

2025 TwΔChE
11.29-11.30

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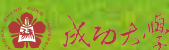
2025 TJK-ISCE

Taiwan-Japan-Korea
International Symposium
on Chemical Engineering

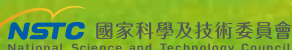
PROGRAM BOOK



Organizers



Co-Organizers



National Cheng Kung University

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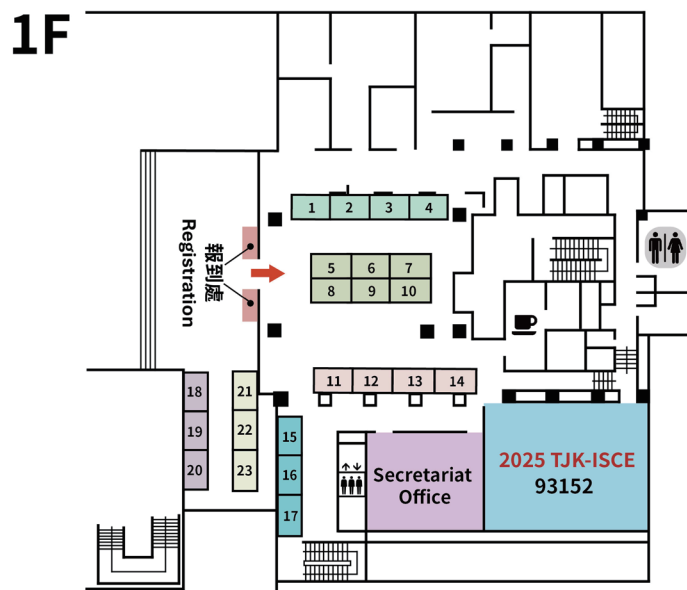
2025 TJK-ISCE

2025 Taiwan-Japan-Korea
International Symposium on
Chemical Engineering

MAP & FLOOR PLAN



- Dept. Chem Eng is located at Tzu-Chiang Campus of NCKU.
- 16 mins walk from The Rear Entrance/Exit of Tainan Railway Station to Dept. Chem Eng of NCKU.
- 15 mins walk from Shangri-La Far Eastern, Tainan to Dept. Chem Eng of NCKU.
- 10 mins walk from Academy Hotel to Dept. Chem Eng of NCKU.



PROGRAM AT A GLANCE

F1 TJK-ISCE I

11/30, 08:30-10:20

Room 93152 柏林講堂 Berlin Hall, 1F

Chair: Bing-Hung Chen (National Cheng Kung University, Taiwan)

Dun-Yen Kang (National Taiwan University, Taiwan)

Presentation Time	Speech Title and Author
08:30-08:50	Opening Ceremony & Group Photo
F1-1 08:50-09:20	[Keynote Speech] Equilibrium and Nonequilibrium Phenomena in Highly Concentrated Emulsions <u>Heng-Kwong Tsao</u> (National Central University, Taiwan)
F1-2 09:20-09:40	[Invited Speech] Influence of Deashing Processes on the Pore Structure of Rice Husk-Derived Activated Carbon <u>Jun'ichi Hayashi</u> , Haruka Yamamura, Isao Hasegawa (Kansai University, Japan)
F1-3 09:40-10:00	[Invited Speech] Na ⁺ -based Near-infrared Electrochromic Modulation from Plasmonic Tungsten Oxide Nanocrystals <u>Sungyeon Heo</u> (Seoul National University of Science and Technology, Korea)
F1-4 10:00-10:20	[Invited Speech] Defying the D ² -Law under Gravity: How Buoyancy and Flame Reshape Droplet Combustion <u>Hsien-Hung Wei</u> (National Cheng Kung University, Taiwan)

F2 TJK-ISCE II

11/30, 10:30-13:00

Room 93152 柏林講堂 Berlin Hall, 1F

Chair: Hsien-Hung Wei (National Cheng Kung University, Taiwan)

Inho Song (Chung-Ang University, Korea)

Presentation Time	Speech Title and Author
F2-1 10:30-11:00	[Keynote Speech] Ion Conducting Membranes via Graft Copolymer Self-Assembly Hyuk Jin Roh, Jin Hyuk Kim, So Youn Lee, <u>Jong Hak Kim</u> (Yonsei University, Korea)
F2-2 11:00-11:20	[Invited Speech] Introduction of Case Studies of Process Development for Efficiency and Energy Savings in the Production of Thermoplastic Resins <u>Ryuki Yasunari</u> , Naoki Deguchi, Kento Kanaya (Kaneka Corporation, Japan)
F2-3 11:20-11:40	[Invited Speech] All-Polymer Electrochromic Display <u>Inho Song</u> (Chung-Ang University, Korea), Jianguo Mei (Purdue University, USA)
F2-4 11:40-12:00	[Invited Speech] Separation of Trivalent Metal Ions via Supported Liquid Membrane with Strip Dispersion: Roles of Ion Hydration <u>Ngan Thi Tuyet Dang</u> (Hanoi University of Science and Technology, Vietnam), Hao-Po Tsai, Feng-Ting Weng, Da-Ming Wang (National Taiwan University, Taiwan)
12:00-13:00	Lunch & Research Collaboration / Industry-Academia Cooperation Kevin Wu (National Taiwan University, Taiwan) & Company

F3 TJK-ISCE III

11/30, 13:10-15:00

Room 93152 柏林講堂 Berlin Hall, 1F

Chair: Tsai-Wei Wu (National Cheng Kung University, Taiwan)

Naoto Ohmura (Kobe University, Japan)

