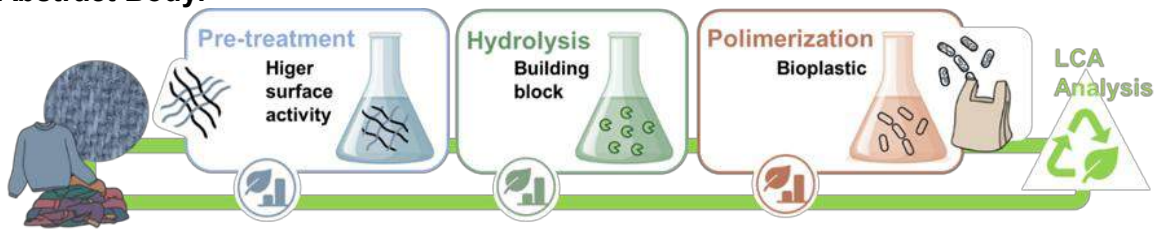

Figure 1 Steps overview of the research method

Introduction. The textile sector is often underestimated source of environmental pollution, land contamination, wastewater generation, and microplastic emissions. The rapid expansion of fast fashion has led to a sharp increase in post-consumer textile waste, particularly blended fabrics containing synthetic and cellulosic fibres, which pose major challenges for separation and recycling. This study aims to convert post-consumer mixed fiber textiles into industrially relevant building block and bioplastic. The work lies in the integration of experimental results into a block-based life cycle assessment (LCA) of the proposed pathway and compared with conventional waste management options, such as landfilling and incineration.

Methods. The laboratory scale experiments were performed to optimise the alkaline pretreatment to increase the enzymatic hydrolysis of the natural fibre fraction of blended textiles. Enzymatic hydrolysis, depending on process requirements, was then carried out to produce fermentable sugars for subsequent conversion into PHAs. The hydrolysis was applied using Cellic CTec3® and Celluclast® enzymes to compare their activities. The treated textiles and the products of hydrolysis and fermentation were characterised by SEM, FTIR spectroscopy, HPLC analysis, the DNS assay, and methanolysis. Two LCAs were developed to quantify environmental impacts of proposed waste valorisation pathway and to compare them with conventional waste management practices.

Results and discussion. The implemented pretreatment strategies increased the enzymatic hydrolysis yield of the cellulosic fraction by up to 40%. Based on the quantification of glucose released by enzymatic hydrolysis, higher yields were observed for rayon and viscose textiles compared to cotton–PET blends. The hydrolysis yield also appeared to increase with the use of different enzymatic cocktails. The PHAs were successfully synthesised with yields comparable to those obtained from commercial glucose. These results enabled the

identification of yield values scalable to industrial conditions and supported comparative analyses under identical hydrolysis parameters, including agro-industrial waste streams characterised by higher industrial Technology Readiness Levels. In alignment with European environmental policies and emerging Extended Producer Responsibility (EPR) frameworks, this study presents a scalable and sustainable strategy for mixed textile waste exploitation, together with a stepwise LCA framework applicable to future recycling scenarios.

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SCW0547

Hydro Upgrading Strategies for Converting Plastic Waste Pyrolysis Oils into Steam Cracker Ready Feedstocks

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Waste Valorization

Keywords: Post-consumer plastic waste, Pyrolysis oil upgrading, Hydroprocessing, Light olefins, Steam cracking

Abstract Body.
Chemical recycling via pyrolysis followed by steam cracking offers a route to convert hard-to-recycle mixed plastic waste into virgin-like monomers, supporting plastics-to-plastics circularity. Despite advances in producing waste-derived pyrolysis oils (Py-oils), their variable quality remains a major bottleneck for large-scale deployment. The heterogeneous contaminant content, including halogens, oxygenates, nitrogenates, and metals, together with a broad boiling range, makes raw Py-oils unsuitable as drop-in feedstocks for steam crackers. Upgrading is therefore required prior to integration into refinery or petrochemical operations. However, compared with fossil feedstocks, the higher variability and contaminant levels of Py-oils can accelerate catalyst deactivation, reduce process stability, increase hydrogen demand, and overall upgrading costs.
This study investigates hydrocracking as an upgrading strategy for a waxy Py-oil derived from post-consumer mixed polyolefin waste, which has a wide boiling range and significant contaminant content. Two configurations are considered: hydrocracking of the whole Py-oil and selective hydrocracking of the heavy fraction (b.p. > 200 °C) after removal of naphtha-range material. Prior to hydrocracking, the nitrogen content of the Py-oil needed to be reduced below 25 mg/kg by hydrotreatment over a sulfided Ni-Mo/γ-Al_2O_3 catalyst. Subsequent hydrocracking is performed over a sulfided NiW zeolite catalyst in a fixed-bed reactor under varying severities to tailor product distributions toward lighter fractions. The upgraded Py-oils were characterized using simulated distillation. As shown in Figure 1, variations in hydrocracking strategy and severity shift the boiling-range distribution toward lighter fractions relevant to steam cracking, whereas hydrotreatment causes negligible changes in boiling ranges. Hydrotreatment is primarily used to improve feed quality by removing contaminants and reducing olefinic content. The hydrocarbon compositions and contaminant content of the feedstocks will be investigated using comprehensive two-dimensional gas chromatography and complementary analytical techniques. The feedstocks have been evaluated for steam cracking in a bench-scale unit, equipped with detailed online product analysis. This work links upstream upgrading intensity and hydrogen consumption to downstream olefin yields, product distribution, and cracker operability. By comparing hydrocracking routes, the study clarifies how upgrading pathways influence hydrogen demand, feed quality, and cracking performance, providing insight into their implications for

overall process efficiency and the technical viability of integrating waste-derived feeds into existing petrochemical infrastructure.

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SCW0569

Highly active Mn-substituted MgAl2O4 spinel catalysts with oxygen defects for glycolysis of waste PET

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Waste Valorization

Keywords: Chemical recycling of PET, Glycolysis, Bis(2-hydroxyethyl)terephthalate (BHET), Heterogeneous catalysis, Oxygen vacancies, Reaction kinetics.

Abstract Body.
Introduction.
The practical application of heterogeneous catalysts in PET glycolysis is often limited by metal leaching, which adversely affects catalyst stability and recyclability and may result in residual metal species in the recovered BHET that can be carried over into subsequently repolymerized PET. These limitations highlight the need for the rational design of stable heterogeneous catalysts that effectively suppress metal leaching while maintaining high catalytic activity. In particular, for metal oxide-based catalysts, it is widely recognized that not only metal components but also oxygen vacancies play important roles in determining catalytic performance. Despite this understanding, systematic and quantitative studies on the role of oxygen vacancies, especially their influence on PET glycolysis reaction kinetics, remain limited.
Methods.
The MgAl2O4 spinel structure was chosen for its strong metal oxygen bonding and high thermal stability, which suppress metal leaching during reaction and regeneration. Within this framework, Mn-substituted MgAl2O4 oxides with varying Mn contents were prepared by coprecipitation and subsequently acid- treated to tune surface properties and oxygen-vacancy density. Structural and spectroscopic analyses were conducted, and catalytic activity, recyclability, and reaction kinetics were evaluated.
Results and Conclusions.
Mn incorporation into the MgAl2O4 lattice generated lattice oxygen defects originating from charge imbalance and local structural distortion, resulting in the formation of oxygen vacancies. Acid treatment further increased the vacancy density by selectively removing amorphous or weakly bound oxide species while maintaining the crystalline spinel structure. Systematic control of defect concentration revealed a clear correlation between oxygen vacancy density and PET glycolysis kinetics, with higher vacancy concentrations facilitating the formation of soluble oligomeric intermediates and accelerating PET conversion. Among the catalysts examined, Mn0.25Mg0.75Al2O4 showed the highest activity, achieving complete PET conversion with a BHET yield of 95.3 % within 4 h at 190 ℃. Stable catalytic performance was maintained over repeated cycles, with full activity recovery after simple calcination, indicating strong structural stability and resistance to metal leaching.
Acknowledgments

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SCW0655

Selective Olefin Production from Waste wet wipes via Catalytic Pyrolysis

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Waste Valorization

Keywords: Polyethylene terephthalate (PET), catalytic pyrolysis, light olefins, zeolite catalysts, product selectivity, reaction pathway control

Abstract Body.
Introduction.
Waste polyethylene terephthalate (PET), although widely available, remains a challenging carbon resource due to its aromatic backbone and high oxygen content. These features inherently favor decarboxylation and aromatization during thermal conversion, thereby complicating precise reaction control [1]. These challenges can be addressed by employing zeolite catalysts, which enable regulation of PET degradation pathways [2]. In this study, a reaction-engineering-based strategy is proposed to redirect PET degradation pathways toward the selective production of light olefins via catalytic pyrolysis.
Methods.
PET-based waste wet wipes were employed as the feedstock, and zeolite catalysts were introduced to enable reaction pathway control. Pyrolysis experiments were conducted above 600 °C in a lab-scale fixed-bed reactor, with catalyst type, reaction temperature, and steam injection systematically varied. Furthermore, co-pyrolysis with waste polypropylene (PP) was performed to evaluate the scalability of the proposed strategy under mixed-waste conditions.
Results and discussion.
The results show that zeolite catalysts effectively suppress coke formation while promoting the conversion of PET into light olefins. In particular, the application of steam under catalytic conditions increased the light olefin selectivity to 15.07 vol%, compared to 4.63 vol% obtained under non-catalytic conditions. These findings indicate that olefin production from oxygen-rich PET can be actively directed through the catalytic regulation of reaction pathways. Notably, synergistic co-pyrolysis with waste PP led to a significant increase in light olefin yield, proving the effectiveness of this strategy in realistic waste scenarios.
This work highlights how chemical reaction engineering can transform recalcitrant PET waste into carbon-neutral chemical feedstocks, offering a viable pathway for closing the carbon loop in future sustainable chemical processes.
Acknowledgments
This work was supported by the National Research Foundation of Korea(NRF) grant funded by the Korea government(MSIT) (2022R1A2C1011106).
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SCW0656

Catalytic pyrolysis of waste toner powder over hierarchical ZSM-5 for selective aromatic hydrocarbon production

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Waste Valorization

Keywords: Waste toner powder, Catalytic pyrolysis, Hierarchical ZSM-5, Aromatization

Abstract Body.
Introduction.
The rapid growth of electronic device consumption has made electronic waste (e-waste) one of the fastest-growing waste streams worldwide [1]. Beyond metals, e-waste contains polymer fractions that can form microplastic-like residues and release hazardous additives. Waste toner powder (WTP) from spent laser printer cartridges consists of micron-sized styrene–acrylate polymers, pigments, charge-control agents, and metal oxides, and is resistant to natural degradation with limited recycling options [2]. Catalytic pyrolysis offers a promising route to convert this polymer-rich waste into valuable chemicals [3]. This study focuses on the selective production of aromatic hydrocarbons, particularly benzene, toluene, and xylenes, through catalytic upgrading of WTP over hierarchical ZSM-5 catalysts.
Methods.
Hierarchical ZSM-5 catalysts were prepared from commercial ZSM-5 (SiO_2/Al_2O_3 = 50 and 80) via controlled desilication using NaOH and mixed alkaline–organic base systems (NaOH/TEAOH and NaOH/TPAOH), and an organosilane-templated hierarchical ZSM-5 was also used. WTP decomposition was analyzed by Py-GC/MS at 600 ℃. The resulting vapors were catalytically upgraded in a lab-scale fixed-bed reactor under N_2, CO_2, or CH_4 atmospheres. Liquid products were quantified by GC-MS, and permanent gases and C1-C4 hydrocarbons were analyzed by GC-TCD/FID.
Results and discussion.
Characterization confirmed that both desilicated and template-derived hierarchical ZSM-5 preserved the crystalline MFI framework while developing increased external surface area and mesoporosity. These textural changes improved access of bulky pyrolysis intermediates to acid sites, enhancing secondary cracking, deoxygenation, and aromatization. Compared with the parent zeolite, hierarchical ZSM-5 showed higher mono-aromatic formation due to improved diffusion and reduced mass-transfer limitations during vapor upgrading. Reaction atmosphere affected product distribution, with CO_2 suppressing coke formation and CH_4 influencing BTEX formation through hydrogen-related effects, while multi-cycle tests showed the highest cumulative BTEX and lowest coke under CO_2.
The synergy between hierarchical porosity and strong acidity enabled efficient upgrading of WTP-derived vapors into valuable aromatics, demonstrating the feasibility of converting toner-derived polymer waste into petrochemical feedstocks via catalytic pyrolysis and highlighting the importance of both catalyst structure and reaction environment in controlling product selectivity.

Acknowledgments
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SCW0700

TiO2-supported Ru-Fe catalysts for the hydrodeoxygenation of PET-derived BHET

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Waste Valorization

Keywords: bis(2-hydroxyethyl) terephthalate, catalyst, hydrodeoxygenation, iron, ruthenium

Abstract Body.
Polyethylene terephthalate (PET) upcycling to petrochemical feedstocks proceeded through catalytic hydrodeoxygenation (HDO) of bis(2-hydroxyethyl) terephthalate (BHET) prepared by glycolysis of PET. HDO of BHET was performed at 250 ℃ under 50 bar H2 balanced with N2 using a high pressure batch reactor. TiO2 -supported ruthenium catalysts produced deoxygenated compounds that included aromatic and cyclohexyl molecules. A hydrogen-pressure-dependent deoxygenation pathway was inferred from the detected intermediates. With iron added to Ru/TiO2 (Ru/Fe/TiO2), the carbon yield to C6–C8 deoxygenated compounds reached 61.1%. TEM, XPS and CO-DRIFTS were analyzed for elucidating the catalyst structure and electronic effects, combined with DFT calculations. Proximity of Ru to Fe oxides depleted the electron density of Ru, adjusted its catalytic activity, and suppressed excessive hydrocracking, which preserved high yields of C6–C7 hydrocarbons.

