INVITATION · PSE ASIA 2026

12TH ASIAN SYMPOSIUM ON

Process Systems Engineering

AI Applications and Carbon Neutrality on
Process Systems Engineering

AI / ML Data analytics	**CARBON NEUTRALITY** CCUS · LCA	**PROCESS SAFETY** Monitoring · Fault	**MULTIDISCIPLINARY** Pharma · Energy

DATE · VENUE

July 5 – 8, 2026

Engineering Building D, Yonsei University
Seoul, Republic of Korea

CONFERENCE MATERIALS

Program · Abstracts · Proceedings

Hosted by Yonsei University · Organized by KIChE
pseasia2026.org · pseasia2026@gmail.com

Conference Materials

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PART I

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Program Book

Overview · Schedule · Sessions · Speakers

3 Plenary · 6 Keynote · 119 Oral · 111 Poster — 239 contributions

PART II

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Abstract Book

Individual Abstracts of All Oral and Poster Presentations

238 abstracts collected (1 placeholder for TBA presentations)

PART III

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Proceedings

Full Papers — Peer-Reviewed Conference Proceedings

9 full papers — 5 from Student Oral sessions and 4 from Poster sessions

Table of Contents

PROGRAM BOOK OVERVIEW

Welcome to PSE ASIA 2026

AI APPLICATIONS AND CARBON NEUTRALITY ON PROCESS SYSTEMS ENGINEERING

On behalf of the Organizing Committee, we cordially welcome you to the **12th Asian Symposium on Process Systems Engineering (PSE ASIA 2026)**, held at Yonsei University in Seoul, Republic of Korea, from July 5 to July 8, 2026. Advancements in AI and carbon neutrality are revolutionizing process systems engineering. AI enhances efficiency and safety through predictive modeling, optimization, and real-time monitoring, contributing to reduced carbon emissions and increased energy efficiency. By combining AI with sustainable technologies, we aim for a safer, greener future.

This year's program features **3 plenary lectures** by world-leading authorities, **6 keynote lectures** opening each oral session, **119 oral presentations** across four parallel tracks, and **111 poster presentations** — totaling **239 contributions** from across Asia and beyond. The symposium concludes with an ISC member meeting, a Division meeting, and a cultural program offering participants an opportunity to experience Korea.

Symposium	12th Asian Symposium on Process Systems Engineering
Dates	July 5 (Sun) – 8 (Wed), 2026
Venue	Engineering Building D & Alen Building, Yonsei University
Address	50 Yonsei-ro, Seodaemun-gu, Seoul 03722, Republic of Korea
Language	English (official)
Format	In-person

Main Topics

Artificial Intelligence	Carbon Neutrality	Process Safety	Multidisciplinary
AI/ML for Data Analytics Process Optimization Emerging applications of AI	Sustainable Process Design Life Cycle Assessment CCUS	Predictive Maintenance Process Safety Management Monitoring & Fault Diagnosis	Pharma Manufacturing Process Integration Energy Transition PSE Education

Venue & Rooms

Room	Building	Used for
D404	Engineering Building D	Plenary (Mon/Tue), Track 1 (A1–D1)
D403	Engineering Building D	Track 2 (A2–D2)
D402	Engineering Building D	Track 3 (A3–D3)
D408	Engineering Building D	Track 4 (A4–D4)
Alen Building	Yonsei Campus	Plenary 2 (Mon evening) & Banquet

Invitation Letter

FROM THE CHAIR OF PSE ASIA 2026

Dear Esteemed Members of the PSE ASIA,

Advancements in **artificial intelligence** and **carbon neutrality** are revolutionizing process systems engineering. AI enhances efficiency and safety through predictive modeling, optimization, and real-time monitoring, contributing to reduced carbon emissions and increased energy efficiency.

By combining AI with sustainable technologies, we aim for a **safer, greener future**. The 12th Asian Symposium on Process Systems Engineering will bring together leading researchers and practitioners from across Asia and beyond to share the latest advances, foster collaboration, and shape the future of our field.

We encourage your active participation in this conference to share the latest research and collaborate. We look forward to welcoming you in Seoul this July.

Thank you for your continued support.

Il Moon
Chair, PSE ASIA 2026
Yonsei University

Organizing Committee

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H2
Decentralized
Low carbon
Hydrogen
Production

Decentralized Low-carbon Hydrogen Production ERC Center (KAIST)

Program at a Glance

FOUR-DAY SCHEDULE OVERVIEW

SUN · July 5	15:00 – 18:00 Registration (Engineering Building D, 1F)

MON · July 6 *Registration desk open 09:00–18:00 · Engineering Building D, 1F*

Time	D404	D403	D402	D408
09:00–10:00	**Plenary 1** **Christos Maravelias** **Princeton Univ. (D404)**			
10:00–12:00	Oral A1	Oral A2	Oral A3	Oral A4
12:00–13:30	Lunch			
13:30–14:30	Poster Session P1 (56 posters) Engineering Building D, 1F			
14:30–16:30	Oral B1	Oral B2 (13:30–16:30)	Oral B3	Oral B4
16:30–17:00	Break / Transfer to Alen Building			
17:00–18:00	**Plenary 2** **Chang Hwan Kim** **Hyundai Motors (Alen Bldg.)**			
18:00–	Banquet (Alen Building)			

** Oral B2 starts at 13:30 (concurrent with Poster Session P1).*

TUE · July 7 *Registration desk open 09:00–18:00 · Engineering Building D, 1F*

Time	D404	D403	D402	D408
09:00–10:00	**Plenary 3** **Hirokazu Sugiyama** **Univ. of Tokyo (D404)**			
10:00–12:00	Oral C1	Oral C2	Oral C3	Oral C4
12:00–13:30	Lunch & ISC Member Meeting			
13:30–14:30	Poster Session P2 (57 posters) Engineering Building D, 1F			
14:30–17:00	Oral D1	Oral D2	Oral D3	Oral D4
17:00–18:00	**Closing & Awards Ceremony**			

WED · July 8	09:00 – 12:00 Division Meeting 12:00 – 18:00 Cultural Program

Information for Presenters

PRESENTATION GUIDELINES

Thank you for presenting at PSE ASIA 2026. Please review the following information regarding your presentation. The official language of the conference is English.