Presentation Time	Speech Title and Author
F3-1 13:10-13:40	[Keynote Speech] Digitalization and AI for Dynamic Process Intensification <u>Hideyuki Matsumoto</u> (Institute of Science Tokyo, Japan)
F3-2 13:40-14:00	[Invited Speech] Digital Chemistry and Engineering of Nanoporous Materials <u>Yongchul G. Chung</u> (Pusan National University, Korea)
F3-3 14:00-14:20	[Invited Speech] Integrating Information Theory into Process Intensification for Complex Chemical Process Synthesis <u>Naoto Ohmura</u> (Kobe University, Japan), Takafumi Horie, Hayato Masuda (Osaka Metropolitan University, Japan)
F3-4 14:20-14:40	[Invited Speech] Process Synthesis of Membrane-Adsorption Hybrid CO ₂ Separation by using Machine Learning Model <u>Keigo Matsuda</u> , Yota Fujii (Nagoya University, Japan)
F3-5 14:40-15:00	[Invited Speech] Optimizing Inter-regional CO ₂ Capture, Transport, and Storage Networks in Taiwan: Cost, Leakage Risk, and Life Cycle Assessment Perspectives <u>Tsai-Wei Wu</u> (National Cheng Kung University, Taiwan)

F4 TJK-ISCE IV

11/30, 15:20-16:50

Room 93152 柏林講堂 Berlin Hall, 1F

Chair: Jui-Yuan Lee (National Cheng Kung University, Taiwan)

Hsiu-Po Kuo (National Taiwan University, Taiwan)

Presentation Time	Speech Title and Author
F4-1 15:20-15:40	[Invited Speech] Multiphase Process Simulations using CFD-DEM <u>Hsiu-Po Kuo</u> (National Taiwan University, Taiwan), An-Ni Huang (National Taiwan University of Science and Technology, Taiwan), Wan-Yi Hsu (Chang Gung University, Taiwan)
F4-2 15:40-16:00	[Invited Speech] Efforts to Accelerate Commercialization through CAE for Sustainable Manufacturing <u>Akiho Itomi</u> , Tomohide Ina, Shota Suzuki (Daicel Corporation, Japan)
F4-3 16:00-16:20	[Invited Speech] Theory-Driven Engineering of Metal–Nitrogen–Carbon Architectures Featuring Single and Dual Atom Sites for Enhanced Electrocatalytic Performance <u>Jeong Woo Han</u> (Seoul National University, Korea)
F4-4 16:20-16:40	[Invited Speech] The Use of Mixing Technology for Process Improvement Toward Energy Saving <u>Soontaree Intasaard</u> , Takaaki Yajima (Sumitomo Heavy Industries (Thailand) Ltd., Thailand), Katsuhide Takenaka (Sumitomo Heavy Industry, Japan)
16:40-16:50	Closing Ceremony



Keynote Speaker - F1-1

HENG-KWONG TSAO

Department of Chemical and Materials Engineering
National Central University
Taiwan

EQUILIBRIUM AND NONEQUILIBRIUM PHENOMENA IN HIGHLY CONCENTRATED EMULSIONS

An emulsion consists of one liquid (the dispersed phase) suspended in the other (the continuous phase). Familiar examples of emulsions include milk, butter, paints, and cosmetics. Highly concentrated emulsions also called high internal phase emulsions (HIPEs) possess a large volume of dispersed (internal) phase. As the volume fraction of the dispersed phase exceeds a critical value ($\Phi > \Phi_c \approx 0.65$), the liquid-like emulsion undergoes a transition to the solid-like state, in which droplets are deformed into polyhedra separated by thin films of continuous phase. This jamming transition associated with close-packing yields a number of peculiar and fascinating viscoelastic properties of soft materials, that benefit numerous applications such as cosmetic products, templates for porous materials, and scaffolds for tissue engineering. In this talk, the interesting solid-like behaviors of highly concentrated emulsions like Young's modulus will be introduced and the factors that influence the rheological behaviors of HIPEs like yield stress and mechanical moduli are discussed.

BIOGRAPHY

Professor Heng-Kwong Tsao holds the position of chair professor in the Department of Materials Science and Engineering at National Central University in Taiwan. His scholarly endeavors center around fundamental research in colloid and interface science, with a particular emphasis on investigating microscopic mechanisms. With a prolific academic record, Professor Tsao has authored close to 300 papers. His recent research is dedicated to the study of wetting phenomena and capillarity. Additionally, he plays a significant role in the academic community, serving as a senior editor for the American Chemical Society's prestigious journal "Langmuir" and holding the position of chief editor for the "Journal of the Taiwan Institute of Chemical Engineers."



Invited Speaker - F1-2

**JUN'ICHI
HAYASHI**

Department of Chemical, Energy and Environmental
Engineering
Kansai University
Japan

INFLUENCE OF DEASHING PROCESSES ON THE PORE STRUCTURE OF RICE HUSK-DERIVED ACTIVATED CARBON

Activated carbon is a widely used material in various industries such as chemicals, food, and pharmaceuticals. Additionally, the demand for activated carbon is expected to continue growing as environmental and energy issues gain increasing attention. Raw materials for activated carbon include wood chips, coconut shells, and coal. Recently, the demand for biomass has surged due to biomass power generation, leading to a shortage of raw materials such as wood chips and coconut shells for activated carbon. Therefore, finding new raw materials has become an urgent priority. Rice husks are one of the raw materials. However, rice husks contain a high ash content, which results in a significant amount of ash remaining in the activated carbon. This leads to a significant reduction in specific surface area, which is undesirable.