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SCW0714

Production of Valuable Petrochemicals from Plastic-Derived Oil Fractions via Catalytic Cracking over ZSM-5 based catalysts

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - Sustainable Chemicals - Waste Valorization

Keywords: Plastic-derived oil, Catalytic cracking, ZSM-5 zeolite, light olefins, BTX aromatics, pyrolysis oil upgrading,

Abstract Body.
The transition toward carbon-neutral chemical production requires alternative, non-fossil carbon feedstocks that are compatible with existing catalytic infrastructure. Plastic-derived oils (PDOs), produced via pyrolysis of mixed plastic waste, represent a promising circular carbon resource; however, their broad boiling range, high olefinicity, and poor stability limit direct utilization. This study investigates the catalytic cracking of a light PDO fraction (<195 °C) over ZSM-5-based catalysts to establish a reaction-engineering pathway for converting plastic waste into value-added petrochemical products.
Catalytic performance was first benchmarked using n-heptane as a model compound over H-ZSM-5 (Si/Al = 40) in a continuous fixed-bed reactor at 350–450 °C. Conversion increased systematically with temperature and catalyst contact time, reaching up to 94% at the highest severity. Product selectivity was strongly governed by reaction conditions, with higher temperatures favoring monomolecular protolytic cracking and β-scission pathways, leading to increased yields of light olefins (C_2 –C_4). Increased contact time promoted secondary reactions such as hydrogen transfer, oligomerization, cyclization, and aromatization, resulting in enhanced BTX formation. The apparent activation energy (75 kJ mol^{-1}) is consistent with carbocation-mediated cracking on acidic zeolites.
The light PDO fraction, dominated by C_5 –C_{12} mono-olefins, cycloalkenes, and mono-aromatics, exhibited cracking behavior analogous to the model compound. Increasing reaction temperature significantly enhanced light olefin yields (up to 45.3 wt.% at 450 °C) and increased BTX production (up to 16.8 wt.%), while heavier olefins and naphthenic species were substantially reduced. These results demonstrate that reaction severity can be used as an effective lever to steer product selectivity toward targeted petrochemical streams. Overall, ZSM-5-based catalytic cracking is shown to be an effective upgrading route for plastic-derived oils, enabling tunable production of light olefins and aromatics from waste-derived feedstocks. Ongoing work focuses on hierarchical and metal-modified ZSM-5 catalysts (Fe- and Pt-loaded) to improve mass transport, heteroatom tolerance, and selectivity control, supporting the development of scalable, circular, and de-fossilized petrochemical processes.

Poster Presentation

Clean Environmental Technologies

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CET0150

Facile and efficient microwave strategy for upcycling of plastic wastes into high-yield hydrogen and carbon nanotubes

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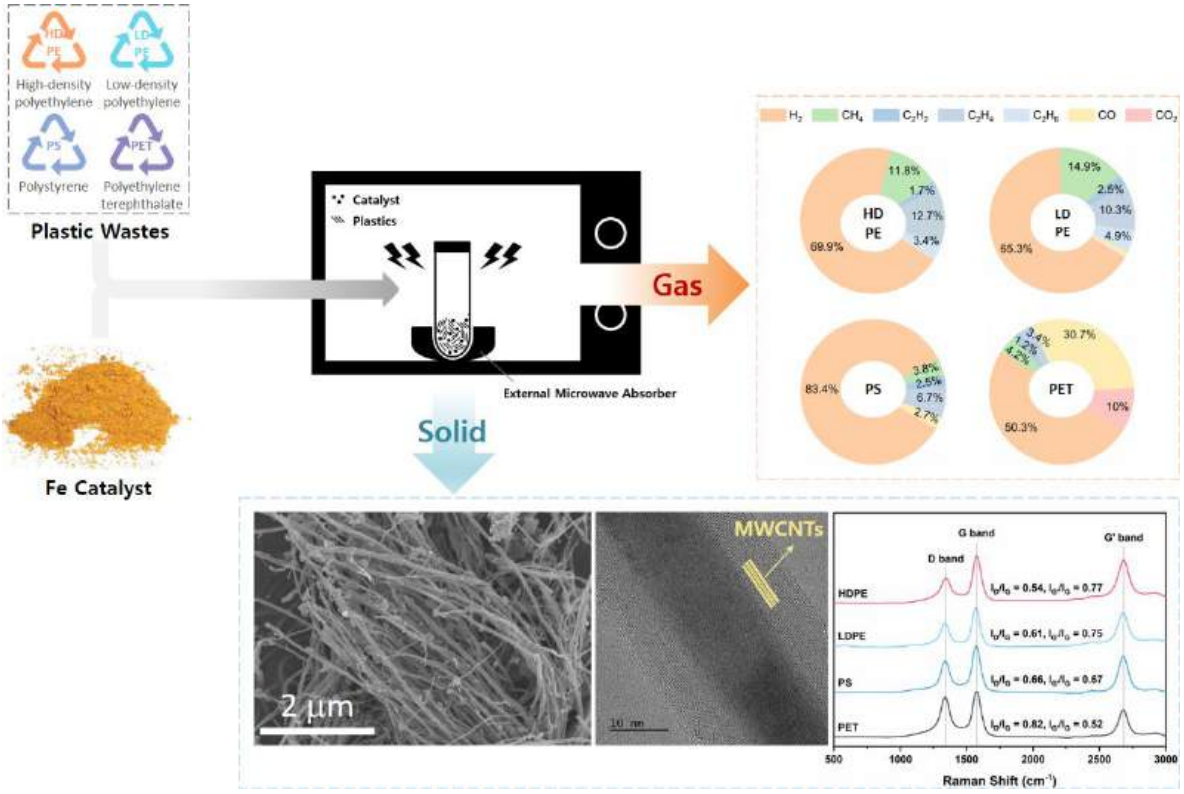
Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: plastic waste upcycling, microwave-irradiated pyrolysis, microwave absorber, hydrogen, carbon nanotube

Abstract Body.
Plastics are indispensable in modern society, yet their persistence and low degradability impose a growing environmental burden. Accordingly, the establishment of sustainable and practical plastic waste management strategies has been considered one of the most urgent and non-negotiable agendas. To address this issue, various thermochemical valorization routes have been widely explored to convert plastic waste into value-added products. Among them, microwave-assisted pyrolysis has been particularly attractive because it has enabled rapid volumetric heating and short reaction times. However, practical implementation of microwave-driven upcycling has often been limited by the need for purpose-built microwave cavities, specially designed reactors, and sophisticated control systems to stabilize temperature profiles and product selectivity. In this work, we present a facile and efficient microwave-assisted plastic-waste upcycling strategy that operates in a common household microwave oven, providing a low-infrastructure alternative for rapid conversion. In the presence of an Fe catalyst and an external silicon carbide (SiC) microwave absorber, plastic wastes (HDPE, LDPE, PS, PET, and their mixtures) were rapidly decomposed into high-yield H2 and carbon nanotubes (CNTs) within 1–2 min of microwave irradiation. SiC played a decisive role by triggering an abrupt thermal surge, raising the reaction temperature to as high as 1123 K, which preferentially accelerated C–H bond cleavage and enabled simultaneous CNT growth. Microwave-irradiated pyrolysis of HDPE and LDPE exhibited high H2 selectivity (up to ~70%) and produced high-quality CNTs (Raman ID/IG = 0.54) with an ~95% filamentous carbon yield after purification, indicating efficient carbon utilization in the solid phase with negligible formation of undesired liquids. Indeed, liquid products were undetectable, and CO2 formation was minimal except for PET. Even for oxygen-rich PET, CO production was approximately three times higher than CO2 production. It is noted that microwave-irradiated pyrolysis of mixed plastic wastes generated syngas with tunable H2/CO ratios (0.75–2.5). Since other gaseous products such as CH4 and C2Hx do not participate in the reaction, the resulting syngas can be directly used for the Fischer–Tropsch reaction for e-fuel production. These results established a practically deployable, SiC-boosted household-microwave pathway that coupled ultrafast H2 liberation with in-situ CNT synthesis from real-world plastic wastes.


HDPE
LDPE
PS
PET
High-density polyethylene
Low-density polyethylene
Polystyrene
Polyethylene terephthalate
Plastic Wastes
Fe Catalyst
Catalyst
Plastics
External Microwave Absorber
Gas
Solid
H2
CH4
C2H2
C2H4
C2H6
CO
CO2
HD PE
LD PE
PS
PET
2 μm
MWCNTs
G band
D band
G' band
HDPE
LDPE
PS
PET
Raman Shift (cm-1)

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2026 / SEOUL, KOREA

CET0021

Rethinking Green Hydrogen: A Smarter Route to Decarbonization for Energy-Abundant Nations

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: Green hydrogen, Decarbonization, LNG

Abstract Body.
Hydrogen plays a pivotal role in global decarbonization, particularly across sectors that are difficult to electrify directly. Its versatility as an energy carrier offers significant potential to reduce greenhouse gas (GHG) emissions across industries and transportation systems. However, realizing this potential requires accounting for the hidden CO_2 emissions embedded throughout the production and lifecycle of green hydrogen, which can remain substantial even in regions with abundant renewable energy resources. This study employs a scenario-based modeling approach to conduct a comparative assessment of green energy utilization for natural gas displacement versus green hydrogen export. The analysis quantifies CO_2 emissions and cost trade-offs associated with converting renewable power to hydrogen compared to its direct use for household consumption. Results show that converting 100 MW of renewable electricity into green hydrogen is approximately twelve times less cost-effective in achieving decarbonization than directly supplying the same power to homes. For energy-rich nations such as Oman, exporting the natural gas conserved through domestic renewable substitution to energy-deficient, coal-dependent countries could reduce emissions by up to 67.5%. The findings highlight that prioritizing green power for domestic use while maintaining liquefied natural gas (LNG) exports can offer a more balanced and globally beneficial decarbonization strategy.

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CET0038

Understanding into the Microstructure and Diffusion behaviors of Water Removal in Nanopores of Wafer by Supercritical Carbon Dioxide

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: Wafer drying, Supercritical carbon dioxide, Molecular Dynamics Simulation

Abstract Body.
In the fabrication of semiconductor devices, especially wafer manufacturing, drying process constitutes a critical processing step. The continuing reduction of critical dimensions in wafer manufacturing has rendered structural collapse (deformation or bending) induced by conventional wet processing techniques an increasingly severe issue. Supercritical carbon dioxide ($scCO_2$), owing to its absence of surface tension, demonstrates significant potential as an effective displacement agent and drying medium of drying process for nanostructure of wafer.
In this work, experiments and simulations were used to investigate the macroscopic phenomena and microscopic mechanisms of removal of residual water from wafer nanostructures using $scCO_2$. Equilibrium molecular dynamics (EMD) simulation and non-equilibrium molecular dynamics (NEMD) simulation were adopted to investigate the effects of different concentrations of IPA on the microstructure and diffusion behavior of residual water removal in the nanopore of silicon wafers.
The experimental validation using patterned wafers confirms that supercritical drying can completely remove residual water from nanostructures, exhibiting both effectiveness and rapidity. Moreover, the drying efficiency exhibits a distinct feature-size dependence, with wider line-width structures demonstrating faster residual moisture elimination rates.
However, current research on supercritical fluid drying primarily focuses on empirical observations, with limited understanding of the underlying displacement mechanisms. Molecular dynamics (MD) simulation was adopted to study the microstructure and diffusion behaviors of water removal in nanopores of wafer by $scCO_2$. The simulations of the interfacial CO_2-IPA supercritical drying system results shows that the enhancement of IPA accumulation induces deeper molecular penetration, thereby increasing the interface thickness and the tendency of the IPA-OH vector to point to the interface, and making a negative contribution to the interfacial tension (IFT). The strong molecular orientation of IPA and the decrease of IFT are related to the hydrogen bond interaction between water and IPA molecules in the interface region. In addition, IPA additives facilitate water dissolution by reducing the energy barrier, thereby enhancing swelling behavior. From an interaction perspective, the presence of IPA enhances the migration and diffusion of residual water, consequently increasing its mobility.
These findings provide a fundamental molecular-level understanding of the moisture removal

process in micro-nano structures during the $scCO_2$ drying process.

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CET0198

Synchronizing Spectrum-Modulated Radiative Cooling and Integrated Heating in Hierarchical Film for All-Season Thermal Management

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: Multifunctional Thermal Regulation, Radiative Cooling, Hierarchical Porous Composite Architecture, Photothermal and Joule heating, Wide-Temperature Adaptive Thermal Management.

Abstract Body.

Achieving energy-efficient and adaptive thermal comfort under dynamically varying and extreme climates remains a major challenge. Existing passive heating or cooling materials often operate in a single mode and lack the flexibility required for year-round thermal regulation, while conventional heating, ventilation, and air-conditioning (HVAC) systems suffer from high energy consumption and carbon emissions. Here, we report a hierarchically architected multifunctional thermal regulation film (MTRF) that integrates passive radiative cooling, passive solar heating, and active Joule heating within a single, stable material system to enable all-season adaptive thermal management.

The MTRF was fabricated via layer-by-layer deposition combined with interface-regulated phase separation and graphene spray coating. The resulting triple-layer architecture consists of a top graphene layer for photothermal conversion and Joule heating, a middle liquid metal (LM)-embedded polyethersulfone (PES) layer forming a continuous conductive network, and a bottom PES/hollow SiO_2 composite layer with hierarchical porosity for radiative cooling. The bimodal porous structure and hollow SiO_2 microspheres promote strong solar scattering and mid-infrared emissivity, while the confined LM and graphene coating ensure high electrical conductivity, mechanical integrity, and suppression of LM leakage and oxidation.

In the cooling mode, the bimodal porous structure of the PES matrix, combined with hollow SiO_2 microspheres, induces strong Mie scattering in the solar spectrum and high emissivity within the atmospheric window, resulting in a solar reflectivity of 97.7% and an emissivity of 91.8%. Outdoor field tests demonstrate an average daytime radiative cooling effect of 5.3 °C below ambient temperature. In the heating mode, flipping the film activates the graphene surface, which exhibits a high solar absorptivity of 94.8% and produces a solar heating effect of 6.7 °C above ambient under winter conditions. Moreover, the efficient conductive network enables rapid low-voltage Joule heating, raising the surface temperature from −20 °C to 20 °C within 31.2 s under an applied voltage of only 0.6 V, providing reliable thermal compensation under ultralow temperatures, nighttime operation, or insufficient solar irradiation.