01 PRESENTATION TIMES

Type	Total	Presentation	Q&A
Plenary Lecture (PL)	60 min	50 min	10 min
Keynote Lecture (K)	30 min	25 min	5 min
Regular Oral (OR)	20 min	15 min	5 min
Student Oral (OS)	15 min	12 min	3 min

02 ORAL PRESENTATIONS (PL / K / OR / OS)

Venue: Engineering Building D & Alen Building, Yonsei University (Seoul Campus)

- Please arrive at the presentation room **10–15 minutes before** your session starts.
- Bring your file on a **USB** (or portable storage) and copy it to the presentation laptop **during the break before your session**.
- To avoid font / formatting issues, **PDF format is recommended**.
- For PowerPoint, set the slide ratio to **16:9** for optimal projection.
- If your presentation includes **video clips**, please bring the original video files as well.

> The presentation order and number may be subject to change. In the event of any changes, the Secretariat will notify you accordingly.

03 POSTER PRESENTATIONS

Venue: Lobby, Engineering Building, Yonsei University (Seoul Campus)

Posting	Presentation & Q&A	Removal
Jul 6 (Mon) & Jul 7 (Tue) 09:00–16:30	Jul 6 (Mon) & Jul 7 (Tue) 13:30–14:30	After 16:30

- Poster size: **90 cm (W) × 120 cm (H)**, portrait orientation.
- **Do not print the presentation number on your poster** (numbers may be adjusted on-site).
- It is strongly recommended that the poster title remain **identical to the submitted abstract**.
- Attach your poster to the board matching your presentation number (**pins / tape provided on-site**).
- Presenters must **stand by their posters during the mandatory presentation time** (13:30–14:30) and answer questions.

- Posters left unattended during the mandatory time are **excluded from the Outstanding Poster Award**; winners are announced at the Closing & Awards Ceremony.
- Please **remove your poster after the session** (after 16:30).

04 REGISTRATION & CONTACT

- **Registration is mandatory for all presenters.** If you have not pre-registered, please complete online registration before the conference begins.
- Withdrawals: please notify the Secretariat at **pseasia2026@gmail.com** as soon as possible.
- Full schedule and updates are available in the Program Book or at **https://pseasia2026.org/**.

> On-site registration will NOT be operated at the front desk.

Plenary Lectures

THREE DISTINGUISHED SPEAKERS

PL-01 Christos Maravelias

Princeton University, USA

July 6 (Monday), 09:00–10:00 · Engineering Building D, D404

Chair: Inkyu Lee (Pusan National Univ.)

Title: *Systems Engineering for Industrial Decarbonization*

PL-02 Chang Hwan Kim

Hyundai Motors, Korea

July 6 (Monday), 17:00–18:00 · Alen Building

Chair: Inkyu Lee (Pusan National Univ.)

Title: *To be announced*

PL-03 Hirokazu Sugiyama

University of Tokyo, Japan

July 7 (Tuesday), 09:00–10:00 · Engineering Building D, D404

Chair: Inkyu Lee (Pusan National Univ.)

Title: *Making real-world impacts through modeling – a perspective from Pharma PSE research*

PL-01 · Plenary Speaker

CHRISTOS MARAVELIAS · PRINCETON UNIVERSITY

SPEAKER

Christos T. Maravelias

Chair of Chemical and Biological Engineering
Anderson Family Professor in Energy and the Environment
Princeton University, USA

SCHEDULE

July 6 (Monday), 09:00–10:00
Engineering Building D, D404

LECTURE TITLE

Systems Engineering for Industrial Decarbonization

ABSTRACT

We present a general optimization-based framework for designing chemical and energy systems that experience variability at multiple timescales. Motivated by the need to decarbonize manufacturing, we seek to understand the viability of chemical and energy systems subject to temporal variability in physical and economic conditions. In the first part of the talk, we discuss how systems thinking can enhance our understanding of novel strategies to produce renewable fuels and chemicals and, importantly, identify technological and economic drivers, thereby guiding future research efforts. In the second part of the talk, we outline the proposed framework which can be applied to determine the basic configuration and size of unit operations, associated material and energy flows, and relevant state variables. It is also possible to study optimal design between different cases and identify how optimal design evolves over time. We apply our framework to study green ammonia synthesis, and identify optimal process designs with distinct operational behavior at hourly, seasonal, and (multi-)yearly timescales. Finally, we discuss how the synthesis of systems based on electricity leads to new types of problems for which traditional approaches are insufficient, and outline progress towards the development of methods to address these challenges, including approaches that use AI techniques.