In this study, rice husk char produced at 600°C was boiled in a 1 mol/L sodium hydroxide solution to remove ash. The ash-free char was then activated with carbon dioxide to produce activated carbon. The pore structure of the char and activated carbon was characterized by measuring nitrogen adsorption isotherms at 77 K. The specific surface area and mesopore pore size distribution were determined using the BET method and the Dollimore-Heal method, respectively. The ash content of the 600°C-char was 42.9%, which decreased to 3.62% after ash removal. Figure 1 shows the influence of ash removal on the adsorption isotherms. Before removal, there was little increase in the amount adsorbed at relative pressures of 0.1 or higher, but after removal, the amount adsorbed increased significantly. This indicates the development of mesopores due to the removal of ash. Figure 2 shows the pore size distribution curve of mesopores. It can be seen that the removal of ash significantly increased the mesopore volume. After ash removal, 600°C char was activated with carbon dioxide at 900°C for 2 h, and the produced activated carbon had a specific surface area of 1,423 m²/g with well-developed mesopores.

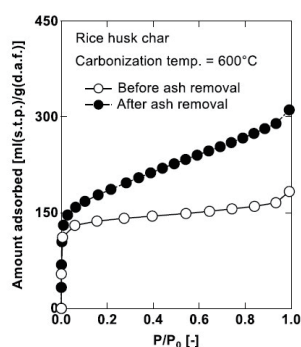


Fig.1 Influence of ash removal on the adsorption isotherms

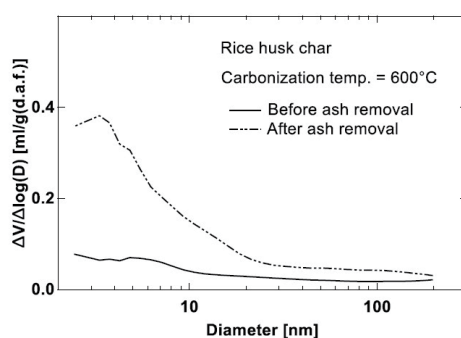


Fig.2 Influence of ash removal on the mesopore size distribution



Invited Speaker - F1-3

SUNGYEON HEO

Department of Chemical and Biomolecular
Engineering
Seoul National University of Science and Technology
Korea

Na⁺-BASED NEAR-INFRARED ELECTROCHROMIC MODULATION FROM PLASMONIC TUNGSTEN OXIDE NANOCRYSTALS

Next-generation electrochromic windows with near-infrared modulation will have a significant impact on energy savings in the building and transportation sectors. The advancement of these technologies can be achieved using plasmonic metal oxide nanocrystals, thanks to their uniquely tunable light absorption in the near-infrared range via localized surface plasmon resonance. However, despite the presence of shape and crystalline anisotropy in some plasmonic metal oxide nanocrystals, such as tungsten oxide, understanding their influence on electrochromic modulation and how to harness these properties remains limited.

In this talk, I will first present how shape and crystalline anisotropy in plasmonic tungsten oxide nanocrystals affect Na⁺-based electrochromic performance. Interplay of shape and crystalline anisotropy influences on the charge capacity and coloration efficiency both of which are major factors that determine the degree of electrochromic modulation. While hexagonal Cs⁺-doped tungsten oxide nanorods exhibit high coloration efficiency than that of platelet, their charge capacity is limited due to Cs⁺ dopants blocking Na⁺ insertion into the hexagonal tunnels. To address this issue, I will also discuss the importance of dopant engineering in hexagonal tungsten oxide nanocrystals to enhance Na⁺-based electrochromic modulation.



Invited Speaker - F1-4

HSIEN-HUNG WEI

Department of Chemical Engineering
National Cheng Kung University
Taiwan

DEFYING THE D^2 -LAW UNDER GRAVITY: HOW BUOYANCY AND FLAME RESHAPE DROPLET COMBUSTION

The D^2 -law is a widely employed model in droplet combustion, stating that the square of a droplet's diameter decreases linearly with time. While this law holds under idealized, diffusion-controlled conditions in stagnant environments, it breaks down in practical settings where gravity plays a significant role. In this talk, I demonstrate both experimentally and theoretically how flame-induced buoyant convection—a natural outcome of gravity—profoundly alters droplet combustion dynamics. Experimentally, the measured shrinkage exponents across a variety of liquid fuels are found to consistently fall within a narrow range of 2.6-2.7, indicating a pronounced positive departure from the D^2 -law. Theoretically, a new $D^{8/3}$ -law is derived to govern the droplet shrinking kinetics, well explaining the observed departures. Importantly, this new law is purely transport-determined, arising from the coupled effects of momentum, heat, and mass transfer driven by flame-induced buoyant convection. Further analysis reveals that the shift to this new law originates from the emergence of an inherent buoyancy length scale specific to each fuel-gas system. Owing to its invariance across fuel types and insensitivity to combustion chemistry and detailed reaction kinetics, the new $D^{8/3}$ -law serves as a robust tool for predicting, characterizing, and ultimately achieving active control of droplet burning in realistic gravitational environments. Its applicability also extends to blended fuel systems where disruptive puffing and micro-explosions are present, providing a universal paradigm for understanding and steering complex droplet combustion phenomena involving multiple coupled transport effects.