This work demonstrates a unified materials design strategy that synergistically combines hierarchical structural engineering, spectral selectivity, and efficient electrical heating within a single system, offering a versatile and energy-efficient pathway toward all-season adaptive thermal management for portable shelters, wearable devices, and

protection in extreme environments.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

CET0204

Alkali fusion with NaOH-KOH hydroxide to convert waste dehydrated clay cake into zeolitic materials

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: Waste dehydrated clay cake, Alkali fusion with alkali hydroxide, Zeolitic material, Kinetic analysis

Abstract Body.
During quarrying, a large amount of dehydrated cake is generated to be landfilled, it is becoming difficult to secure landfill sites, and effective utilization of dehydrated cake is desired. Zeolite has attracted attention for its potential application in environmental purification and other fields, due to its ion exchange capacity and so on. In a previous study, a zeolitic product with high cation exchange capacity was successfully prepared by alkali fusion of dehydrated stone cake with NaOH at more than 400 ℃ to convert the insoluble contents of Si and Al in mineral into soluble contents with high reactivity in the reaction solution. The key point in this process is the fusion reaction with alkali hydroxide to convert waste cake into zeolitic product. However, little information is available on the fusion reaction with alkali hydroxide to waste cake. In this study, alkali fusion with NaOH-KOH hydroxide was examined to convert waste clay cake into zeolitic materials. Dehydrated clay cake, discarded from one of the quarries in Japan, containing 56.8% SiO_2, 27.8% Al_2O_3, 7.9% Fe_2O_3, 3.1% MgO and 2.7% TiO_2 in the form of mainly silicate minerals, such as quartz [SiO_2], albite [$Na_2Al_2Si_2O_8$], and muscovite [$KAl_3Si_3O_{10}(OH)_2$]. was used. The mixture of NaOH and KOH at a weight ratio (NaOH: KOH) of 1:0, 3:1, 1:1, 1:3 and 0:1 was heated in an electric furnace at 400 ℃ for 1 hour, and naturally cooled at room temperature for 40 minutes to prepare a mixed alkali hydroxide. A cake was added to the iron crucible, then a mixed alkali hydroxide was added to the cake and heated at 200 - 400 ℃ for 0 – 240 min. The soluble contents of Si and Al in the fused cake were calculated from the dissolution amounts from the fused cake in 1 M HCl solution. The fused cake was added to distilled water in the tube, then the tube was shaken for 24 h, and heated at 80 ℃ for 12 h to synthesize the zeolitic product. As a result, with increasing heating temperature on alkali fusion, reaction rate of alkali fusion promoted, and the highest reaction rate is indicated using alkali hydroxide with NaOH: KOH = 1 : 3. Zeolitic product including faujasite can be synthesized from the cake fused with alkali hydroxide (NaOH: KOH = 1 : 3) at 250 ℃ for 60 min, and showed higher ion exchange capacity than natural zeolite.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

CET0242

Reversible Photochromic Films Constructed based on Meticulous Defect and Interfacial Engineering strategies for Energy-saving Smart Window

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: Thermal management, Energy saving, Meticulous defect, Interfacial engineering

Abstract Body.
In response to the global energy crisis and climate change, passive thermal management plays a vital role in building energy conservation. However, widespread adoption of photochromic smart windows is hindered by critical bottlenecks such as low modulation efficiency, slow response, and insufficient cycling stability. An ultrafast, robust photochromic W18O49-based smart window was prepared via a defect-interface co-engineering strategy that enables triple-mode spectral regulation, large modulation amplitude, and markedly improved durability. The assembled photochromic smart window exhibited three distinct optical modes under illumination: bright mode (high Tlum and high TNIR), transparent mode (high Tlum and low TNIR), and shading mode (low Tlum and low TNIR), enabling dynamic modulation of Vis and NIR transmission under varying climatic conditions. the smart window achieved a Tlum ~ 84.15% in transparent mode and demonstrated strong solar modulation ability (ΔTsol) around 77.31% via switching to shading mode. Besides, the photochromic smart window demonstrates excellent reversible light response characteristics: under UV irradiation, a modulation of ΔTNIR = 57.04% was realized within 10 s, while the recovery of ΔTlum = 53.42% occurred within 30 s under NIR irradiation. This work provides a simple, yet effective strategy via defect-interface co-engineering to enhance the performance and stability of W18O49-based photochromic smart window and offers both theoretical and practical guidance for performance enhancement in smart windows and other advanced thermal management technologies.

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CET0256

Accelerated Design of Wide-Temperature-Range Molten Salts via Transfer Learning with Small Sample Sizes of data

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: Energy Storage Molten Salts; Wide Temperature Range; Machine Learning

Abstract Body.
Introduction. Concentrated Solar Power (CSP) and thermal power retrofits extensively utilize molten salts.[1] The current commercial salt, Solar Salt, operates within a limited temperature range (220–565°C). However, the development of advanced multi-component salts faces distinct challenges.[2] Traditional approaches are inefficient for exploring the vast compositional space. While machine learning strategies offer acceleration, they are severely constrained by the small sample size of data.[3] Direct training on such limited datasets is prone to noise, which obscures the true chemical trends. This study proposes a transfer learning framework to design wide-temperature-range molten salts, specifically to overcome small sample size limitations.
Methods. To address the challenge of small sample sizes in energy storage materials, a hierarchical dataset was constructed. This comprised a foundational dataset of low-fidelity historical data to capture general trends and a high-quality dataset generated via strictly controlled experiments. A non-linear regression model was utilized as the base learner to capture interactions between salt components (KNO3, NaNO3, NaNO2, LiNO3, Ca(NO3)2). A transfer learning strategy was employed, where the model was pre-trained on lower-fidelity data and subsequently fine-tuned using the small set of high-fidelity experiment data. This approach avoids the noise and bias introduced by simply aggregating datasets of varying fidelity. Screening was then applied to predict candidates with optimal thermal properties.
Results and discussion. The transfer learning strategy successfully mitigated the limitations imposed by the small sample size of data, allowing the model to accurately predict thermal stability limits even when the data is noisy and sparse. The model-guided screening identified novel multi-component molten salt formulations with temperature range exceeding 500°C. Remarkably, this represents a 50% increase over commercial salts. This study provides a framework for accelerating the discovery of next-generation thermal energy storage materials despite limited data.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

CET0266

Effects of Acid Sites in Nanosheet MCM-22 on Plasma-Assisted Depolymerization of Poly(methyl methacrylate)

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: Wasted PMMA recycling, depolymerization, nonthermal plasma, MCM-22, Nanosheet zeolites

Abstract Body.
In recent years, improving the efficiency of poly(methyl methacrylate) (PMMA) depolymerization has gained attention due to the limitations of conventional thermal processes, particularly for additive-containing PMMA, which suffer from low selectivity and high energy demand [1]. To address these challenges, zeolite-based solid acid catalysts have been applied to the chemical recycling of additive-containing PMMA, mainly focusing on methacrylic acid (MAA) retrieval [2]. In this study, PMMA depolymerization over MCM-22 catalysts is investigated using a dielectric barrier discharge (DBD) plasma-assisted system. Nanosheet MCM-22 (NS-MCM-22) was synthesized using carbon spheres as a hard template, followed by calcination and ion exchange to obtain the H+ form. PMMA depolymerization was performed in a lab-scale dielectric barrier discharge (DBD) plasma reactor at 300oC (10 kV, 1 kHz) using helium, with a packed bed of physically mixed waste PMMA pellets and catalyst. SEM images and thickness histograms show that the nanosheet morphology reduces the particle thickness of MCM-22, increasing external surface exposure without altering overall particle dimensions. XRD patterns of NS-MCM-22 confirm that the MWW framework remains intact after morphology modification. Pyridine-adsorbed FT-IR spectra show that the Na+ form NS-MCM-22 is dominated by Lewis acid sites associated with Na+ cations, whereas Brønsted acid sites are predominant in the H^+ form. Under identical plasma conditions, the difference in acidity is reflected in the depolymerization behavior, with the H^+ form favoring selective MMA formation and the Na^+ form promoting oxygenated byproducts such as methanol. This behavior is attributed to Brønsted acid sites in the H^+ form enabling more controlled chain unzipping, whereas Lewis acidity associated with Na^+ cations leads to less selective fragmentation in the plasma environment.

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2026 / SEOUL, KOREA

CET0288

Revealing the active Cu species in Cu/ZSM-5 catalysts for the selective catalytic oxidation of ammonia

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: NH3-SCO, Cu/ZSM-5, ammonia, oxidation, active sites

Abstract Body.

Introduction.

Ammonia slip, a by-product of NH_3 processes such as selective catalytic reduction (SCR) of NO_x and emerging NH_3 -fueled energy systems, poses significant environmental and health risks, necessitating its removal via the selective catalytic oxidation of ammonia (NH3-SCO; 4NH3 + 3O2 → 2N2 + 6H2O). Recent studies have demonstrated the potential of Cu/zeolite catalysts for NH_3 -SCO reactions, owing to their intrinsic oxidation activity and high N2 selectivity. However, the precise nature of the active Cu sites governing NH3-SCO has not been fully established and remains controversial.

Methods.

In this study, a series of Cu/ZSM-5 catalysts with varying Cu loadings was synthesized via an aqueous ion-exchange method. The structural properties were characterized by XRD and BET, while the nature and distribution of Cu species were examined using H2-TPR, EPR, and UV-Vis DRS. In addition, NH3 adsorption behavior and reaction pathways were investigated through NH3-TPD and in situ DRIFTS. The reaction rate and apparent activation energy (E_a) were determined under conditions with NH_3 conversion maintained below 20% to avoid mass diffusion limitations.

Results and discussion.

Among the catalysts with various Cu loadings, the 2.1Cu/ZSM-5 catalyst, corresponding to the maximum Cu content achievable via ion exchange, exhibited up to 99.5% NH_3 conversion and 99.4% N_2 selectivity at 400 °C. To investigate the active Cu sites in the NH3-SCO reaction, the distribution of the Cu species quantified by H2-TPR and EPR was correlated with the reaction rate, revealing that isolated Cu2+ ions exhibited the strongest linear correlation. A controlled experiment involving the selective reduction of Cu2+ to Cu+ resulted in a significant decrease in the NH3 conversion, confirming that Cu2+ ions are more active than Cu+ ions in the NH3-SCO reaction. Furthermore, the turnover frequency (TOF), calculated based on the number of Cu2+ ions, remained nearly constant with a slight increase at higher Cu loadings, confirming the primary role of Cu2+ ions in the catalytic oxidation process and the minor contribution of other Cu species. Further NH3-TPD and in situ DRIFTS analyses demonstrated that Cu ion-exchange enhances NH3 adsorption capability, thereby contributing to the improved catalytic activity in the NH3-SCO reaction. These results collectively indicate that both the population and intrinsic reactivity of isolated Cu^{2+} ions are key factors governing NH3-SCO performance. This study identifies the most active Cu sites and their role in NH_3 oxidation within ion-exchanged Cu/ZSM-5 catalysts, providing insights for developing future strategies to achieve enhanced NH3-SCO performance.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

CET0312

Mechanistic Insights into the Trace BCl3/PCl3 Removal from SiHCl3 through Nitrogen-Containing Functional Groups and Pore Size Tuning: GCMC and DFT Simulation Study

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Abstract Category: Environmentaly-friendly and Sustainable Chemicals - 선택 없음

Keywords: Keywords: Chlorosilane purification; Adsorption behavior; Nitrogen-containing functional groups; Porous carbons; GCMC simulation; DFT simulation.

Abstract Body.
Introduction.
The deep purification of SiHCl3 is critical for high-purity polysilicon production. Removing trace BCl3 and PCl3 is extremely challenging due to their molecular similarity to SiHCl3 and part-per-billion concentration limits. Adsorption on activated carbon is promising but limited by insufficient capacity (leading to deactivation) and a low removal limit (causing unstable performance). Enhancing performance requires tuning both pore structure and surface chemistry. Introducing nitrogen-containing functional groups is a common strategy, yet how they interact with B/P impurities and synergize with pore confinement remains unclear. This study integrates DFT and GCMC simulations to bridge molecular mechanisms with macroscopic adsorption, elucidating the synergy between nitrogen-containing functional and pore structure to guide adsorbent design.
Methods.
A combined computational-experimental approach was employed. DFT calculations probed the adsorption configurations, charge transfer, and binding energies of BCl3, PCl3, and SiHCl3 on nitrogen-functionalized carbon sheet models(-NH2, -NO2, -N6, -N5, -NQ). GCMC simulations then investigated the effects of nitrogen-group type, content, and pore size on equilibrium capacity, competitive isotherms, and adsorbate distribution in amorphous and slit-pore models. Guided by the theoretical predictions, N-doped activated carbons were synthesized via urea-assisted pyrolysis. Static adsorption experiments were conducted to measure the removal limit at trace concentrations and the adsorption capacity at higher concentrations. The samples were characterized using XPS, BET, and elemental analysis validating the proposed adsorption mechanism and the accuracy of the simulations.
Results and discussion.
DFT calculations show that the binding energy of nitrogen-containing groups with BCl3 increases as their electrostatic potential decreases, while the opposite trend holds for PCl3. Notably, groups like -NH2 and -N6 form stable complexes with both impurities via strong electron donation and spatial matching. Experimentally, increasing pyrolysis temperature raised the -N6 content, enhancing removal performance. At a pyrolysis temperature of 800 ℃, BCl3 and PCl3 concentrations were reduced from 150 ppb to 2.23 ppb and 47.26 ppb, respectively. GCMC simulations confirm that nitrogen doping does not alter the optimal pore-size range (6-10 Å) but significantly boosts selectivity and capacity

through stronger surface interactions. At 50 ppm, adsorption capacities reached 4.46 mg/g for BCl_3 and 2.34 mg/g for PCl_3. These results demonstrate that precise tuning of surface nitrogen chemistry enables adsorbents with both high capacity and deep removal limits, providing a clear design strategy for $SiHCl_3$ purification.