BIOGRAPHY

Christos Maravelias is the Chair of Chemical and Biological Engineering, and the Anderson Family Professor in Energy and the Environment at Princeton University. Before joining Princeton, he was the Vilas Distinguished Achievement Professor at the Department of Chemical and Biological Engineering at the University of Wisconsin–Madison, USA.

His research interests lie in the general area of process and energy systems engineering and optimization. Specifically, his group develops optimization and other computational methods to study production planning and scheduling, supply chain management, and energy systems synthesis and analysis with emphasis on renewable energy technologies. He has authored a research monograph on *Chemical Production Scheduling*. He is the recipient of numerous awards including the Computing in Chemical Engineering Award and the Sustainable Engineering Forum Research Award from AIChE, the Production and Operations Management Society Applied Research Challenge Award, and the Horizon Prize from the Royal Society of Chemistry.

Christos obtained his Diploma in Chemical Engineering at the National Technical University of Athens, an MSc in Operational Research from the London School of Economics (London, UK), and a PhD from Carnegie Mellon University.

PL-02 · Plenary Speaker

CHANG HWAN KIM

Photo
to be provided

SPEAKER

Chang Hwan Kim

Vice President
Hyundai Motors, Korea

SCHEDULE

July 6 (Monday), 17:00–18:00
Alen Building

LECTURE TITLE

To be announced

ABSTRACT

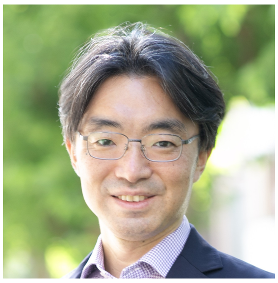
The abstract will be provided by the speaker prior to the symposium. Please refer to the official website (pseasia2026.org) for the most up-to-date information.

BIOGRAPHY

The biography of Chang Hwan Kim will be provided shortly. This page is reserved and will be updated in the final printed program.

PL-03 · Plenary Speaker

HIROKAZU SUGIYAMA · THE UNIVERSITY OF TOKYO



SPEAKER

Hirokazu Sugiyama

Full Professor & Department Head (FY2025/26)
Department of Chemical System Engineering
The University of Tokyo, Japan

SCHEDULE

July 7 (Tuesday), 09:00–10:00
Engineering Building D, D404

LECTURE TITLE

Making real-world impacts through modeling – a perspective from Pharma PSE research

ABSTRACT

Recent advances in Pharmaceutical Process Systems Engineering (Pharma PSE) at The University of Tokyo demonstrate the transformative role of model-based approaches in pharmaceutical process design and operation. This plenary lecture highlights key achievements across small molecules, biopharmaceuticals, and regenerative therapy products, emphasizing the critical role of hybrid modeling in addressing industrial challenges.

For small molecule manufacturing, our research focuses on the flow synthesis of drug substances. We proposed novel models for various reaction systems, such as the Grignard reaction, which have been successfully applied to determine design spaces and identify optimal operating conditions. In biopharmaceuticals, we investigated cell cultivation for model development, utilizing an automated bioreactor system to generate experimental datasets. This enabled the creation of a robust hybrid model capable of mapping the design space across a wide range of cultivation conditions for a new cell line. Furthermore, in stem cell and regenerative medicine, we developed models for 2D cell cultivation and cryopreservation, with model-based design spaces and optimal conditions being experimentally validated for real-world applications. Beyond these achievements, our lab conducts social-scale research, including an indicator-based assessment of potential supply risks for pharmaceutical excipients, which successfully identified critical compounds requiring mitigation. Together, these studies illustrate the efficacy of model-based process development and underscore the necessity of close collaborations between experimental and simulation researchers.

Finally, this talk addresses critical open discussions, such as balancing modeling costs against realized benefits as well as the cyclic interactions between reality and modeling. Through these themes, a forward-looking perspective will be provided on the evolving role of PSE in the pharmaceutical industry.

BIOGRAPHY

Hirokazu Sugiyama is a full professor in the Department of Chemical System Engineering at the University of Tokyo (UTokyo), where he serves as the department head for FY2025/26. He studied chemical engineering at UTokyo (BEng in 2001, MEng in 2003), and earned his PhD from ETH Zurich (2007). Subsequently, he joined Roche in Switzerland, holding various positions of increasing responsibility within biopharmaceutical manufacturing. His final position was Head of Prefilled Syringe Production. In 2013, he returned to UTokyo to begin his academic career as an associate professor, and was promoted to full professor in 2021.

Prof. Sugiyama's research focuses on design and operation support for pharmaceutical manufacturing processes using mechanistic, data-driven, and hybrid modeling approaches. His work spans multiple modalities including small molecules, biopharmaceuticals, and regenerative therapy products, and addresses multiscale challenges across molecular/cellular, process, and societal perspectives. His research is supported by several public grants (e.g., JSPS, AMED) as well as industrial funding.

To date, he has published 116 papers. His accomplishments include the Young Investigator Researcher Award from the Division of System, Information and Simulation in the Society of Chemical Engineers, Japan (2015), the Bioindustry Research Award from the Japan Bioindustry Association (2022), and the 2023 Class of Influential Researchers - Asia and Pacific by *Industrial & Engineering Chemistry Research*. He served as a board member of the Society of Chemical Engineers, Japan from 2022 to 2025 (acting as chief administrative director in 2024/25), and has been an editorial board member of *Computers & Chemical Engineering* since 2025.