Keynote Speaker - F2-1

JONG HAK KIM

Department of Chemical and Biomolecular
Engineering (HoD)

Yonsei University

Korea

ION CONDUCTING MEMBRANES VIA GRAFT COPOLYMER SELF-ASSEMBLY

Ion-conducting membranes have become a cornerstone technology in the pursuit of carbon neutrality, offering sustainable energy solutions with high efficiency, zero emissions, and broad applicability in systems such as polymer electrolyte membrane fuel cells, anion exchange membrane water electrolyzers, lithium-ion batteries, and supercapacitors. A key requirement for these membranes is to achieve high ionic conductivity while maintaining excellent mechanical strength. Over the past decades, extensive research has been devoted to understanding and optimizing the transport properties of various polymer membranes to improve their performance in energy conversion and storage devices—including fuel cells, batteries, and water electrolyzers—as well as in separation technologies like electrodialysis, desalination, and industrial ion removal. However, a well-known trade-off between ionic conductivity and mechanical robustness continues to limit the practical application of ion-conducting membranes. In this talk, I will present our recent advances addressing this challenge through the following approaches: 1) Synthesis of SEBS-g-PSSA block-graft copolymers, derived from commercially available hydrocarbon triblock copolymers, to achieve balanced conductivity and elasticity. 2) Development of a rapid, energy-efficient fabrication process for anion-exchange membranes based on poly(arylene piperidinium) (PAP), in contrast to the conventional solution casting method that requires high-boiling aprotic solvents (e.g., DMSO), prolonged drying times, and high energy input. 3) Design of thermoplastic elastomeric graft copolymer "glue" electrolyte membranes, featuring nanoscale domain architectures, dual-ion transport pathways, and strong universal interfacial adhesion for advanced solid-state applications. These strategies offer promising pathways toward the scalable production of high-performance ion-conducting membranes for next-generation electrochemical systems.

BIOGRAPHY

Prof. Jong Hak Kim earned his Ph.D. in Chemical Engineering from Yonsei University in 2003. Following this, he conducted postdoctoral research at the Massachusetts Institute of Technology (MIT) before joining Yonsei University as a faculty member in 2005. His research primarily centers on the synthesis of polymers for gas separation membranes and polymer electrolyte membranes. He has published over 410 papers, including works in *Nat. Comm.*, *Energy Environ. Sci.*, *Adv. Mater.*, and *Angew. Chem.*, with an H-index of 69.

Invited Speaker - F2-2

Kaneka, Japan



Presenter

**RYUKI
YASUNARI**



**MASAHIRO
TSUJINAKA**

INTRODUCTION OF CASE STUDIES OF PROCESS DEVELOPMENT FOR EFFICIENCY AND ENERGY SAVINGS IN THE PRODUCTION OF THERMOPLASTIC RESINS

Polyester-based thermoplastic resins are crystalline materials that can be easily molded by melting with heat and allowing them to solidify upon cooling. These resins are known for their many useful properties, such as being lightweight, chemically resistant, and mechanically strong. They are used in a variety of applications, including packaging materials and industrial components.

Kaneka's thermoplastic resin is manufactured by spray drying a slurry of micrometer-sized particles dispersed in water. However, the spray drying process consumes a large amount of energy due to water evaporation, which is a cause for environmental concern. This manufacturing process also has several issues including poor handling in downstream processes and a risk of dust explosion due to the presence of fine particles smaller than 100 μ m in the manufactured dry powder.

In this study, we established a new resin manufacturing process consisting of dewater, drying, and compression granulation to solve the above issues.

In the dewatering process, the pH of the slurry is first adjusted to create microflocs. These microflocs are then dewatered using a filter press, and their moisture content is reduced further by air replacement [1]. This operation significantly reduces the energy required for drying. We were able to significantly reduce the risk of dust explosions by using a dryer that prevents dust from flying around during the drying process [2]. Furthermore, using the dry compaction pelletizer produces resin pellets with excellent handling properties without fine dust [3].

This process effectively reduces environmental impact while improving operability, and it is expected to contribute to a sustainable resin manufacturing process.

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- [2] Liu X, Jiang J. Mass and Heat Transfer in a Continuous Plate Dryer. *Drying Technology*. 2004, 1621-1635
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Invited Speaker - F2-3

**INHO
SONG**Department of Chemical Engineering and Material
ScienceChung-Ang University
Korea

ALL-POLYMER ELECTROCHROMIC DISPLAY

Electrochromic displays (ECDs) offer a promising alternative to emissive technologies, featuring low power consumption, superior outdoor readability, and reduced eye strain. However, conventional ECDs suffer from complex multi-layered architectures and limited flexibility due to the reliance on rigid, brittle transparent conductors such as indium tin oxide (ITO). Here, we report a flexible, fully polymer-based electrochromic display platform utilizing an n-doped poly(3,7-dihydrobenzo[1,2-b:4,5-b']difuran-2,6-dione) (n-PBDF) as a dual-function material that serves both as a transparent conductor and ion-storage layer.[1,2] The n-PBDF film exhibits high mixed ionic-electronic conductivity, minimal color change across electrochemical cycling, and excellent optical transparency across the visible spectrum, allowing it to replace multiple functional layers in conventional ECDs. Its solution processability and mechanical flexibility enable facile integration into passive-matrix, see-through, full-color displays on flexible substrates. Using in situ photolithographic patterning, we constructed 8×8 pixelated displays with four functional photopatterned layers: electrochromic polymers (ECPs), ion-conducting polymer electrolyte, and n-PBDF layers as both working and counter electrodes. The localized patterning of both ECPs and electrolyte layers effectively suppresses crosstalk, a common challenge in passive-matrix display architectures. These displays demonstrated high bistability, excellent electrochromic efficiency, and extremely low power consumption, making them highly suitable for applications with infrequent content updates. Moreover, the displays retained their electro-optical performance under repeated mechanical deformation and harsh environmental conditions, showcasing their robustness and practical viability. The flexible platform further enabled the realization of wearable, segmented, and full-color displays, including graphics on plastic bands and human skin. Our findings highlight the potential of n-PBDF as a next-generation capacitive transparent electrode that not only simplifies fabrication but also broadens the applicability of electrochromic displays to wearable, foldable, and transparent electronics. This work lays the groundwork for scalable manufacturing of energy-efficient, lightweight displays across emerging optoelectronic and electrochemical device platforms.