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CET0340

Separation of intentionally-added substances from plastic waste, including legacy substances

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Keywords: dissolution recycling; plastic waste; additives; extraction; solid-liquid separation
Introduction. In 2025, approximately 10% of the total produced plastic worldwide came from recycled content,[1] highlighting the need to close the loop for plastic materials. Plastic waste contains several intentionally- and non-intentionally added substances, (N)IAS, including additives, labels, inks, and contaminants such as organic residues, wood, paper and metals.[2] Dissolution recycling is an emerging promising recycling route for plastics, as it allows to deal with complex streams without the need to depolymerize the polymer. The principle is to dissolve the target polymer, followed by purification steps to remove (N)IAS and a recovery step to obtain the polymer back from solution.[3] In this work we investigate the separation of several additives from polystyrene (PS) waste, including organic and inorganic substances. **Methods.** Solvent screening for polystyrene and additives was based on Hansen Solubility Parameters and COSMO-RS simulations. Different techniques were employed for the removal of the additives, including solid-liquid separation processes such as filtration and centrifugation, and adsorption batch experiments using activated charcoal. **Results and discussion.** The results show that solvent selection is key for the separation of the majority of additives. These exhibit diverse molecular structures, resulting in an heterogeneous mixture of soluble and insoluble components. Thus, a combination of extraction technologies is needed to obtain high-purity recyclate. This work shows that successful technologies are adsorption and solid-liquid separation processes. For instance, (legacy) flame retardants could be removed up to 99% using activated charcoal[4] and 100% retention of inorganic (N)IAS from real PS waste.

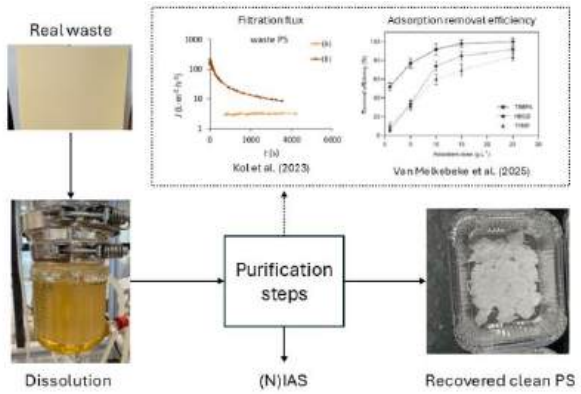

Figure 1. Figure illustrating the removal of

pigments was obtained with solid-liquid separation processes[5]. Additionally, the findings indicate that the removal of carbon black colorant is more challenging due to its finer particles and two-step process may be needed to achieve 100% removal. This work shows the potential of dissolution recycling towards closing the loop for PS-based waste, which can be extended to other polymeric materials.

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ISCRE29 & APCRE11
2026 / SEOUL, KOREA

CET0367

Enhanced sulfur resistance of the zeolite-mixed bulk vanadium oxide catalyst for NH3-SCR

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: Bulk vanadium oxide catalyst; Physical mixing; Y zeolite; ABS migration

Abstract Body.

Bulk vanadium oxide (VOx) catalyst has drawn attention due to its superior low-temperature catalytic activity [1], while no thorough study on the deactivation process of the VOx catalyst due to SO2 has been conducted. Previously, our group reported that physical mixing of zeolite can effectively alleviate the sulfur poisoning of the V2O5-WO3/TiO2 (VWTi) catalyst via the migration and trapping of ABS species to the zeolite domain [2]. In this study, we have investigated the origin of the different deactivation behavior of the VOx catalyst and the VWTi catalyst. We have also elucidated the effect of zeolite mixing on the sulfur resistance of the VOx catalyst, which further demonstrated the potential applicability of the mechanical mixing method to a wider range of catalysts to enhance their sulfur resistance.

The VOx catalyst was prepared from the vacuum evaporation of the vanadium oxalate solution. The physically mixed (PM) catalyst was prepared by grinding VOx and zeolite Y together in the mortar with a mass ratio of 2:1. The catalytic activity of the catalysts was measured with NOx analyzer (42i-HL, Thermo Scientific) To investigate the distribution of sulfur species on the SO2-aged catalyst, TEM-EDS and TPD-MS analysis was performed.

The deactivation behavior of the VOx, VWTi, and VOx+Y(5.1) catalyst during the exposure to SO2 is shown in Fig. 1(a). It can be seen that the deactivation rate of the VOx catalyst is notably higher in the initial stage. This behavior stems from the rapid formation and saturation of ABS on the catalytic surface. Compared to the VOx catalyst, the VOx+Y(5.1) catalyst shows significantly lower deactivation rate and retains high catalytic activity after exposure to SO2, which shows that the mechanical mixing strategy also effectively enhanced the sulfur resistance of the VOx catalyst. The TEM-EDS and TPD-MS analysis result shown in Fig. 1(b) and (c) shows that the sulfur species mostly exist on the zeolite domain for the VOx+Y(5.1) catalyst, which confirms the migration of ABS from the VOx to the zeolite. Our findings highlight the deactivation behavior of the VOx and PM catalyst, which would further contribute to elucidating the method to utilize the VOx catalyst for real-life application.

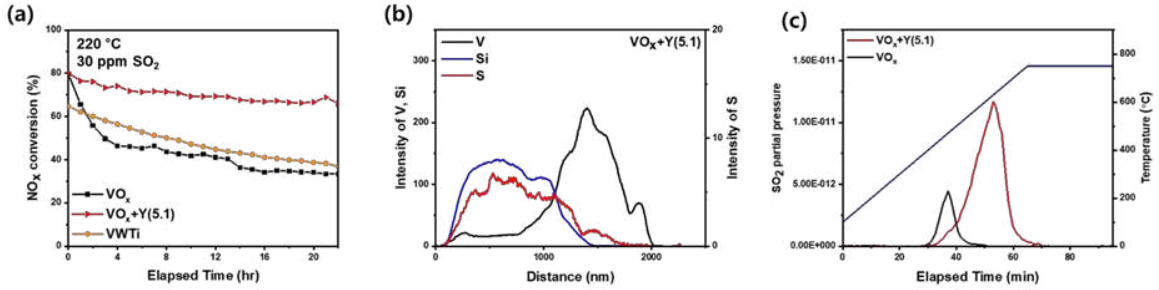

Fig. 1. (a) NOx conversion profile of VOx, VWTi and VOx+Y(5.1) catalyst (b) TEM-EDS analysis of the SO2-aged VOx+Y(5.1) catalyst (c) TPD-MS analysis of the SO2-aged VOx and VOx+Y(5.1) catalyst

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

CET0369

Depolymerization of Poly(Methyl Methacrylate) over Heteropoly Acid Catalysts in a Dielectric Barrier Discharge Plasma Reactor

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: Wasted PMMA recycling, Depolymerization, nonthermal plasma, Polyoxometalates

Abstract Body.
Introduction. Plastic recycling remains a significant global challenge due to the continuous increase in plastic waste generation. Among various plastic, poly(methyl methacrylate) (PMMA) has been widely used due to its excellent properties; however, the depolymerization of commercial additive-containing PMMA is highly energy-intensive and typically results in lower monomer yields compared to pristine PMMA. Previous studies have shown that dielectric barrier discharge (DBD) plasma combined with acidic catalysts enhances both methyl methacrylate (MMA) conversion and yield. In this study, a DBD plasma reactor was constructed and coupled with Heteropoly acid possessing strong Brønsted acid sites to promote PMMA depolymerization.
Methods. HPMo(H3[P(Mo3O10)4]·xH2O) was prepared from Merck. ZSM-5 were purchased from Zeolyst (USA). ZSM-5 was calcined under aeration at 550°C for 6 hr to obtain the H-form zeolites. Depolymerization of Poly (Methyl Methacrylate) was performed in a lab-scale dielectric barrier discharge (DBD) plasma reactor at 300oC (10 kV, 1 kHz) using Helium, with a packed bed of physically mixed wasted PMMA pellets and catalyst.
Results and discussion. XRD spectra show that HZSM-5 was confirmed to possess a well-developed MFI structure with uniform facets, indicating successful crystallization, while HPMo exhibited a highly crystalline nature. DT/TGA analysis of the spent sample indicated that the DT curves could be deconvoluted into two distinct peaks, which were attributed to the combustion of PMMA and dehydration of AlOOH, respectively. NH_3 -TPD analysis revealed dominant weak acid sites on HZSM-5 and strong acid sites on HPMo at higher temperatures, accounting for the observed differences in PMMA depolymerization performance.

ISCRE29 & APCRE11
2026 / SEOUL, KOREA

CET0397

Effect of zeolite framework on NOx operating cycle in Pd/zeolite Passive NOx adsorbers

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: Zeolite framework, Passive NOx adsorber, Pd speciation, site interconversion

Abstract Body.
Introduction. Pd/zeolites are the preferred materials for Passive NOx adsorbers (PNAs) due to their high low-temperature NOx storage capacity and optimum NOx desorption temperature.1,2 Experimental studies suggest that NOxstorage capacity and release temperatures are influenced by the zeolite framework, though the underlying reason for the same is unclear.1,2 Moreover, variation in Pd speciation (Pd2+, Pd1+, [PdOH]+, [Pd-O-Pd]2+ and [PdOH]+[PdOH]+) could also influence the Pd transformation mechanism and subsequent NOx adsorption. Thus, elucidating the effect of zeolite framework on NOx adsorption-desorption behavior is critical.

Methods. DFT simulations are performed using the plane-wave code as available in Vienna ab initio simulation package (VASP). For exchange-correlation functionals, the generalized gradient approximation (GGA) developed by Perdew, Burke, and Ernzerhof (PBE) is invoked. The structures of the transition state (TS) on the minimum energy path (MEP) are located using the Climbing Image Nudged Elastic Band (CI-NEB) method. Free energy for various surface reactions is determined using first principles thermodynamic analysis.

Results and discussion. Pd speciation and their interconversion, and the energetics of NO adsorption, oxidation, and desorption across different zeolite frameworks are computed theoretically to propose framework-dependent NOxadsorption-desorption cycle. The proposed NO operating cycles in Pd/BEA and Pd/CHA are depicted in Figure 1a and 1b, respectively. Irrespective of the zeolite framework, NO binds strongly on Pd1+ sites making them the main adsorption site. NO binding on Pd(II) species is relatively weak except on Pd2+ sites in BEA and ZSM-5 wherein the NO binding is comparable to Pd1+ sites. Thus, both Pd1+ and Pd2+ are principal adsorption sites in BEA and ZSM-5 whereas other Pd sites with relatively weak binding are more suited for desorption. In contrast, only Pd1+ site is found to be the optimum adsorption site in CHA and FER. The energetics of redox transformation of dimeric Pd(II) species ([PdOH]+[PdOH]+ and [Pd-O-Pd]2+) to Pd1+ with simultaneous NO oxidation are strongly dependent on the zeolite framework. Framework dependent variations in NO binding strength, Pd interconversion and reoxidation energetics collectively could explain the effect of the zeolite framework on the NOx adsorption-desorption characteristics. Further, the effect of exhaust components such as H2O and CO on NOx operating cycle would be discussed in detail in the full paper.

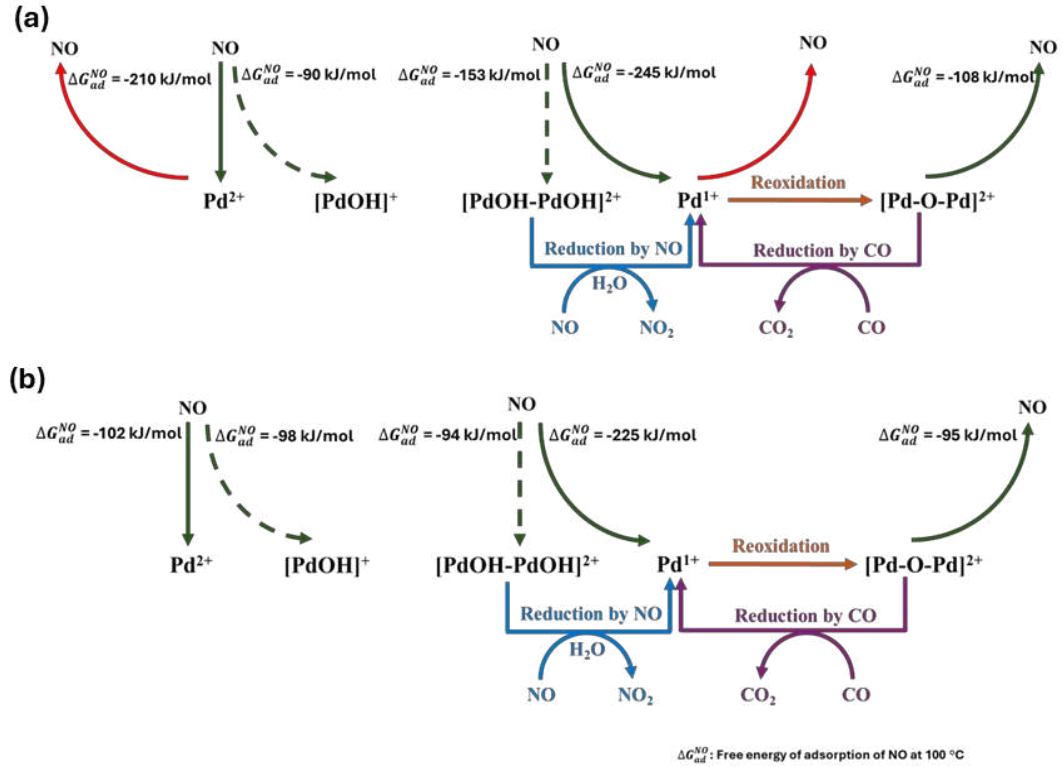

Figure 1: NO operating cycle in (a) Pd/BEA and (b) Pd/CHA.