Special Session

ERC-SPONSORED SPECIAL SESSION

ERC-sponsored special session

Process systems engineering for hydrogen energy and carbon neutrality

Monday, July 6, 2026 · 13:30 – 16:30 · Oral Session B2 (Engineering Building D, D403) · 6 presentations

ORGANIZERS

- **Professor Jae W. Lee** Korea Advanced Institute of Science and Technology (KAIST), Korea
- **Professor Seongmin Heo** Korea Advanced Institute of Science and Technology (KAIST), Korea

SPEAKERS

OR-B2-01	**Jae W. Lee**	Korea Advanced Institute of Science and Technology, Korea
OR-B2-02	**Seongmin Heo**	Korea Advanced Institute of Science and Technology, Korea
OR-B2-03	**Bor-Yih Yu**	National Taiwan University, Taiwan
OR-B2-04	**Jong Min Lee**	Seoul National University, Korea
OR-B2-05	**Ung Lee**	Korea Institute of Science and Technology, Korea
OR-B2-06	**Jinsu Kim**	Chonnam National University, Korea

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Oral Presentations

125 PRESENTATIONS · 16 SESSIONS · 4 PARALLEL TRACKS

Oral presentations are organized into **16 sessions across 4 parallel rooms**, held on Monday (A & B sessions) and Tuesday (C & D sessions). Sessions are color-coded by category: **Regular Oral** (with opening Keynote ●), **Special Session**, and **Student Oral**.

Regular Oral	Special Session	Student Oral	● Keynote
Sessions A1, A2, B1, C1, C2, D1	Session B2	Sessions A3, A4, B3, B4, C3, C4, D2, D3, D4	Opens each Regular Oral session

MONDAY, JULY 6 · Sessions A & B

Oral Session A1

REGULAR ORAL

Location: Engineering Building D, D404

Chair: Seongbin Ga (Ulsan Univ.)

K-A1-01 ● KEYNOTE	10:00~10:30	**Responsible AI for the Future of Process Systems Engineering: From Materials Discovery to Adaptive Operation** Hyeon Yang, **Jiyong Kim**[*] *School of Chemical Engineering, Sungkyunkwan University, Korea*
OR-A1-01	10:30~10:50	**Digital-Twin-Oriented Pedagogical Integration of BatchSep for Dynamic Modeling and Validation of EtOH/H_2O Batch Distillation** **Anawin Ampaipisut**, Chayut Chokkhanapitak, Vorravit Saelee, Phongsakon Bangsai, Yuthachai Srivaree, Aknarin Nonbudsri, Patcharapon Saranuttee, Atitaya Naknon, Sureeporn Kromthin, Phavanee Narataruksa, and Piyapong Hunpinyo[*] *Department of Chemical Engineering, King Mongkut's University of Technology North Bangkok, Thailand*
OR-A1-02	10:50~11:10	**Pathways to Decarbonization for a Garment Manufacturing Facility: LEAP Modeling & Optimization Analysis** Tin Nok Mak[1], **Charlle Sy**[2,*] [1] *The Hong Kong University of Science and Technology, Hong Kong* [2] *Cornell University, USA*
OR-A1-03	11:10~11:30	**Adaptive Model Predictive Control for Cyclic Distillation Columns** **Chengtian Cui**[1,2,*], Ali Moradvandi[1], and Anton A. Kiss[1] [1] *Department of Chemical Engineering, Delft University of Technology, Netherlands* [2] *Faculty of Science and Engineering, Åbo Akademi University, Finland*
OR-A1-04	11:30~11:50	**Adaptive Reinforcement Learning–Based Energy Management of Electrolyzer-Coupled District Heating Systems under Uncertainty** **Nikita Gupta**[1], Vahid Khaligh[1], Jay Liu[2,*] [1] *Institute of Cleaner Production Technology, Korea* [2] *Pukyong National University, Korea*
OR-A1-05	11:50~12:10	**Physics-Informed Machine Learning Approaches for Accelerating Chemical Process Development** **Seokyoung Hong**[1,2] and Jong Min Lee[2,*] [1] *School of Energy and Chemical Engineering, Ulsan National Institute of Science and Technology, Korea* [2] *Department of Chemical and Biological Engineering, Seoul National University, Korea*

Oral Session A2

REGULAR ORAL

Location: Engineering Building D, D403

Chair: Yeonsoo Kim (Kwangwoon Univ.)