References

- [1] Zhifan Ke, Ashkan Abtahi, Jinhyo Hwang, Ke Chen, Jagrity Chaudhary, Inho Song, Kuluni Perera, Liyan You, Kyle N. Baustert, Kenneth R. Graham, Jianguo Mei J. Am. Chem. Soc. 2023, 145, 3706–3715.
- [2] Inho Song, Won-June Lee, Zhifan Ke, Liyan You, Ke Chen, Sumon Naskar, Palak Mehra, Jianguo Mei Nat. Electron. 2024, 7, 1158–1169.



Invited Speaker - F2-4

NGAN THI TUYET DANG

Department of Chemical Engineering
Hanoi University of Science and Technology
Vietnam

SEPARATION OF TRIVALENT METAL IONS VIA SUPPORTED LIQUID MEMBRANE WITH STRIP DISPERSION: ROLES OF ION HYDRATION

The selective removal of metal ions from impure mixtures is crucial in various chemical processes, including ore processing, radiochemistry, post-synthetic purification, environmental remediation, wastewater treatment, and the recovery of precious metals and rare earth elements from industrial and waste streams. Supported Liquid Membrane with Strip Dispersion (SLMSD) is an emerging technique for metal recovery from waste sources. Theoretically, simultaneous extraction and stripping through a hydrophobic membrane could greatly enhance separation efficiency and allow for high metal concentrations in the receiving phase.

This presentation will explore the mechanisms influencing the permeability of trivalent metal ions during SLMSD, especially the roles of ion hydration. It will also highlight the effects of the dissociation mechanisms of metal aqua ion complexes. In addition, we will report suitable operating conditions for efficient separation of various trivalent metal ions.



Keynote Speaker - F3-1

HIDEYUKI MATSUMOTO

Department of Chemical Science and Engineering
Institute of Science Tokyo
Japan

DIGITALIZATION AND AI FOR DYNAMIC PROCESS INTENSIFICATION

Dynamic Process Intensification (DPI) is a model-based approach to chemical process design that improves efficiency by intentionally introducing dynamic changes instead of relying solely on steady-state operation. Chemical processes based on the DPI technologies are cyclic distillation, cyclic adsorption, simulated moving bed chromatography, and oscillatory baffled reactors (OBRs). Design of the intensified dynamic process requires simultaneous consideration of equipment structure and unsteady operation, beginning with conceptual design, where goals, levers, and constraints are hypothesized. Based on these, a dynamic model stack is developed.

This keynote presents the development and application of dynamic models using conceptual design of OBRs as an example. OBRs are advantageous for reactions requiring long residence times, avoiding impractically long conventional plug flow reactors. This DPI technology is also effective for multi-phase flows where precise control of mass and heat transfer is needed. Design parameters for OBRs include tube diameter, baffle spacing, and free baffle area. Performance is often evaluated using dimensionless numbers such as net flow Reynolds number, oscillatory Reynolds number, Strouhal number, and velocity ratio. In our prior work on the three-phase hydrogenation of 3-butyne-2-ol using a Pd/Al₂O₃ catalyst, OBRs outperformed packed bed reactors. At the same oscillatory Reynolds number, lower amplitude of oscillatory flow achieved higher conversion, suggesting that frequency and amplitude influence internal flow patterns and reaction behavior. This insight motivated the development of dynamic model stacks for distributed parameter systems to guide OBR structural design.

Efficient simulation of unsteady flows for the OBR design was pursued via a systems approach integrating reduced-order modeling (ROM) with machine learning [1]. ROM methods such as principal component analysis and proper orthogonal decomposition (POD) reduce the dimensionality of complex data. POD applied to flow pattern data from particle image velocimetry identified modes and time-varying mode coefficients useful for predicting flow patterns with neural networks. Fourier series expansion of time-varying mode coefficients improved reduced-order model formulation. While this black-box modeling approach showed promise, its reliance on purely data-driven methods limits generalizability across reactor conditions. Bridging machine learning with first-principles models based on idea of multiple model fidelities is proposed.

Finally, I discuss the challenges of digitalization and AI application in process design based on DPI technologies from the perspective of multiple model fidelities. Although computational fluid dynamics (CFD) can analyze unsteady flows, it demands high computational resources. To address this, lumped ODE models and 1D/2D PDE distributed models incorporating reaction kinetics and mass transfer are effective alternatives. Parameter estimation is essential for these models, especially under uncertainty, where Bayesian estimation methods can be applied.

BIOGRAPHY

Professor, Department of Chemical Science and Engineering, School of Materials and Chemical Technology, Institute of Science Tokyo

Cross Appointment Fellow, Renewable Energy Research Center, Department of Energy and Environment, National Institute of Advanced Industrial Science and Technology (AIST)

- 1996 Master of Engineering in Department of Chemical Engineering, Tokyo Institute of Technology
- 1999 Doctor of Engineering in Department of Chemical Engineering, Tokyo Institute of Technology
- 1999 Assistant Professor, Department of Chemical Engineering, Tokyo Institute of Technology
- 2010 Associate Professor, Department of Chemical Engineering, Tokyo Institute of Technology
- 2015 Principal Researcher (transferred), Renewable Energy Research Center, Department of Energy and Environment, AIST
- 2018 Associate Professor, Department of Chemical Science and Engineering, Tokyo Institute of Technology
- 2024 Professor, Department of Chemical Science and Engineering, Institute of Science Tokyo (Formerly Tokyo Institute of Technology)



Invited Speaker - F3-2

YONGCHUL G. CHUNG

Department of Chemical & Biomolecular Engineering
Pusan National University
Korea