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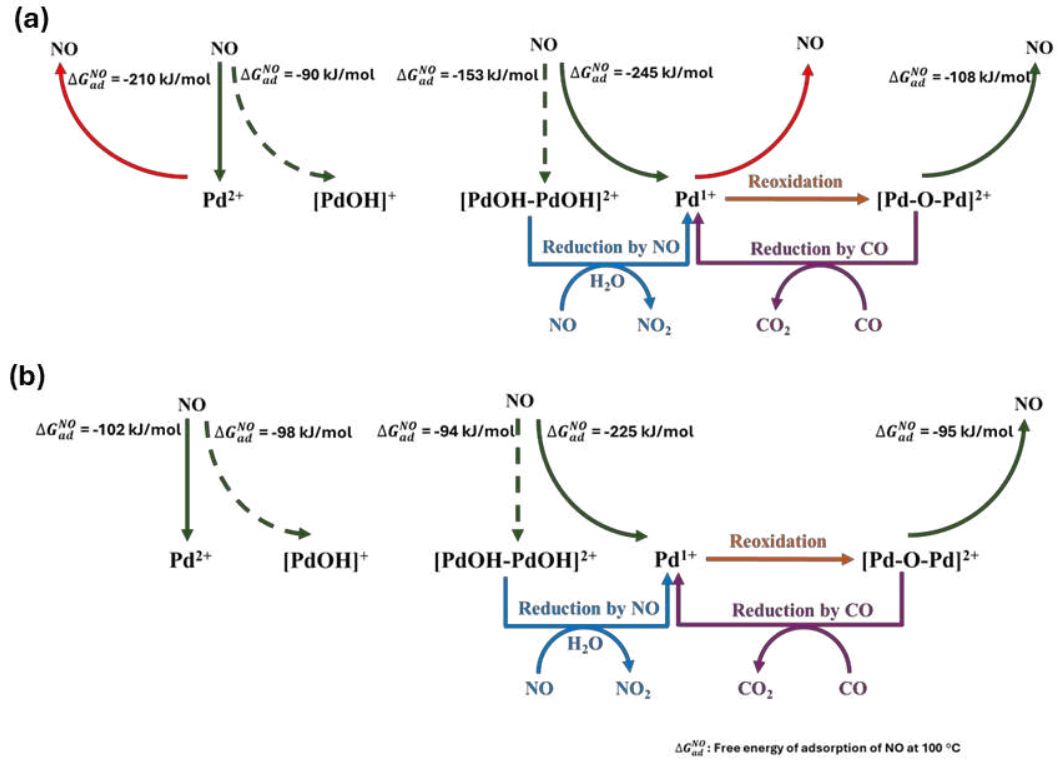
(a)
NO
ΔG_{ad}^{NO} = -210 kJ/mol
NO
ΔG_{ad}^{NO} = -90 kJ/mol
Pd^{2+}
$[PdOH]^{+}$
NO
ΔG_{ad}^{NO} = -153 kJ/mol
ΔG_{ad}^{NO} = -245 kJ/mol
NO
NO
ΔG_{ad}^{NO} = -108 kJ/mol
$[PdOH\text{-}PdOH]^{2+}$
Pd^{1+}
Reoxidation
$[Pd\text{-}O\text{-}Pd]^{2+}$
Reduction by NO
Reduction by CO
H_2O
NO
NO_2
CO_2
CO
(b)
NO
ΔG_{ad}^{NO} = -102 kJ/mol
ΔG_{ad}^{NO} = -98 kJ/mol
Pd^{2+}
$[PdOH]^{+}$
NO
ΔG_{ad}^{NO} = -94 kJ/mol
ΔG_{ad}^{NO} = -225 kJ/mol
NO
ΔG_{ad}^{NO} = -95 kJ/mol
$[PdOH\text{-}PdOH]^{2+}$
Pd^{1+}
Reoxidation
$[Pd\text{-}O\text{-}Pd]^{2+}$
Reduction by NO
Reduction by CO
H_2O
NO
NO_2
CO_2
CO
ΔG_{ad}^{NO}: Free energy of adsorption of NO at 100 °C

ISCRE29 & APCRE11
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CET0403

DFT Mechanistic Insights into Selectivity in Alkaline Glucose Electrooxidation on Au(111)/Au(OH) and CuO(111): Branching Between Aldehyde Oxidation and C–C Scission Governed by OH Coverage

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: DFT, biomass, catalyst

Abstract Body.

This DFT-focused study aims to explain why alkaline glucose electrooxidation shows catalyst-dependent selectivity, with Au favoring C6-retaining oxidation products while CuO promotes C–C bond cleavage. We target the mechanistic origin by quantifying how catalyst identity and potential-dependent hydroxylation govern early pathway branching.

Spin-polarized DFT calculations were performed with VASP using PAW and the vdW-DF2 functional. Au(111) and CuO(111) slabs were modeled, applying DFT+U (Ueff = 7 eV) for CuO. Electrochemical energetics were evaluated via the computational hydrogen electrode framework referenced to RHE, formulating alkaline steps with OH-. Surface Pourbaix analysis guided the construction of hydroxylated surface models to represent potential-dependent OH coverage.

Relative energy profiles indicate that on Au and hydroxylated Au, the aldehyde (C1) oxidation branch from adsorbed glucose is generally more favorable than C–C bond cleavage, consistent with a preference for C6-retaining products and suggesting additional stabilization of oxidation intermediates under OH-rich conditions. On CuO(111), the energetic landscape favors C–C bond cleavage already at the branching stage, aligning with predominant formation of fragmented products. Structural analysis shows metallic Au can stabilize deprotonated, ring-opened (diolate-like) motifs, whereas increased OH coverage promotes ring-closed (pyranose) configurations via hydrogen bonding and site blocking.

DFT identifies catalyst composition and potential-driven hydroxylation as key descriptors controlling glucose electrooxidation selectivity by reshaping adsorption motifs and the competition between aldehyde oxidation and C–C bond cleavage. These insights provide a mechanistic basis for rationally tuning product distributions through catalyst choice and control of OH coverage.

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2026 / SEOUL, KOREA

CET0410

Performance Evaluation of Cation-Exchanged Zeolites for CO_2/CH_4 Separation

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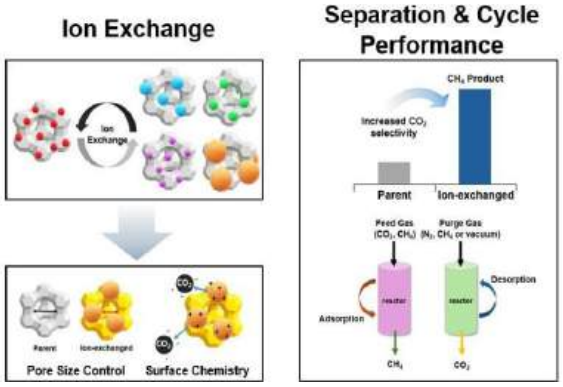
Keywords: Ion-exchanged zeolite; CO_2/CH_4 Separation; Vacuum pressure swing adsorption (VPSA)

The technology for efficiently separating CO_2 and CH_4 from natural gas and biogas is crucial for achieving energy sustainability and climate goals. Zeolite-based adsorption processes are well-recognized as promising technologies due to their high stability and structural tunability. However, to enhance separation efficiency, it is necessary to simultaneously optimize physical pore size and chemical surface properties. This study aimed to confirm the enhancement of CO_2/CH_4 separation performance by controlling the pore structure and surface charge density (acid sites) through cation exchange in zeolites, utilizing both electrostatic interactions and kinetic mechanisms between the zeolite framework and CO_2 molecules.

Cation-exchanged zeolites were synthesized using a conventional ion-exchange method. Typically, 10g of the base zeolite was dispersed in a 1.0 M metal-nitrate aqueous solution and stirred at 80°C for 6h. To ensure maximum exchange capacity, the process was repeated four times by replacing it with a fresh solution. The ion-exchanged zeolites were washed with deionized water, dried in an oven for 12h, and calcined at 500°C for 5h. The physicochemical properties of synthesized samples were characterized using X-ray diffraction (XRD), X-ray fluorescence (XRF), X-ray photoelectron spectroscopy (XPS), temperature-programmed desorption (TPD), and N_2 and CO_2 specific surface area analysis (BET). Dynamic separation properties were investigated using vacuum pressure swing adsorption (VPSA), where CO_2 adsorption capacity, CO_2/CH_4 separation performance and cyclic stability were evaluated under various purge gas conditions.



As a result of study, it was identified that the effective pore size of the zeolite was precisely controlled according to the ionic radius of the introduced cations. Furthermore, characterization results revealed that changes in surface acid sites and electrostatic interactions following cation introduction were key factors determining CO_2 adsorption affinity. These changes in physicochemical properties effectively restricted CH_4 diffusion while maintaining CO_2 accessibility, resulting in differences in kinetic selectivity. In particular vacuum pressure swing was performed to confirm CO_2 adsorption capacity and CO_2/CH_4 separation performance. Cyclic experiments using various purge gases suggest that desorption efficiency and adsorbent regeneration are influenced by the type of purge gas.

Acknowledgments

This study wasconductedwith thesupportofthe Korea Institute of Energy Technology Evaluation and Planning (KETEP) asanew and renewable energy core technology development project funded by the Ministry of Trade, Industry and Energy in 2024. (No. 202400459131). This work was supported by the Korea Institute of Energy Technology Evaluation and Planning(KETEP) and the Ministry of Trade, Industry & Energy(MOTIE) of the Republic of Korea (RS- 2025-02422969).

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CET0429

Electro-Mechanical Piston Reactor to Drive Propane Chemistry

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: Electrification, Piston-reactor, Energy-storage, Clean-chemicals

Abstract Body.

Introduction.

This work investigates an electrically driven piston-reactor as a concept for converting intermittent renewable electrical energy into mechanical and subsequently chemical energy. The piston reactor operates similarly to a conventional engine and can be implemented as a compact, modular reactor for distributed and decentralized chemical production. Rapid compression generates short-duration temperature and pressure pulses on millisecond timescales, enabling chemical reactions to occur within this short operating window.

Methods.

Experimental studies were conducted using a propane/air mixture in a 25-cc spark-ignition piston reactor operated under fuel-rich conditions, with equivalent ratios ranging from 1.5 to 3.9. Propane was selected as the feedstock since it produces a wide range of chemically relevant products, including syngas and light olefins. The experiments aimed to determine ignition limits, operating windows, product distributions, and the effect of intake preheating. In parallel, a two-zone spark-ignition reactor model was developed, capturing the coupled thermodynamic and kinetic processes, including flame formation and propagation. The model was validated against experimental data and was used to explore operating conditions that could not be accessed experimentally.

Results and discussion.

Propane conversion levels of up to 90% were observed experimentally at atmospheric intake pressure and temperature for equivalence ratios (around 1.5, while co-producing excess work. At higher intake temperatures of approximately 500 °C, propane conversions of around 80% were achieved at richer conditions ($\varphi \approx 1.93$), as shown in Figure 1. Most experiments produced a syngas-rich product stream, with small traces of light olefins such as ethylene and acetylene. In addition to mechanical work, the hot exhaust stream contained recoverable thermal energy. The model showed good agreement with experimental results, with mean square errors below 2×10^{-3}.In air-fed operation implemented experimentally, nitrogen acts as an inert diluent, limiting the maximum in-cylinder temperature. Parametric studies showed that replacing air with pure oxygen, while co-feeding CO_2 to control heat release, allows the heat released from propane oxidation to drive non-catalytic dry reforming

reactions, achieving over 50% conversion of CO_2 and more than 90% conversion of propane to syngas.

This approach is valuable for assessing the piston reactor, and the parametric studies performed with the validated model provide data to evaluate the technology at both economic and environmental levels. More broadly, the combined experimental–modeling framework enables rapid, model-guided screening of piston reactor operation for other fuels and the production of alternative chemical products, providing a fast and effective method to assess the broader potential of this technology.

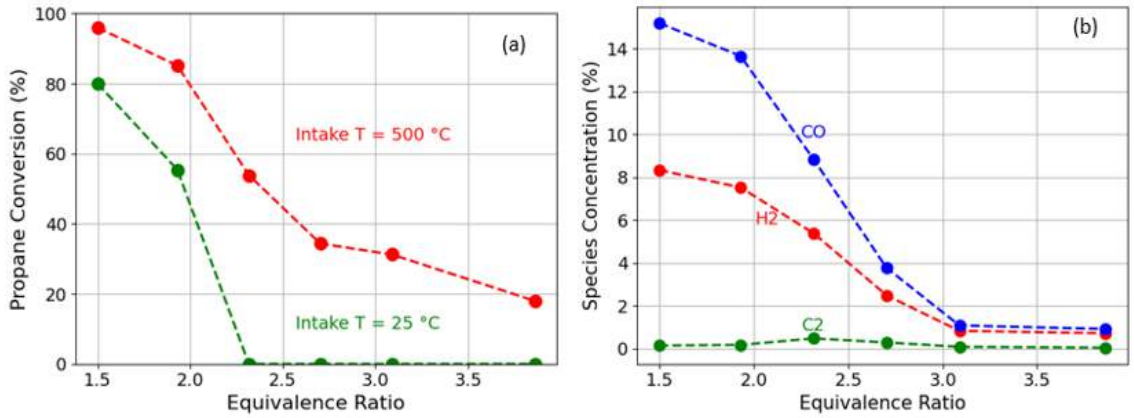

Figure 1: (a) Propane conversion as a function of equivalence ratio for intake temperatures of 25 °C and 500 °C (b) Exhaust gas mole fractions of H_2, CO, and C_2 species for an intake temperature of 500 °C. All cases were operated at an engine speed of 1300 rpm

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CET0438

Preliminary techno-economic Analysis (TEA) of cultivated meat using hazelnut press cake proteins

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: TEA; side streams; circular economy; cell agriculture; plant protein

Abstract Body.
Introduction. Cultivated meat is an edible product derived from cell engineering technologies, where cells are extracted from animal tissues and multiplied using culture media in laboratory settings. Specifically, cultivated cells are maintained with basal media supplemented with Fetal Bovine Serum (FBS). Media constitutes over 90% of current production costs, hampering commercial viability [1] with albumin is the most concentrated protein in FBS. To enable the scale-up of cultivated meat, cheap sources of proteins need to be identified (e.g., hazelnut press cake proteins). This study addresses the possibility of using a side-stream formulated cell culture medium for cultivated meat production as shown in Figure 1.
Methods. The TEA has been conducted using a performance modeling framework that is built around three components: cell growth model, bioreactor environment model and bioreactor system model [2]. With this approach, the cellular response can be applied to multiple potential microenvironments in the bioreactor while the overall operating mode and control dynamics of the bioreactor are captured computationally by the bioreactor system model. The software used for modelling is BioSTEAM.
Results. Three preliminary scenarios evaluated FBS replacement with hazelnut protein isolate (HPI, €3.50/kg from press cake, 1 mg/mL concentration): (1) partial replacement (5% FBS + HPI), (2) total replacement (0% FBS + HPI), (3) recombinant albumin benchmark (0.8 mg/mL). Media costs decreased by 30%, 52%, and 20% respectively. The results underlined several parameters as critical in the modelling for different species and optimized bioprocesses as dry cell measurements, dynamic growth modeling.