K-A2-01 ● KEYNOTE	10:00~10:30	**Adaptive Machine Learning Models for Fault Detection and Control of Process Systems** Deepak Kumar[1], Amal Anto[1], Hariprasad Kodamana[1,2,3], and **Manojkumar Ramteke**[1,2,*] *[1]Department of Chemical Engineering, Indian Institute of Technology Delhi, India* *[2]Yardi School of Artificial Intelligence, Indian Institute of Technology Delhi, India* *[3]ANSK School of Information Technology, Indian Institute of Technology Delhi, India*
OR-A2-01	10:30~10:50	**Optimization for the design and operation of flexible Power-to-ammonia systems** **Li Zhou**[*], Xudong Zhou, Zhang Qingqing, Tian Qiu, Xu Ji *School of Chemical Engineering, Sichuan University, China*
OR-A2-02	10:50~11:10	**Evaluating Methanol Production Pathways from CO_2 and H_2O via High-Temperature Electrolysis Systems** Edward Egbert[1], Alif Syafiq Zaahir Zaidan Hartono[1], Matthew Putrafael Situmorang[1], **Riezqa Andika**[1,2,*] *[1]Process Systems Engineering Lab, Department of Chemical Engineering, Universitas Indonesia, Indonesia* *[2]Center of Excellence for Low Carbon Fuels, Universitas Indonesia, Indonesia*
OR-A2-03	11:10~11:30	**A process simulator of cryopreservation for human induced pluripotent stem cells** **Maimi Nakano**[1], Yusuke Hayashi[1,*], Yuki Uno[2,3], Masahiro Kino-oka[2,3], Hirokazu Sugiyama[1] *[1]Department of Chemical System Engineering, The University of Tokyo, Japan* *[2]Department of Biotechnology, The University of Osaka, Japan* *[3]Research Base for Cell Manufacturability, The University of Osaka, Japan*
OR-A2-04	11:30~11:50	**Superstructure-based Optimization for E-fuel Production using Solid Oxide Electrolysis Cells** **Meng Qi**[1,2,*], Zhengyang Song[2], and Haoshui Yu[2] *[1]College of Chemistry and Chemical Engineering, China University of Petroleum (East China), China* *[2]Department of Chemistry and Bioscience, Aalborg University, Denmark*
OR-A2-05	11:50~12:10	**Process development and demonstration for olefin production from steel mill gases** Myung Kyun Lim[1], Cheonwoo Jeong[2], Doowook Kim[3], Kosan Roh[4], Yong-Ki Park[1,*], **Kiwoong Kim**[1,*] *[1]Green Carbon Research Center, Korea Research Institute of Chemical Technology (KRICT), Republic of Korea* *[2]Industrial Gas Research Cell, Research Institute of Industrial Science & Technology (RIST), Republic of Korea* *[3]Hydrogen Research Department, Korea Institute of Energy Research, Republic of Korea* *[4]Department of Chemical Engineering and Applied Chemistry, Chungnam National University, Republic of Korea*

Oral Session A3

STUDENT ORAL

Location: Engineering Building D, D402

Chair: Sang Hwan Son (Pusan National Univ.)

OS-A3-01 10:00~10:15

Development of a Cost-Effective Green LH_2–NH_3 Hybrid Value Chain via LN_2 Circulation and a Heat-Integrated Power Cycle

Yejin Lee, and Inkyu Lee[*]

School of Chemical Engineering, Pusan National University, Korea

OS-A3-02 10:15~10:30

Targeting CO_2 emission in a Carbon Capture and Utilisation facility with epistemic uncertainty in the parameters

Abhishek Kumar Pandey[*], Santanu Bandyopadhyay

Department of Energy Science and Engineering, Indian Institute of Technology Bombay, India

OS-A3-03 10:30~10:45

Rigorous and Robust Equation-Oriented Phase Equilibrium Formulation via Phase Stability-Driven Characteristic Variables

Luoyu Zhang[1], Xijun Wang[1], Jun Zhao[1], Jianping Wang[2], Shaohui Tao[1,*], Li Xia[1], Lili Wang[1], Xiaoyan Sun[1,*], and Shuguang Xiang[1]

[1]*Qingdao University of Science and Technology, China*
[2]*Petro-Cyber Works Information Technology Co. Ltd, China*

OS-A3-04 10:45~11:00

Electrified Reheating of Circulating Sand for Biomass Fast Pyrolysis Toward Low-Carbon Marine Fuels

Aditia Aulia, Daejun Chang[*]

Department of Mechanical Engineering, Korea Advanced Institute of Science and Technology, Korea

OS-A3-05 11:00~11:15

Optimization of Methanol Synthesis from Blast Furnace Gas using Surrogate Model

Akihide Wakita[1], Sagar Saren[1], Tomoyuki Yajima[1], Kohei Yoshikawa[2], Yuta Nishikawa[2], Nobuyuki Shigaki[2], and Yoshiaki Kawajiri[1,3,*]

[1]*Department of Materials Process Engineering, Nagoya University, Japan*
[2]*Steel Research Laboratory, Japan*
[3]*School of Engineering Science, LUT University, Finland*

OS-A3-06 11:15~11:30

A computer-aided screening of cryoprotective agents for stem cells utilizing transfer learning

Akihiro Kimura[1], Rei Tamaki[1], Yusuke Hayashi[1,*], Yuki Uno[2], Masahiro Kino-oka[2], and Hirokazu Sugiyama[1]

[1]*Department of Chemical System Engineering, The University of Tokyo, Japan*
[2]*Department of Biotechnology, The University of Osaka, Japan*

OS-A3-07 11:30~11:45

Comparative Analysis of Karnopp and He-Based Valve Stiction Models Incorporating Valve Characteristic Transfer Functions for Temperature Control in Deferasirox Purification

Anuchit Wuttitrairat[1], Soottiwan Thamsakona, Wachira Daosud[2] ,Paisan Kittisupakorn[1,*]

[1]*Faculty of Engineering, Chulalongkorn University Bangkok, Thailand*
[2]*Department of Chemical Engineering, Burapha University, Thailand*

OS-A3-08 11:45~12:00

Multi-objective optimization of non-adiabatic reactor configurations for renewable diesel production from waste cooking oil

Bangkit Gotama[1,2], and Hao-Yeh Lee[1,*]

[1]*Department of Chemical Engineering, National Taiwan University and Science and Technology, Taiwan*
[2]*Department of Chemical Engineering, Institut Teknologi Kalimantan, Indonesia*

Oral Session A4

STUDENT ORAL

Location: Engineering Building D, D408

Chair: Donghwi Jeong (Ulsan Univ.)