DIGITAL CHEMISTRY AND ENGINEERING OF NANOPOROUS MATERIALS

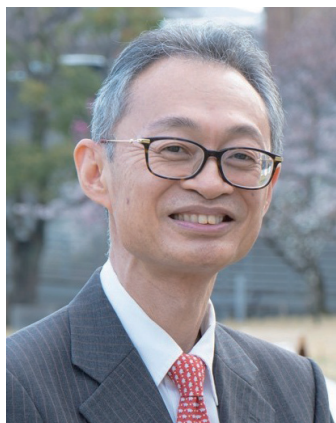
Digital Chemistry, an emerging frontier in chemical science, integrates computational methods, data science, and automation to accelerate chemical research and applications. By leveraging automated workflows and data-driven insights, this approach optimizes important industrial processes such as drug discovery, materials design, and chemical synthesis, bridging theoretical innovation with practical implementation.

Nanoporous materials, including zeolites, metal-organic frameworks (MOFs), and porous organic polymers (POPs), hold transformative potential for tackling global challenges related to energy and the environment, such as hydrogen storage, carbon capture, and water harvesting. However, the extensive chemical and structural diversity of these materials presents significant challenges in identifying optimal candidates for specific applications.

In this presentation, I will demonstrate how our research group employs a Digital Chemistry framework, integrated with chemical engineering processes, to streamline the discovery, characterization, and evaluation of nanoporous materials. First, I will highlight the impact of the Computation-Ready, Experimental (CoRE) MOF database, demonstrating how open-access datasets enabled accurate prediction of high-surface area MOFs and accelerated the identification of high-performing materials for hydrocarbon separations.

Next, I will present a crystal graph convolutional network (GCN) model that we developed which could rapidly estimates DFT-derived partial atomic charges and band gaps in MOFs. This method has been applied to the newly updated CoRE MOF database, enabling large-scale accurate computational screening for carbon capture scenarios.

Finally, I will discuss the importance of multi-scale modeling in the real-world performance of nanoporous materials, particularly in complex multi-component gas separations. By coupling macrostate probability distributions (MPD) obtained from transition matrix Monte Carlo (TMMC) simulation with process modeling, we enhance both the efficiency and accuracy of mixture predictions.



Invited Speaker - F3-3

NAOTO OHMURA

Department of Chemical Science and Engineering
Kobe University
Japan

INTEGRATING INFORMATION THEORY INTO PROCESS INTENSIFICATION FOR COMPLEX CHEMICAL PROCESS SYNTHESIS

Process intensification (PI) for sustainable production requires process design approaches that integrate flow, reaction, and separation phenomena as interconnected functional modules rather than isolated unit operations [1]. Designing new processes represented by such functional modules requires accurate transmission of information—such as concentration, structure, and temperature—between modules. However, uncertainties inherent in the process, along with external noise and fluctuations (disturbances), can leave ambiguity in the transmitted information. As a result, process designs often become redundant to tolerate errors, which limits the realization of ultra-compact processes with highly integrated functions. To address this challenge, we propose a methodology that quantifies noise and uncertainty in process information transfer via metrics such as entropy, coding, and quantization, combined with the nonlinear characteristics of process elements [2]. By exploring the interaction between noise and nonlinearity, we seek conditions where stochastic resonance and related effects enhance transport, mixing, and reaction performance beyond conventional design limits [3].

The study addresses two challenges:

1. Reaction control in imperfectly mixed fields: Lagrangian tracking and CFD of Taylor–Couette flows and oscillatory baffled reactors (OBRs) quantify information gain of fluid elements in spatially distributed fields (temperature, viscosity, density), revealing beneficial noise effects on transport [1,3].
2. Flow/reaction control in hysteretic processes: Laminar vortex flows are perturbed with periodic/apperiodic noise to induce nonlinear transport enhancement, with hysteresis quantified using fractal analysis [4].

Acknowledgment

This work was supported by JSPS KAKENHI Grant Number JP24H00396.

References

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Invited Speaker - F3-4

KEIGO MATSUDA

Department of Complex Systems Science, of
Informatics
Nagoya University
Japan

PROCESS SYNTHESIS OF MEMBRANE-ADSORPTION HYBRID CO₂ SEPARATION BY USING MACHINE LEARNING MODEL

Carbon dioxide capture and storage (CCS) technology has become important to reduce carbon dioxide emissions. Adsorption and membrane separation processes for CO₂ capture have gained attention as they are considered more energy efficient than gas absorption using amine. However, the capture efficiency of these processes is low and their application to CCS has not yet progressed¹⁾. While combining these two processes is one way to improve separation performance, research on the configuration of these combinations or multi-stage processes is still insufficient.

Membrane separation is operated in a steady state and adsorption separation is in an unsteady state, which makes the design a hybrid process complex²⁾. Recently, the use of machine learning for process design has been proposed³⁾. We have applied machine learning to the design of multi-stage CO₂ separation processes.

Models were developed for each adsorption and membrane process with variables such as operating pressures of compressors and vacuum pumps, CO₂ composition in the feed gas, and flow rates. This data was used to build statistical models with neural networks to perform multi-objective optimization. Adsorption and membrane separation processes were optimized and found that neither process could achieve the CCS requirements. Adsorption has a higher separation performance than membrane, but it also consumes more energy. Next, a two-step process was developed by combining statistical models of the adsorption and membrane processes.

In the multi-objective optimization performed for this process, it was shown that the combined membrane and adsorption process meets the CCS requirements and reduces the energy consumption of the compressor and vacuum pumps compared to the single-stage process. This research indicated the potential of using statistical models to synthesize multi-stage processes.