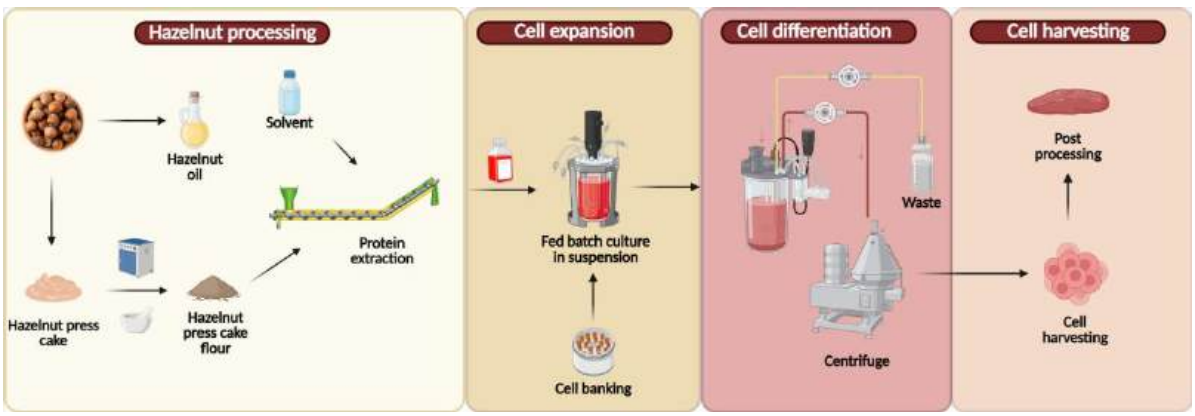

Figure 1. Simplified process diagram.

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CET0447

Anaerobic digestion of raccoon dog (Nyctereutes procyonoides) manure and co-digestion with rice straw

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: Raccoon dog manure, Anaerobic digestion, Methane production, Energy potential

Abstract Body.

Purpose: With the improvement of living standards, the market demand for fur products has been growing rapidly. As a high-quality fur raw material, raccoon dog skin has high market recognition. Currently, China has become the world's largest country in raccoon breeding, with a breeding scale of 24 million per year. While raccoon dog manure (RM), as a source of bioenergy, has not been effectively utilized. Most of the RM is only simple composted into organic fertilizer, failing to fully explore its energy potential. This not only results in resource waste but also has become a prominent problem restricting industrial and regional development. Thus, it is urgent to find an efficient and reasonable treatment method. Anaerobic digestion (AD), a key process of anaerobic catabolism, is a series of complex biochemical reactions driven by microorganisms in which organic matter is transformed into methane and carbon dioxide through four stages: hydrolysis, acidogenesis, acetogenesis and methanogenesis. AD can not only promote the biochemical circulation, optimize energy structure, advance carbon emission reduction, and achieve sustainable economic and social development, but also is one of the most important means to treat organic wastes such as agricultural waste, food waste and livestock manure and so on. However, the feasibility of AD for RM and its methane production potential have not been reported so far.

Methods: In this study, the resource utilization of RM was carried out by AD. The composition and AD characteristics of RM were analyzed. The daily methane production and experimental methane production were monitored simultaneously. The cumulative methane production, theoretical methane production, biodegradability and synergistic effect index were calculated.

Results: The results showed that RM is a feasible substrate for AD, and the methane production potential was 309.2 m3/t. Then it was co-digested with rice straw to optimize the carbon-nitrogen ratio, and the methanogenic potential was increased to 355.6 m3/t, with the

synergistic effect index of 13.56%. If all RM is converted into methane by co-digestion, 8.56×107 m3 can be prepared each year, the total energy output reaches 5.10×108 MJ, 1.74×104 t of standard coal combustion is reduced, and the particulate matter emission is reduced by 5.60×109.

Conclusions: It can be seen that the treatment of RM by AD can not only produce clean energy, helping optimize the energy structure, but also contribute to achieving the goal of “carbon peak and carbon neutralization”, with remarkable economic, environmental and social benefits.

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CET0455

Co-pyrolysis Characteristics of Plastics and Biomass in a Bubbling Fluidized Bed

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: plastic waste, biomass, co-pyrolysis, fluidized bed, pyrolysis oil

Abstract Body.
Due to global population growth, the production and consumption of waste plastics have steadily increased, making recycling a critical challenge. Meanwhile, biomass is a carbon-neutral resource that can be utilized as a clean fuel through appropriate treatment. This study evaluated the potential for waste resource circulation by comparing the pyrolysis characteristics of plastics (PE and PP) and woody biomass under both single and co-pyrolysis conditions. Experiments were conducted in a lab-scale fluidized-bed reactor at 600, 700, and 800 ℃ under a nitrogen atmosphere with a superficial gas velocity to minimum fluidization velocity ratio (ug/umf) of 1.5. The produced gases were analyzed using NDIR and GC-FID, while the pyrolysis oils were characterized by GC–MS. Concentrations of H2, CO, CH4, CO2, and C2–C3 hydrocarbons in the pyrolysis gas were quantified, and oil compositions were determined by integrating the mass spectrometric peak areas of individual compounds. Co-pyrolysis was carried out using a 1:1 mixture of PE and biomass, or PP and biomass. Biomass exhibited a maximum oil yield at 600 ℃, whereas PE predominantly produced wax rather than oil at the same temperature. Gas yield of biomass was up to 0.867 at 800℃, and gas yield of PE was up to 0.899 at 700℃. Biomass-derived oils consisted mainly of phenolic and ester compounds, with phenolic concentrations increasing as the temperature rose. This study demonstrates the potential of converting waste plastics and biomass into pyrolysis oils as a viable pathway for waste recycling and sustainable resource circulation.

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CET0462

Low-temperature NOx Reduction over Pd/ZSM-5 by H2: Effect of Catalyst Composition and Preparation Method

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: deNOx, Catalyst, Zeolite, Palladium, Hydrogen

Abstract Body.

NOx is a significant air pollutant, serving as a primary precursor to both photochemical smog and secondary particulate matter. Selective catalytic reduction of NOx with NH3 (NH3-SCR) is the most established technology for NOx control, but its catalytic activity is significantly limited at low temperatures, particularly during cold-start or start-up conditions. With the increasing utilization of H2-containing fuels, H2-assisted NOx reduction (H2-SCR) has emerged as a promising alternative due to its remarkable low-temperature performance. Nevertheless, this approach suffers from a narrow operating temperature window and the formation of byproducts (e.g. N2O).

Pd has been widely used as an active metal for H2-SCR. Metallic Pd species promote hydrogen spillover, thereby facilitating NOx reduction. Previous studies on Pd-based catalysts supported on conventional metal oxides have generally reported high NOx conversion at relatively high temperatures, whereas under low-temperature conditions (≤ 100 °C) these catalysts tend to exhibit limited NOx conversion. In contrast, ZSM-5, a microporous zeolite with Brønsted acid sites, stabilizes Pd species in a highly dispersed state and provides adsorption sites for NOx and reaction intermediates, thus enhancing the overall deNOx performance. Despite these advantages, a comprehensive understanding of how preparation methods and catalyst compositions synergistically influence the active species and the resulting performance remains limited.

In this study, a series of Pd/ZSM-5 were prepared by varying preparation method and catalysts composition. Pd/ZSM-5 prepared by incipient wetness impregnation (IWI) revealed slightly better performance compared to those by ion-exchange (IE). When the Pd loading was varied, the 1 wt.% Pd/ZSM-5 catalyst exhibited a pronounced operating temperature window, achieving around 90% NO conversion between 75 and 150 °C. In contrast, the 0.5 wt.% Pd/ZSM-5 catalyst reached 100% NO conversion at 100 °C and showed insufficient activity below this temperature. Further increasing Pd content to 2 wt.% led to decreased activity below 200 °C. In addition, variation of the ZSM-5 Si/Al ratio (SAR) significantly altered catalytic behaviors. Pd/ZSM-5 with SAR = 50 exhibited low NO conversion across

the entire temperature range, whereas higher-SAR catalysts (80 and 200-400) achieved high NO conversion only in a very narrow low-temperature range around 50 °C. To gain further insight, various characterizations were employed to probe Pd species and surface intermediates. By correlating these results with H2-SCR performance, we clarify the structural and surface factors responsible for the low-temperature activity of Pd/ZSM-5.

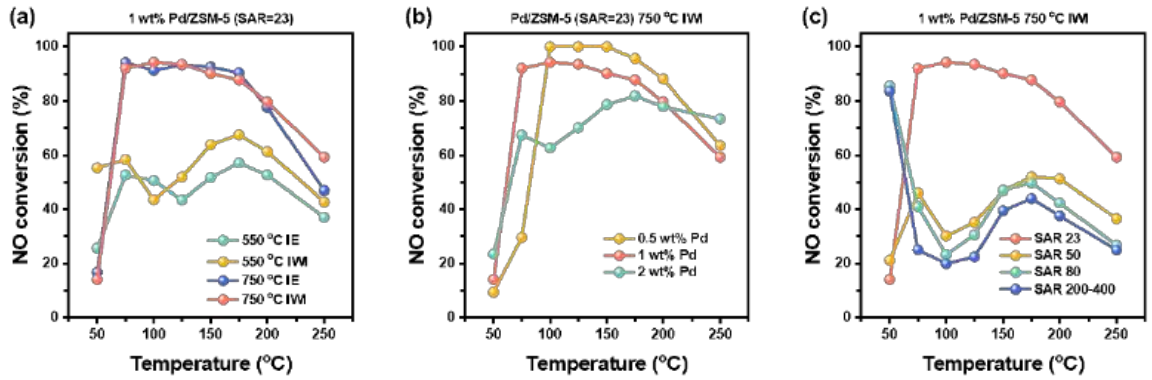

Figure 1. NO conversions of Pd/ZSM-5: (a) preparation method, (b) Pd loading, and (c) Si/Al ratio

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CET0463

NOx-N2O simultaneous reduction over desilicated Fe/Beta prepared by solid-state ion exchange

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: NO-N2O simultaneous reduction, NH3-SCR, Fe-zeolite

Abstract Body.
Introduction.
Simultaneous reduction of NOx and N2O in NH3-containing exhaust streams remains challenging due to the sensitivity of catalyst performance to preparation methods. Fe-exchanged Beta zeolites are active under NH3-SCR conditions, yet conventional aqueous ion exchange offers limited control over Fe distribution and generates wastewater. In this study, solid-state ion exchange (SSIE) combined with desilication was applied to Fe/Beta to examine how mesostructural modification influences catalyst properties and NOx–N2O reduction behavior.
Methods.
4+ to remove residual alkali species. Fe was introduced by ball-milling-based SSIE. Catalysts prepared with and without desilication were compared with Fe/Beta obtained by aqueous ion exchange. Textural properties were evaluated by N2 physisorption, while Fe-moieties were characterized using H2-TPR and UV–Vis spectroscopy. Catalytic performance was evaluated under NH3-SCR conditions by monitoring NO, N2O, NO_2, and NH_3 conversions.
Results and discussion.
Desilication increased the mesopore volume of Beta zeolite while preserving its framework structure. For SSIE-prepared Fe/Beta, H2-TPR profiles showed an additional reduction feature in the intermediate temperature range after desilication, reflecting altered reduction behavior of Fe species introduced by ball milling. UV–Vis spectra exhibited increase area of 200–300 nm and 300–500 nm regions, indicating a redistribution of Fe species rather than differences in total Fe content. In catalytic tests, N2O conversion over Fe/Beta increased from approximately 66% to 73% upon desilication, reaching a comparable performance to that of Fe/Beta prepared by aqueous ion exchange.
Conclusion
Desilication combined with solid-state ion exchange modifies the pore structure of Beta zeolite and affects the state of Fe species formed during ball milling. These changes are accompanied by a moderate increase in N2O conversion under NH3-SCR conditions, demonstrating that desilication provides a practical means to tune the performance of Fe/Beta catalysts for NOx– N2O simultaneous reduction.
Acknowledgement
This work was supported by Hydrogen & Low-Carbon R&D Lab, POSCO N.EX.T Hub,

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CET0464

Elucidation of Phase-Dependent Structure-Activity Relationships: Cu-Ag/ZrO2 Catalysts for Simultaneous NH3/CO Oxidation

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: Ammonia, Carbon monoxide, Catalytic oxidation, ZrO2, Cu-Ag

Abstract Body.
NH3 and CO are critical air pollutants that pose significant risks to human health and air quality. While NH3 is a key precursor to secondary particulate matter, it is increasingly emitted not only from conventional aftertreatment systems, such as NH3-SCR, but also from emerging NH3-fueled combustion processes. Meanwhile, CO, a toxic byproduct of incomplete combustion, remains a ubiquitous pollutant across various industrial and transportation sectors. Since the simultaneous emission of NH3 and CO has become a pressing technical challenge, developing highly efficient catalysts for their co-removal is crucial to comply with increasingly stringent emission regulations.

Among non-PGM catalysts, Cu/CeO2 has been widely used for NH3 or CO oxidation reactions. To further improve its performance, Ag has been introduced to enhance NH3 oxidation activity, while Zr has been incorporated to improve the thermal stability of the ceria support. However, most studies have focused on Zr as a secondary additive to Ce-Zr composites, and attempts to utilize ZrO2 as a single-component support for the Cu-Ag system remain rarely investigated. Although ZrO2-based catalysts are reported to exhibit higher N2 selectivity compared to CeO2 despite slightly lower activity, their potential has not been fully realized in simultaneous NH3 and CO removal over Cu-Ag catalysts. Notably, ZrO2 allows for diverse phase control depending on the synthetic conditions, enabling the modulation of metal–support interactions and thereby optimizing catalytic pathways for simultaneous NH3/CO oxidation.