OS-A4-01	10:00~10:15	**Multiscale Simulation and Mechanism Analysis of R23-R116 Separation by Ionic Liquid Extractive Distillation** **Kexin Yin**, Chun Deng[*] *College of Chemical Engineering and Environment, China University of Petroleum, China*
OS-A4-02	10:15~10:30	**Techno-Economic Analysis of Sustainable Aviation Fuel Production Process Incorporating Aromatics from Waste Plastic Pyrolysis** **Jeongheon Kim**, and Inkyu Lee[*] *School of Chemical Engineering, Pusan National University, Korea*
OS-A4-03	10:30~10:45	**Behavioral Modelling in Eco-Industrial Parks Using Game Theory and Personality Traits** **Leap Wun Yip**, and Jui-Yuan Lee[*] *Department of Chemical Engineering, National Cheng Kung University, Taiwan*
OS-A4-04	10:45~11:00	**MPEC-Based Dynamic Optimization of Packed Column Batch Distillation Startup** **Na Gyeong Lee** and Jong Woo Kim[*] *Department of Chemical Engineering, Incheon National University, Korea*
OS-A4-05	11:00~11:15	**A Generalized and Robust Initialization Framework for Complex Distillation Columns Using a Pseudo-Transient Hybrid Integration Strategy** **Yadi Gao**[1], Yiqing Luo[1,2,*], Shengkun Jia[1,2] , Xigang Yuan[1,2] [1] *School of Chemical Engineering and technology, Tianjin University, China* [2] *National Engineering Laboratory of Chemical Engineering and Low Carbon Technology (Tianjin University), China*
OS-A4-06	11:15~11:30	**Al-rich Beta Zeolite Acidity Tuning for Enhanced C4 Alkylation Selectivity via Cobalt Modification** **Ming Wen**, Yijie Ding, Minglei Yang[*], Yichun Li, Weizhong Zheng, Weizhen Sun[*], and Ling Zhao *School of Chemical Engineering, East China University of Science and Technology, China*
OS-A4-07	11:30~11:45	**Hydrogen Supply Chain Modeling and Optimization to Decarbonize Steel, Fertilizer, and Steel Sectors** Harsh Bajpai, **Nikhil Sharma**, Ishan Bajaj[*] *Department of Chemical Engineering, Indian Institute of Technology, India*
OS-A4-08	11:45~12:00	**Green mixed-solvent extractive distillation for ether-containing azeotropes: Mechanistic insights and energy-saving intensification** **Ning Sun**, Wenna Liu, and Peizhe Cui[*] *Qingdao University of Science and Technology, China*

Oral Session B1

REGULAR ORAL

Location: Engineering Building D, D404

Chair: Jui-Yuan Lee (National Taiwan Univ.)

K-B1-01
● KEYNOTE
14:30~15:00

Enumerating Full Potential of Process Integration using Graph-theoretic Approach

Bing Shen How[1,*], Ákos Orosz[2], Jean Pimentel[3], Ferenc Friedler[3]

[1] Research Centre for Sustainable Technologies, Faculty of Engineering, Computing and Science, Swinburne University of Technology, Malaysia
[2] Department of Computer Science and Systems Technology, University of Pannonia, Hungary
[3] Department of Systems Science, Széchenyi István University, Hungary

OR-B1-01
15:00~15:20

Techno-Economic and Life Cycle Assessment of Electrified Naphtha Cracking with Integrated Methane Valorization

Eprillia Intan Fitriasari[1], Hojae Kim[1], Dae Hoon Lee[2], Hohyun Song[2], Minho Jeong[2], Heesoo Lee[2], Jeongan Choi[2], You-Na Kim[2], Chanmi Jung[2], Donghyun Cho[2], Subin Choi[2,3], Tesfalem Aregawi Atsbha[1,4], J. Jay Liu[5], and Chul-Jin Lee[1,*]

[1] Department of Chemical Engineering, Chung-Ang University, Korea
[2] Korea Institute of Machinery and Materials (KIMM), Korea
[3] Department of Mechanical and Design Engineering, Hongik University, Korea
[4] Department of Chemical and Metallurgical Engineering, Aalto University, Finland
[5] Department of Chemical Engineering, Pukyong National University, Korea

OR-B1-02
15:20~15:40

Hybrid Absorption-Adsorption Separation Process using Porous Slurry for Light Hydrocarbon Recovery from Natural Gas

Chun Deng[*], Gao Ninghan, Ruihang Zhang, Kun Li, Bei Liu, Changyu Sun, and Guangjin Chen

College of Chemical Engineering and Environment, China University of Petroleum, China

OR-B1-03
15:40~16:00

INTHOP: A Second-Order Globally Convergent Method for Nonconvex Optimization

Krishan Kumar[1], Ashutosh Sharma[1], Gauransh Dingwani[2], Nikhil Gupta[1], Vaishnavi Gupta[1] and Ishan Bajaj[1,*]

[1] Department of Chemical Engineering, Indian Institute of Technology Kanpur, India
[2] Department of Chemical Engineering, Indian Institute of Technology Roorkee, India

OR-B1-04
16:00~16:20

Dynamic Life Cycle Assessment with AI and Digital Technologies: Standards-Aligned Pathways for Climate and Regulatory Compliance

Malik Sajawal Akhtar[1], Francesc Romero Gómez[2], Arka Pandit[3], Hira Mahmood[4], Muhammad Ansub Khan[4], Jay Liu[1,4,*]

[1] Institute of Cleaner Production Technology, Pukyong National University, Korea
[2] Cappi Sustainability B.V., Netherlands
[3] Dematic, USA
[4] Department of Chemical Engineering, Pukyong National University, Korea