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Invited Speaker - F3-5

**TSAI-WEI
WU**

Department of Chemical Engineering
National Cheng Kung University
Taiwan

OPTIMIZING INTER-REGIONAL CO₂ CAPTURE, TRANSPORT, AND STORAGE NETWORKS IN TAIWAN: COST, LEAKAGE RISK, AND LIFE CYCLE ASSESSMENT PERSPECTIVES

The roadmap of achieving carbon neutrality in Taiwan demonstrates that we should have CO₂ reduction amount of 40 MT/yr from CO₂ capture, utilization and storage (CCUS) technology by 2050. Given the significant potential identified for CO₂ storage in both onshore and offshore saline aquifers around Taiwan, developing an optimized CO₂ capture, transport, and storage (CCTS) network is of critical interest. To understand how to cost-effectively achieve this goal, a network connecting the CO₂ emission large sources to the storage sites is discussed and optimized by using mixed-integer linear programming (MILP) in this study. Geological data were used for selection of suitable saline aquifers, both offshore and near-shore, as primary storage options. Large fossil fuel power plants in Taiwan are targeted, and the evolution of emission amount as energy structure changes according to Taiwanese government's roadmap up to 2050 will be also considered. Given Taiwan's high seismic activity, an essential part of this research is to include the estimation of appropriate monitoring systems to minimize leakage risks associated with geological storage. While site locations dominantly affect the cost, this study aims to also discuss the monitoring cost corresponding to the characteristics of different storage sites, reflecting the risk-related cost in seismic regions. Finally, a life cycle impact assessment (LCIA) is performed for the optimal scenarios to understand the consequences or alternative environmental impacts of implementing CCS technologies to address the excessive amount of CO₂ in the atmosphere.



Invited Speaker - F4-1

HSIU-PO KUO

Department of Chemical Engineering
National Taiwan University
Taiwan

MULTIPHASE PROCESS SIMULATIONS USING CFD-DEM

Most processes are multiscale and multiphase, and involve multiple physical quantities. Recent advances in computational power have enabled the application of Computational Fluid Dynamics (CFD) and Discrete Element Method (DEM) numerical simulation methods to analyse fluid and particle motion, respectively. By coupling CFD and DEM, most multiphase flow dynamics can be reasonably approached. Besides, CFD-DEM can further couple reaction kinetics, heat (and mass) transfer equations, and thermodynamics, comprehensive information such as power consumption, reaction rate distribution, product yield, and phase changes can be predicted satisfactory. In this talk, we will show our recent advances in designing several processes using CFD-DEM simulation technique. Also, we recently used Micron-scale Computed Tomography (μ -CT) to unveil the internal structure of the object. The comprehensive flow patterns, heat and mass transfer phenomena, as well as the intricate details of reaction behaviors inside a catalytic reactor are initially conducted by our CT-CFD-DEM method.

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Invited Speaker - F4-2

Daicel Chemicals, Japan



Presenter

**AKIHO
ITOMI**



**TOMOHide
INA**

EFFORTS TO ACCELERATE COMMERCIALIZATION THROUGH CAE FOR SUSTAINABLE MANUFACTURING

To realize a sustainable society, the manufacturing industry is increasingly required to reduce environmental impact and develop products more efficiently. In response to these demands, Computer Aided Engineering (CAE) plays a vital role in improving the accuracy of design and evaluation, as well as shortening development cycles. It contributes to the efficient use of resources and the reduction of energy consumption by reducing the number of prototypes and experiments, making it a key technology for lowering environmental impact. Due to its various benefits, CAE has been increasingly adopted across various industries, including chemical manufacturing.

Our company is a chemical manufacturer that handles a wide range of products, including organic solvents, polymers, films, and explosives. We have a wide range of processes, from the manufacture of raw materials to final product assembly. In various areas, we utilize CAE-based simulations to support product design, process optimization, quality improvement, and safety evaluations, thereby contributing to the resolution of various technical challenges.

The introduction of CAE at our company has led to a shift from conventional experiment-based development processes to simulation-driven evaluations. By applying it in the early stages of development, we aim to enhance the accuracy of evaluations and enable faster decision-making while minimizing rework. To promote its effective use, we are actively promoting internal awareness initiatives. In addition to establishing a foundation for simulation-based development, we are also working to improve engineers' skills and enhance the analysis environment to maximize the benefits of CAE. These efforts have contributed to accelerating commercialization by enabling faster problem-solving and reducing the number of experiments required. In this presentation, we will introduce use cases from our company to illustrate how CAE is being utilized to address technical challenges in manufacturing.

Invited Speaker - F4-3



JEONG WOO HAN

Department of Materials Science and Engineering
Seoul National University
Korea

THEORY-DRIVEN ENGINEERING OF METAL–NITROGEN–CARBON ARCHITECTURES FEATURING SINGLE AND DUAL ATOM SITES FOR ENHANCED ELECTROCATALYTIC PERFORMANCE

Atomically dispersed single and dual metal sites in metal–nitrogen–carbon (M–N–C) catalysts are crucial for driving redox reactions in CO₂ utilization and fuel cells. However, fine-tuning atomic coordination environments remains a key challenge, as it directly affects intermediate adsorption.

To address this, we developed a theory-guided design framework that tunes metal nuclearity and coordination geometry.¹ High-throughput DFT screening revealed coordination and orbital control as central strategies, identifying Fe, Co, and Ni single-atom sites as effective for CO₂ reduction.² Ni–N₄ activity was further boosted by mesoporous, graphitic carbon supports,³ while Cu–N₄C₈ sites in micropores reached 96% CO selectivity via orbital modulation.⁴

We expanded this approach to dual-atom systems, where Fe₂–N–C doubled CO₂RR turnover frequency,⁵ and FePd–N–C⁶ and FeCo–N–C⁷ achieved superior ORR activity compared to Pt/C.