In this study, Cu and Ag were supported on both commercial ZrO2 [Cu-Ag/ZrO2 (com)] and precipitation-derived counterpart [Cu-Ag/ZrO2 (p)] to evaluate NH3 and CO conversions. Cu-Ag/ZrO2 (com) reached 100% NH3 conversion at 300 oC, whereas Cu-Ag/ZrO2 (p) achieved complete conversion at a much lower temperature (200 oC) with high N2 selectivity. A similar trend was observed for CO oxidation over both catalysts. This performance gap suggests that the synthesis-dependent physicochemical properties of ZrO2 play a crucial role in enhancing low-temperature activity. To further elucidate the origin of this enhancement, we compare the NH3/CO oxidation activity of Cu-Ag supported on various phase-controlled ZrO2 (cubic, monoclinic, and tetragonal). Advanced

characterization techniques are employed to identify how ZrO2 phase differences modify surface active sites and metal–support interactions. Finally, these insights are correlated with simultaneous NH3/CO oxidation performance and N2 selectivity.

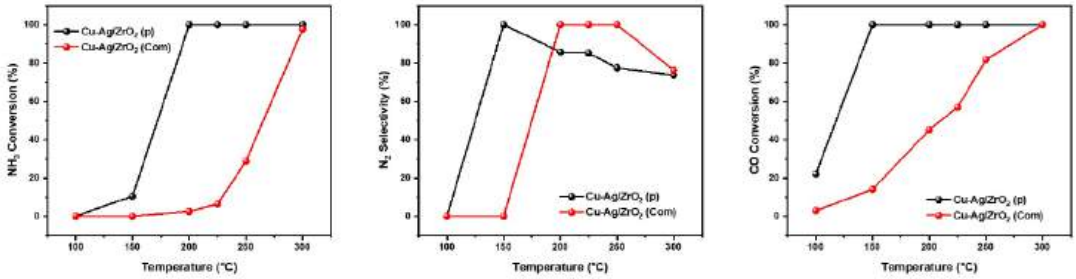

Figure 1. (a) NH3 conversion, (b) N2 selectivity and (c) CO conversion of Cu-Ag/ZrO2 catalysts.

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CET0513

Low-Carbon Portland Cement Produced from Industrial Carbide Slag with Reduced CO2 Emissions

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: carbide slag; Portland clinker; low-carbon cement; hydration heat; life-cycle assessment; CO2 reduction

Abstract Body.
This study evaluates carbonaceous slag (CS) as a total limestone substitute for low-carbon Portland clinker production. At a fixed modulus (KH/SM/IM = 0.91/2.50/1.50), increasing calcination temperatures (1300–1400 °C) transition the clinker from dolomite-rich to C3S-dominant phases, maintaining free CaO below 1% even at 100% CS replacement. The resulting cements demonstrate 28-day strengths up to 47.72 MPa, albeit with delayed hydration and lower heat release. Notably, life cycle assessment indicates a 45.6% reduction in CO2 emissions, confirming CS as a viable raw material for sustainable, large-scale waste valorization in the cement industry.

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CET0522

Bimetallic Pd-Ag Sorbents for High Temperature Mercury Removal from Syngas

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Keywords: Core–shell structure, bimetallic sorbents, Elemental mercury (Hg^0) removal, In- situ DRIFTS, XPS

Introduction

Elemental mercury (Hg^0) in syngas presents serious environmental and operational challenges for integrated gasification and chemical production. Most commercial sorbents are effective only at low temperatures (<120 °C), necessitating cool down and reheating, leading to reduced process thermal efficiency. Thus, there is a need to develop sorbents which can adsorb Hg^0 at high temperatures (>200 °C), thereby obviating the need to cool syngas in an integrated gasification and chemical production plant.

Methods

Core-shell bimetallic Pd–Ag sorbents with varying metal loadings were synthesized on a SIRAL-40 support using galvanic displacement [1]. These were benchmarked against monometallic Pd/SIRAL-40 and Ag/SIRAL-40 sorbents prepared by the incipient wetness impregnation method. Structural, morphological, and textural properties were characterized using XRD, HR-TEM, ICP-MS, and BET. Mercury removal performance was evaluated in a fixed-bed reactor at 270 °C. XPS and in-situ DRIFTS were employed to elucidate mercury adsorption mechanisms and to investigate the influence of individual syngas components (CO, CO_2, and H_2).

Results

The Hg^0 removal performance with various sorbents is shown in Figure 1a. The optimized bimetallic Pd-Ag/SIRAL-40 sorbent (Pd-Ag1) exhibits superior Hg^0 removal performance, maintaining >95% efficiency for over 27 hours at 270 °C. In contrast, the efficiency dropped below 95% in less than 8 hours over monometallic Pd/SIRAL-40. Moreover, Ag/SIRAL-40 shows negligible Hg^0 adsorption. XPS analysis reveals the coexistence of Pd^0 and Pd^{2+} species in the fresh sorbent, with the Pd^{2+} fraction remaining nearly constant after Hg exposure, identifying metallic Pd^0 as the primary active phase. The appearance of Hg 4f peaks at higher binding energies and new low-binding-energy Pd 3d features in the used sorbent provides direct evidence for electron transfer from Hg to Pd and the formation of Pd–Ag–Hg amalgam species. Experiments in the presence of various syngas components show that CO_2 has a negligible impact on Hg^0 capture, whereas CO and H_2 cause reversible inhibition (Figure 1b) due to competitive adsorption on Pd sites, as confirmed by DRIFTS analysis. Variations in the Pd:Ag ratio strongly influence sorption performance, underscoring the importance of surface composition and architecture. These results will be discussed in the full paper.

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CET0535

Design of Waste-Derived Supports for Ni–CeO_x Catalysts toward Enhanced CO_2 Utilization

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: Catalyst; CO2 Utilization; C1 Molecules; Heterogeneous Reaction; Hydrogen; LCA; Waste to Wealth;

Abstract Body.

Detailed abstract is attached. Below is the short abstract.

Large volumes of industrial and agricultural solid wastes present significant opportunities for valorization into value-added materials. The use of waste-derived materials as catalyst supports offers a sustainable and cost-effective alternative to conventional catalysts while simultaneously addressing waste management challenges. In parallel, carbon dioxide (CO_2) capture and utilization has emerged as a critical global priority for mitigating greenhouse gas emissions. This work investigates the conversion of waste materials such as fly ash, coconut shell–derived activated carbon, and slag into catalytically active supports, followed by the incorporation of Ni–CeO_x as active sites for CO_2 utilization reactions aimed at producing value-added chemicals.

Catalysts were synthesized via a facile route involving pretreatment of waste-derived supports and incipient wetness impregnation, followed by calcination and oxygen plasma activation to enhance surface properties. Fresh, reduced, and spent catalysts were comprehensively characterized using XRD, BET, XPS, XRF, HRTEM, TPR, TPD, TGA, DSC, and chemisorption techniques. Catalytic performance was evaluated in a packed-bed reactor equipped with online gas chromatography over a range of temperatures and weight hourly space velocities at atmospheric pressure, and stability tests were conducted under optimized conditions.

Among the catalysts studied, Ni–CeO_x supported on fly ash exhibited superior performance, achieving approximately 80% CO_2 conversion at 300 °C with methane selectivity exceeding 95%, along with stable operation for 24 h without significant deactivation. Structure–activity correlations revealed that the higher density of surface basic sites and the dynamic nature of the fly ash support enhanced metal–support interactions and CO_2 adsorption. Oxygen plasma treatment primarily influenced surface defect formation, as evidenced by XPS analysis. The catalytic activity followed the order: Ni–Ce/Slag < Ni–Ce/Activated Carbon < Ni–Ce/Fly Ash. Kinetic analysis enabled estimation of activation energy for the best-performing catalyst. Furthermore, life cycle assessment using ASPEN Plus simulations indicated reduced carbon emissions for the waste-supported catalytic route compared to conventional processes.

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Optimization of VPSA Process for H2 and CO2 Separation from Biomass-Derived Syngas Using CFD Simulation

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: Bio-oil; Computational Fluidization Dynamics; Gasification; Hydrogen; Vacuum Pressure Swing Adsorption.

Abstract Body.
Introduction. The amount of waste forest biomass in South Korea has steadily increased, yet much remains unutilized due to high collection costs. To address this, a "decentralized-pyrolysis and centralized-gasification" system has been proposed to convert low-value biomass into energy-dense bio-oil and subsequently into syngas. While this bio-oil gasification process effectively recovers energy, the resulting syngas contains a mixture of hydrogen, carbon monoxide, and carbon dioxide, necessitating an efficient separation process to support the hydrogen economy. This study aims to optimize a Vacuum Pressure Swing Adsorption (VPSA) process using Computational Fluid Dynamics (CFD) to separate high-purity hydrogen and recover carbon dioxide from biomass-originated syngas by analyzing the detailed dynamic adsorption behaviors within the column.
Methods. The feed gas composition for the simulation was derived from experimental bio-oil gasification conducted at 800°C with an oxygen equivalence ratio of 0.2, which exhibited the highest hydrogen yield of approximately 24%. The gas composition was normalized to a binary mixture of H2 and CO2. A 3D CFD model representing a lab-scale single-column was developed and validated against experimental data. To simulate the transport phenomena in the porous adsorbent bed, the model solved the conservation equations of mass, momentum, and energy coupled with species transport equations. The Extended Langmuir Isotherm model was employed to describe the competitive adsorption equilibrium between H2 and CO2, while accounting for the heat of adsorption generated during the process. The simulation investigated the effects of key operating parameters, including adsorption pressure, temperature, and cycle time, to determine the optimal operating conditions.
Results and discussion. Based on the normalized binary composition, the CFD analysis characterized the internal flow dynamics and the adsorption behavior of H2 and CO2 within the column. The separation characteristics of H2 and CO2 were compared under varying pressure swing cycles, and optimal operating conditions for selective separation of H2 and CO2 were determined. The results indicated that the pressurization and desorption steps influenced the thermal stability of the bed and the desorption efficiency of H2 and CO2.
These findings suggest that integrating a transportable pyrolysis system with centralized gasification is a technically feasible method for utilizing waste forest biomass. By applying advanced CFD simulations to elucidate the complex internal dynamics, this study provides a robust framework for optimizing downstream hydrogen recovery, contributing to the realization of a carbon-neutral hydrogen economy.

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Role of Ionomer Overlayers and Membrane–Ionomer Matching on PEMFC Performance under Variable Humidity

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: PEM fuel cells; ionomer overlayer; Aquivion®; relative humidity; proton transport; water management

Abstract Body.
Introduction. Water management and interfacial proton transport critically limit polymer electrolyte membrane fuel cell (PEMFC) performance, particularly under reduced relative humidity (RH). Gas diffusion electrode (GDE)–based membrane–electrode assemblies (MEAs) enable scalable fabrication but often suffer from imperfect catalyst layer (CL)–membrane contact and local dehydration. Here, an ionomer overlayer strategy is employed to enhance interfacial continuity and hydration stability. The approach is systematically applied to Nafion®-based, hybrid Aquivion®/Nafion®, and fully Aquivion®-based MEAs to elucidate the role of ionomer chemistry and membrane–ionomer compatibility under variable humidity conditions.
Methods. MEAs were prepared via a GDE-based process. A Nafion®-based MEA without overlayer served as reference. In overlayer-based architectures, a thin ionomer film was spray-deposited onto the cathode CL prior to assembly. Five configurations were investigated: an all-Nafion® MEA; two hybrid systems using Aquivion® D79 or D98 as CL binders with Nafion® membrane/overlayer; and two fully Aquivion®-based MEAs combining Aquivion® D79 or D98 CLs with a matching Aquivion® D72 membrane and overlayer. Single-cell tests were conducted at 80 °C and 150 kPa(abs), with RH varied from 100% to 25%. Polarization curves and electrochemical impedance spectroscopy (EIS) under air and N_2 were used as in situ diagnostics to assess performance, interfacial resistance, and proton transport in the cathode CL, while ex situ FESEM analysis provided microstructural correlation.
Results and discussion. The ionomer overlayer significantly improves MEA performance and humidity tolerance across all architectures. Under fully humidified conditions, hybrid Aquivion®/Nafion® MEAs match or exceed the performance of the all-Nafion® reference at high current densities, indicating effective mitigation of interfacial flooding. With decreasing RH, hybrid systems outperform Nafion®, benefiting from the higher ion-exchange capacity and water retention of Aquivion® ionomers. The strongest enhancement is observed for fully Aquivion®-based MEAs, which maintain high performance down to 25% RH. EIS reveals lower ohmic resistance, reduced cathodic charge-transfer resistance, and markedly lower protonic resistivity within the cathode CL for MEA with overlayer compared to Nafion®-based MEA without overlayer. Chemical matching between SSC ionomers and SSC membranes minimizes hydration mismatch and preserves continuous proton-conduction pathways under

dry operation. Overall, the results highlight a clear synergy between ionomer overlayer and membrane–ionomer compatibility, identifying fully Aquivion®-based architectures as particularly promising for low-RH PEMFC operation.

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Elucidating the mechanism of NOx adsorption and reduction on dual-functional Ag/MgO/Al2O3

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: Passive NOx Adsorber; Non-PGM; Cold Start Emissions; in-situ DRIFTS

Abstract Body.
Introduction. Non-PGM passive NOx adsorbers such as Ag/MgO-Al2O3 have been shown to be promising for reducing cold-start NOx emissions [1]. However, the effect of feed speciation on the NOx storage mechanism and the evolution of surface species remains insufficiently resolved. Accordingly, this study uses in-situ DRIFTS to elucidate NOx adsorption-desorption mechanisms and their correlation to bench-scale reactor studies.