OR-B1-05
16:20~16:40

Range-specific Sensitivity Analysis with Kolmogorov-Arnold Network

Hyein Jung[1], Suk Hoon Choi[1], Damdae Park[2], TaeUng Lee[3], Hyerim Kim[4], and Kyeongsu Kim[1,5,*]

[1] Clean Energy Research Center, Korea Institute of Science and Technology, Korea
[2] Chungnam National University, Korea
[3] Department of Mechanical Engineering, Korea University, Korea
[4] Heat Pump Research Center, Korea
[5] Division of Energy and Environment Technology, University of Science and Technology, Korea

Oral Session B2

SPECIAL SESSION

ERC-sponsored special session

Process systems engineering for hydrogen energy and carbon neutrality

Location: Engineering Building D, D403

Chair: Seongmin Heo (KAIST)

OR-B2-01	13:30~13:55	**Sustainable Hydrogen Production through Dry and Chemical Looping Reforming: Techno-Economic and Environmental Assessment** **Jae W. Lee**[*] *Department of Chemical and Biomolecular Engineering, Korea Advanced Institute of Science and Technology (KAIST), Korea*
OR-B2-02	13:55~14:20	**Integrated Design of Hydrogen–Electricity Supply Chains: System-Level Insights from Joint Planning Frameworks** **Seongmin Heo**[*] *Department of Chemical and Biomolecular Engineering, Korea Advanced Institute of Science and Technology (KAIST), Korea*
OR-B2-03	14:20~14:45	**Pathways to Net-Zero in Taiwan: Bridging Rigorous Process Modeling and Comprehensive Evaluation with Strategic Planning** **Bor-Yih Yu**[*] *Department of Chemical Engineering, National Taiwan University, Taiwan*
OR-B2-04	15:15~15:40	**Algorithmic Techno-Economic Optimization of CO_2 Liquefaction Processes for Low-Carbon CCUS Infrastructure** Sung Hyun Ju[1], Jisung Byun[1], Seokjin Yoon[1], Heesung Kim[2], Unpil Hwang[2], Minji Kim[2], Mina Kong[2], **Jong Min Lee**[1,*] *[1] Department of Chemical and Biological Engineering, Seoul National University, Korea* *[2] Samsung E&A; Co., Korea*
OR-B2-05	15:40~16:05	**Achieving Net-Negative CO_2 Emissions in Methanol Synthesis via High-Yield Reactive Capture and Conversion** Damdae Park, Margareth, Jaehyung Choi, Chun-Jae Yoo, Kyeongsu Kim, and **Ung Lee**[*] *Clean Energy Research Center, Korea Institute of Science and Technology (KIST), Korea*
OR-B2-06	16:05~16:30	**From Air to Fuel: Process Systems Engineering of Carbon and Water Capture for Scalable Negative Emissions** **Jinsu Kim** *Department of Petrochemical Materials, Chonnam National University, Korea*

Oral Session B3

STUDENT ORAL

Location: Engineering Building D, D402

Chair: Seongbin Ga (Ulsan Univ.)

OS-B3-01 14:30~14:45

Optimization of Reclamation Strategies for Managing MEA Degradation in Rate-Based CO_2 Capture Simulation

Yu-Sheng Chen and Bor-Yih Yu*

National Taiwan University

OS-B3-02 14:45~15:00

Rigorous Process Modeling of Lignin-to-SAF Production via Integrated Hydrothermal Liquefaction and Hydrodeoxygenation

Yi-Ming Chen and Bor-Yih Yu*

National Taiwan University, Taiwan

OS-B3-03 15:00~15:15

Real-time Prediction of M2 Monomer Concentration in Organosilicon Synthesis using Near-Infrared Spectroscopy and Enhanced Deep Learning

Chen Zhang, Zhongmei Li, Qinhao Sun, and Enbo Feng*

East China University of Science and Technology, China

OS-B3-04 15:15~15:30

Modeling of mesenchymal stem cell cultivation processesbased on metabolic flux analysis

Daiki Ikuta, Hiroki Kikukawa, Gaku Shimodaira, Yusuke Hayashi,Masaki Nishikawa and Hirokazu Sugiyama*

Department of Chemical System Engineering, The University of Tokyo, Japan

OS-B3-05 15:30~15:45

Literature-Driven Physical Model Building by Graph Neural Network with Context-Embedded Equation Nodes

Ding Yiyang, Shota Kato*, Manabu Kano

Department of Informatics, Kyoto University, Japan

OS-B3-06 15:45~16:00

Thermal Conductivity Evaluation of Thermal Interface Materials Using a Hybrid Particle Random Packing Algorithm

Dong-Gi Lee, Boram Gu*

School of Chemical Engineering, Chonnam National University, Korea

OS-B3-07 16:00~16:15

Superstructure-free multi-objective optimization of supercritical CO_2 power cycles: Extensive topology generation and tightened heat exchanger network synthesis

Donghyeon Kim, Chanmok Kim, Heehyun Choi, Hyeonseo Im, and Jiyong Kim*

School of Chemical Engineering, Sungkyunkwan University, Korea

OS-B3-08 16:15~16:30

Hydrogen network synthesis considering multi-stage separation system and compressor layout

Duankanghui Yang, Linlin Liu*

School of Chemical Engineering, Dalian University of Technology, China

OS-B3-09 16:30~16:45

Meta-Learning for Dementia-Related Disease Prediction with Limited Brain MRI Data

K. Fujii, K. Matsuda*

Nagoya University, Japan

OS-B3-10 16:45~17:00

Effects of a Third Component on CO_2 Absorption in Tetrabutylammonium Bromide-Based Deep Eutectic Solvents

Guilin Wen, Zhaoyou Zhu*

College of Chemical Engineering, Qingdao University of Science and Technology, China

Oral Session B4 STUDENT ORAL

Location: Engineering Building D, D408

Chair: Yeonsoo Kim (Kwangwoon Univ.)