These results highlight atomic coordination as a key design parameter and demonstrate a unified strategy—merging computation, synthesis, and machine learning—for accelerating catalyst development across clean energy technologies.

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2. J. W. Han*, Effective Screening Route for Highly Active and Selective Metal–Nitrogen-Doped Carbon Catalysts in CO₂ Electrochemical Reduction. *Small* 17, 2103705 (2021).

3. J. W. Han*, Rational Design of Nitrogen-Doped Porous Carbon Support on Single Atom Catalysts for Efficient CO₂ Electroreduction. *J. Mater. Chem. A* 13, 4861-4869 (2025).

4. J. W. Han*, Tailoring Local Structures of Atomically Dispersed Copper Sites for Highly Selective CO₂ Electroreduction. *Carbon Energy* 6, e419 (2024).

5. J. W. Han*, Precisely Constructing Orbital Coupling-Modulated Dual-Atom Fe Pair Sites for Synergistic CO₂ Electroreduction. *ACS Energy Lett.* 7, 640-649 (2022).

6. J. W. Han*, Synergistic Fe,Pd Diatomic Sites Anchored on Porous Nitrogen-Doped Carbon for Efficient Oxygen Reduction in the Entire pH Range. *J. Mater. Chem. A* 13 (2025) 21462-21471.

7. J. W. Han*, Reaction Pathway Shift Enabled by Atomic-Level Engineering of FeCo Dual-Atom Catalysts for Enhanced Oxygen Reduction Reaction. submitted (2025).

Invited Speaker - F4-4

Sumitomo Heavy Industry, Japan



Presenter

**SOONTAREE
INTASAARD**

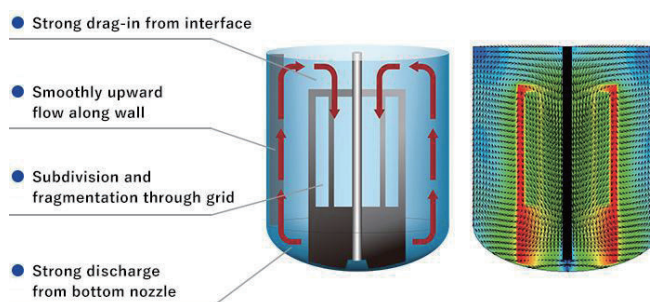


**KATSUhide
TAKENAKA**

THE USE OF MIXING TECHNOLOGY FOR PROCESS IMPROVEMENT TOWARD ENERGY SAVING

Since the latter half of the 1980s, Japanese petrochemical manufacturers have been focusing on the production of high-performance and high-value-added plastics. Sumitomo Heavy Industries Process Equipment as one of the leader companies in mixing business has developed the large blade impeller, MAXBLEND [1], and supported to the chemical manufacturers. By means of unique impeller shape, MAXBLEND can provide an ideal flow that cannot be realized with other conventional impellers. A variety of mixing purposes e.g. single-phase blending and multi-phase mixing, such as solid suspension, gas absorption/dispersion have been applied with our MAXBLEND and received great satisfaction from customers with over 2,000 units around the world.

In recent years, the direction of world chemical industries is toward the reduction of energy consumption. In addition to the modification from chemistry point of view, engineering design of the equipment is one of the keys to improve the production process. By selecting an appropriate design of agitator and internals, proper operation could be achieved resulting in the reduction not only agitation power, but also energy saving due to the depletion in removal/recovery process of waste and solvent. Likewise, challenge conditions in chemical process could be overcome by modification of conventional equipment with suitable design, uncovering the sustainable research and enhancing feasibility in scaling up to larger scale production. In this presentation, the comparison study of mixing performance between conventional type impeller and our SHI mixing technology "MAXBLEND" in all process types: liquid-liquid, solid-liquid, and gas-liquid mixing will be described emphasizing on the total energy reduction.



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FEMALE CHEMICAL ENGINEER AWARDEES



**HYUNJOO
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Prof. Hyunjoo Lee is a full professor in the Department of Chemical and Biomolecular Engineering and a director of Heterogeneous Atomic Catalysts Research Center, KAIST, South Korea. She received Ph.D. from Chemical Engineering, Caltech, USA (2005). Her research interest is to understand the fundamentals of heterogeneous catalysts and develop the catalyst for sustainable chemical industries. She published ~180 papers trying to elucidate how the surface of heterogeneous catalysts can be controlled to have better activity, selectivity, and durability. She had ~50 registered patents about fuel cell, water electrolyzers, CO₂ electrolyzers, and automobile exhaust treatment. She currently serves as an associate editor of JACS Au and has served as an editorial board member of various journals of ChemSusChem, Nano Letters, Molecular Catalysis, Catalysis Today, etc.



**MINA
OKOCHI**

Institute of Science Tokyo
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Mina Okochi received the Ph.D. degree in Technology, Tokyo University of Agriculture and Technology, Japan, in 1998. After conducting DC2 and PD research as a Research Fellow of the Japan Society for the Promotion of Science, she became an Assistant Professor in the Department of Biotechnology at Tokyo University of Agriculture and Technology; subsequently, she served as a Lecturer and then an Associate Professor in the Department of Biotechnology at Nagoya University, Japan. In 2014, she became a Professor at the Tokyo Institute of Technology, which is now the Institute of Science Tokyo. The lab focuses on biotechnology, including the design and biofunctionalization of functional peptides, as well as their applications in biosensing, medicine, and bioengineering. In addition, the group is focusing on cell-cell interactions mediated by extracellular vesicles such as migrasomes.