Methods. Catalysts were prepared by incipient-wetness impregnation of AgNO3 onto MgO(5)/γ-Al2O3 support (PURAL MG 5, Sasol), followed by drying and calcination. DRIFTS was performed using undiluted pre-treated catalyst powders at a total flowrate of 50 sccm. NOx adsorption was performed at 115 °C, followed by N2 purge and N2-TPD (115 to 500 °C, 10 °C min^{-1}). Feed consists of 1000 ppm NO, 1000 ppm NO + 3% O2, 1000 ppm NO + 3% O2 + 1000 ppm H2, 3% CO2, and 3% CO2 + 1000 ppm NO to probe NOx uptake behavior and competitive effects.

Results and discussion. The formation of nitrite/nitrate surface species on Ag/MgO-Al2O3 and MgO(5)/γ-Al2O3 was observed during in-situ DRIFTS, with bands assigned to monodentate, bidentate, and bridging nitrates as well as linear nitrites. Ag/MgO-Al2O3 shows a higher peak intensity at 1555 cm-1 compared to the support (Figure 1 (a)). This denotes enhanced NOx storage in the presence of Ag, which supports the spill-over mechanism for NOx storage. Under the flow of NO + O2 + H2, monodentate (1513-1518 and 1555 cm-1), bidentate (1314 cm-1), and bridging nitrates (1613 and 1628 cm-1) were significantly enhanced while the intensity of nitrites (1474 cm-1) decreased, supporting H2-driven nitrate enrichment (Figure 1 (a)). This explains the measured positive role of H2 in promoting NOx storage. CO2 adsorbed as bicarbonates (1658, 1433, and 1228 cm-1) and carbonates (1516, 1531, and 1560 cm-1) and delayed NO adsorption, consistent with competitive site occupation by CO2-derived species (Figure 1 (b)).

Conclusions. Ag/MgO/Al2O3 shows a high low-temperature NOx storage, evidenced from in-situ DRIFTS by the formation of adsorbed nitrite/nitrate species. Moreover, H2 promotes NOx uptake by favoring nitrate formation, while CO2 competitively occupies sites as carbonate/bicarbonate species and inhibits NOx adsorption. The influence of reductants on the stability of stored NOx species will be discussed in the full paper.

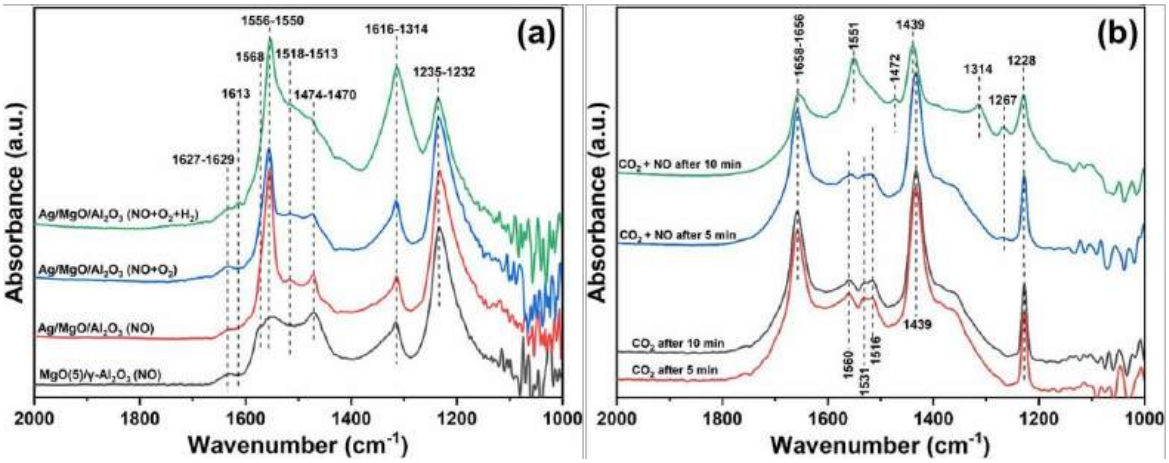

Figure 1. In-situ DRIFTS spectra over the support and catalyst for different feed gases.

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Development of Zeolite Membranes and Cu-ZnO-Al2O3 Catalyst for an Integrated Membrane Reactor for CO2 Hydrogenation to Methanol

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: CO2 hydrogenation; Methanol synthesis; Zeolite membrane; Cu-ZnO-Al2O3 catalysts

Abstract Body.
Introduction: Hydrogenation of CO2 to methanol is a promising pathway for carbon utilization and sustainable fuel production. Water creation, however, limit the reaction equilibrium, reduces the production of methanol, corrodes the catalyst and reduces its life and performance. The membrane reactor technology combining the CO2 hydrogenation catalyst and water selective membrane can solve this problem and can provide higher methanol yield and CO2 conversion due to Le-Chatelier's principle. The current work focuses on synthesis of water selective membrane and catalysts for CO2 hydrogenation. Finally, both catalysts and membranes are placed in the same unit and the performance of membrane reactor is optimized targeting higher methanol yield.
Methods: Zeolite membranes, such as silicate, zeolite A Type, Zeolite 3A and ZSM-5 were prepared by hydrothermal secondary growth on the porous alumina substrates. Permeation tests were used to assess the membrane performance, with a particular emphasis on H2O selectivity over the H2 and CO2.
The Co-precipitation method was used to prepare the Cu based catalysts. The total metal loading was varied from 10-70 weight percent. Catalytic activity for the CO2 hydrogenation was initially investigated in the fixed under the regulated operating conditions following calcination and reduction [2]
Results and discussion: Initially, the synthesized membrane performance was tested in a specially designed membrane separator. It is found that the zeolite structure has a significant impact on the membrane performance. Zeolite A and Zeolite 3A membrane demonstrated significant H2O selectivity and high water permeance, demonstrating their feasibility for the dehydration under the methanol synthesis conditions. ZSM-5 membranes, on the other hand, showed the moderate separation performance determined whereas silicate membranes showed the decreased water transport because of their hydrophobic structure. Thereafter synthesized catalyst performances were tested in a packed bed reactor. It is found that the methanol production is greatly impacted by the Metal loading. The excessive metal loading resulted in the particle agglomeration and decreased activity; intermediate metal amounts improve the Cu dispersion and increased CO2 conversion [2]. Finally, both the membrane and catalysts are integrated in single unit called membrane reactor. The performance of the same is evaluated at different temperature, pressure, feed flowrate in terms of CO2 conversion, water permeability through membrane and methanol selectivity.

The detailed results will be presented in final submission.

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CET0734

Recovery of Electrolyte Solvents from Spent Commercial EV Lithium-Ion Batteries Using Mild Vacuum Distillation

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: Recycling, lithium-ion battery, electrolyte solvents, vacuum distillation.

Abstract Body.

Lithium-ion batteries (LIBs) are widely regarded as one of the most effective energy-storage devices because of their high energy density, high operating voltage, low self-discharge, and strong power performance. Their use has expanded rapidly, particularly in electric vehicles (EVs). Global EV production increased from just 0.01 million units in 2010 to 11.26 million units in 2020 and is expected to reach 21.5 million units by 2030. However, the relatively short service life of LIBs—typically only 3–5 years—has led to a steadily growing volume of end-of-life batteries. Although carbonate solvents account for approximately 85–90 wt.% of the electrolyte, they are largely neglected in conventional recycling processes, which mainly focus on recovering electrode materials and lithium salts. This neglect is mainly due to the flammability, toxicity, and leakage risks associated with these solvents.

In this study, a simple and cost-effective mild vacuum distillation process was developed to recover electrolyte solvents from spent commercial EV lithium-ion batteries. Deionized (DI) water was used not only to trap evaporated electrolyte solvents but also to convert hazardous degradation gases into easily collectable liquid byproducts. To avoid acid-induced corrosion of the thermocouple inside the reactor, calibration experiments were performed to estimate cell temperatures without direct thermocouple contact. The cells were heated at temperatures ranging from 60 to 140 °C for 7.5 h under a combination of atmospheric and reduced pressure conditions. When heated to 140 °C, the evaporated electrolyte solvents accounted for approximately 9 wt.% of the total cell mass, and about 80 wt.% of these vapors were successfully recovered as condensed liquids. GC–MS analysis showed that the condensed liquid consisted mainly of EMC (92.8 wt.%) and DEC (4.6 wt.%) in their original chemical forms, which are commonly used electrolyte solvents in commercial LIBs. Several ethylene carbonate (EC) degradation products—including 1,3-dioxolane, 2-hydroxyethyl carbonate, 2-(2-methoxyethoxy) ethyl methyl carbonate, and 1,2-diyl diethyl decarbonate-ethane—were also detected, indicating that EC was present as an electrolyte component in the cells. Ion chromatography revealed approximately 7000 ppm of fluoride ions formed through $LiPF_6$ decomposition, while ICP-OES analysis detected only trace amounts of cationic impurities. Overall, this work demonstrates that the proposed mild vacuum distillation approach is a practical and scalable method for recovering electrolyte solvents from spent commercial EV lithium-ion batteries, offering a cost-effective alternative to existing recycling technologies and supporting more sustainable battery recycling practices.

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NH3 production from integrated capture and hydrogenation of waste NOx emissions

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: Environmental catalysis, NOx abatement, green NH3, NOx storage-reduction

Abstract Body.
Introduction. NH3 is gaining momentum as energy vector, and it is likely to play a central role in the near future. However, its traditional production is energy intensive and relies on the consumption of natural gas: new processes based on the utilization of renewable H2 for the production of e-NH3 aim to decouple its production from fossil fuels. In this work, e-NH3 has been synthesized starting from H2 and waste NOx emissions (e.g., power plant flue gases), allowing the coupling of NH3 production with the abatement of a harmful compound.
Methods. Pt-Ba, Rh-Ba and Ru-Ba catalysts with equimolar PGM contents and 16% Ba, supported over γ-Al2O3 have been characterized and tested in isothermal transient conditions in the range 125 -350 °C by cycling an oxidizing adsorption atmosphere 500 ppm NO + 3% O2, optionally enriched with 1% CO2 or/and 2.5% H2O; 5 min) and a reducing atmosphere (4% H2, 5 min), spaced out by an inert purge (He; 5 min). Experiments have been performed using microreactors as well as a custom-made operando FT-IR cell to enable the collection of time- and space-resolved spectra, which enables the direct quantification of surface adsorbates along the axial coordinate of the catalytic bed.
Results and discussion. At high temperatures, N2 is the dominant reduction product for all investigated materials, whereas decreasing temperature leads to a progressive increase in NH3 selectivity. However, at low temperatures NOx storage is also kinetically limited by NO oxidation, resulting in a reduced amount of stored NOx and ultimately constraining the overall NH3 yield. These observations highlight the existence of an intrinsic trade-off between adsorption and reduction activities, which must be optimized depending on the operating conditions.
In the absence of CO2, Rh–Ba emerges as the most suitable catalyst, combining high NO_x uptake with favorable NH3 selectivity at low temperatures. In contrast, the presence of CO2 strongly suppresses NOx uptake over Rh- and Ru-based catalysts, due to their limited ability to oxidize NO at low temperature, while Pt–Ba remains largely unaffected. During the reduction phase, carbonyl species are formed on all catalysts; however, on Rh- and Ru-based materials these species are partially hydrogenated to methane, while on Pt–Ba no carbon-containing products are detected in the gas phase. Spatially resolved FT-IR measurements indicate that surface carbonyls persist under H2 and suppress N2 formation kinetics, thereby enhancing NH3 selectivity.

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KOH-modified Iron-impregnated Bamboo Biochar for the Adsorptive Removal of Doxycycline Hyclate

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Abstract Category: Clean Environmental Technologies - Clean Environmental Technologies

Keywords: bamboo biochar, adsorption, DOX removal

Abstract Body.

The presence of antibiotic residues in wastewater is a growing environmental concern due to their contribution to antimicrobial resistance and persistence in aquatic systems. Doxycycline hyclate (DOX), a widely used antibiotic, exhibits pH-dependent speciation with multiple charge states, leading to inconsistent removal efficiencies in conventional treatment processes. This study reports the development of a sustainable, alkali-modified iron-impregnated bamboo biochar (KFBC) with enhanced surface functionality for efficient DOX adsorption across a wide pH range.

KFBC was synthesized using bamboo sawdust as a renewable carbon precursor through pyrolysis, followed by chemical activation and iron impregnation. Material characterization was conducted using scanning electron microscopy with energy-dispersive spectroscopy (SEM-EDS), Fourier transform infrared spectroscopy (FTIR) and point of zero charge (pHpzc) analysis. Batch adsorption experiments were performed to evaluate the effects of solution pH, adsorbent dosage, and initial DOX concentration. Process optimization and modeling were carried out using a Box–Behnken experimental design, while adsorption kinetics and equilibrium behavior were analyzed using established kinetic and isotherm models.

SEM-EDS analysis confirmed successful iron incorporation and revealed a roughened surface morphology with reduced pore size, indicating increased adsorption site availability and well-dispersed iron species. FTIR spectra showed Fe–O–Fe stretching vibrations, confirming effective surface modification. Results showed that iron impregnation alone increased DOX removal from 51.25% to 54.28%, while KOH activation enhanced removal to 83.19% and adsorption capacity to 33.28 mg/g. The combined KFBC treatment achieved 94.38% removal with a capacity of 37.75 mg/g, highlighting the synergistic effect of surface morphology enhancement and Fe-functionalization. The pHpzc of KFBC was 7.44, indicating that electrostatic interactions between the biochar surface and pH-dependent DOX species strongly influence adsorption. The quadratic model predicted an optimal DOX removal of 97.51%, experimentally validated at 98.74% within a 95% confidence level. Adsorption kinetics followed a pseudo-second-order model (R^2 = 0.9996), while equilibrium data fit the Redlich–Peterson isotherm (R^2 = 0.9879), suggesting chemisorption on a heterogeneous surface with a maximum capacity of 95.02 mg/g.

The findings demonstrate that KFBC is an effective adsorbent for the removal of doxycycline from aqueous solution. The enhanced adsorption is attributed to the synergistic effects of KOH activation, which increases surface roughness and functional groups, and iron impregnation, which introduces additional active sites. Bamboo-derived biochar thus represents a sustainable material for advanced wastewater treatment, supporting clean environmental technologies.