OS-B4-01	14:30~14:45	**A Hybrid Modelling Framework: Integrating Machine learning Models for anaerobic digestion of rice straw** **Pragya Singh**, Asad Hasan Sahir* *Indian Institute of Technology Ropar, India*
OS-B4-02	14:45~15:00	**PINN-driven modeling and optimization of green ammonia reactors across wide operating regimes under intermittent renewable feedstocks** **Qingqing Zhang**, Jiaming Wang, Xudong Zhou, Li Zhou*, Xu Ji *School of Chemical Engineering, Sichuan University, China*
OS-B4-03	15:00~15:15	**Capacity Configuration of Power-to-Methanol Systems: A Bi-level Optimization Approach Based on Bayesian and Clustering Algorithms** Yi Wang[1], **Tian Qiu**[2], Miao Yang[1], Qingqing Zhang[2], Xu Ji[2], Li Zhou[2,*] *[1]China Petroleum Engineering & Construction Co. Ltd. southwest branch, China* *[2]School of Chemical Engineering, Sichuan University, China*
OS-B4-04	15:15~15:30	**Hybrid Auxiliary Heating Optimization for Solar Thermal Integration in Industrial Processes: A Screening Curve Approach** **Rohit K. Yadav**[1,2,*], Santanu Bandyopadhyay[1], Andrew Hoadley[2] and Roger Dargaville[2] *[1]Department of Energy Science and Engineering, Indian Institute of Technology Bombay, India* *[2]Department of Chemical and Biological Engineering, Monash University, Australia*
OS-B4-05	15:30~15:45	**Prospective Life Cycle Assessment of Succinic Acid Production from Cyanobacteria** **Roja K**, and Yogendra Shastri* *Department of Chemical Engineering, Indian Institute of Technology Bombay, India*
OS-B4-06	15:45~16:00	**Spatiotemporal Data Analysis for the Development of Physics-informed Machine Learning Models to Design Pre-Swelling Processes for Green Peptide Synthesis** **Rui Tsukui**, Thossaporn Wijakmatee, Hideyuki Matsumoto* *Department of Chemical Science and Engineering, Institute of Science Tokyo, Japan*
OS-B4-07	16:00~16:15	**Achieving Sustainable Ammonia by Multiple Hydrogen Production Technologies: From A Comparative Techno-Economic-Environmental Perspective** **Ruiyang Duan**[1], Lixia Kang[1,2,*], Le Wu[3], Yongzhong Liu[1,2] *[1]Department of Chemical Engineering, Xi'an Jiaotong University, China* *[2]University of Shaanxi Province, China* *[3]Department of Chemical Engineering, Northwest University, China*
OS-B4-08	16:15~16:30	**Comprehensive Analysis and Life Cycle Assessment of Combined Cycle Power Generation and Cogeneration Systems** **Ruru Ma**, Wenwu Xu, Lili Yang, Zhaoyou Zhu, Yinglong Wang, Peizhe Cui* *Qingdao University of Science and Technology, China*
OS-B4-09	16:30~16:45	**Integrated Modeling and Evaluation of a Green Dimethyl Ether–Based Energy Supply Chain** **S.-C. Lien**, C.-W. Ong, C.-C. Li, Z.-Q. Lin, and C.-L. Chen* *Department of Chemical Engineering, National Taiwan University, Taiwan*

OS-B4-10 16:45~17:00

Uncertainty Quantification and Reliability Evaluation Approaches for Multiscale Complex Systems

Yang Sun[1], Zhe Cui[1], Wei Wang[2], and Wende Tian[1,*]
[1]*College of Chemical Engineering, Qingdao University of Science & Technology, China*
[2]*Department of Mechanical Engineering, City University of Hong Kong, China*

TUESDAY, JULY 7 · Sessions C & D

Oral Session C1

REGULAR ORAL

Location: Engineering Building D, D404

Chair: Jia-Lin Kang (National Chung Cheng Univ.)

K-C1-01 ● **KEYNOTE**	10:00~10:30	**AI-Driven Design and Optimization for Complex Chemical Processes** Xiaodong Hong, **Zuwei Liao**[*] *State Key Laboratory of Chemical Engineering and Low-Carbon Technology, College of Chemical and Biological Engineering, Zhejiang University, China*
OR-C1-01	10:30~10:50	**AI Chemical Process Designer Using LLM Agents and the Model Context Protocol: From Aspen Plus Flowsheet Generation to Heat Exchanger Design** **Jia-Lin Kang**[1,*], Yuan Yao[2], and David Shan Hill Wong[2] [1]*Department of Chemical Engineering, National Chung Cheng University, Taiwan* [2]*Department of Chemical Engineering, National Tsing Hua University, Taiwan*
OR-C1-02	10:50~11:10	**What Chemical Engineers can Learn from the Digestive System: Multiscale Modeling for Knowledge Discovery and Engineering Innovation** **Jie Xiao**[*] *School of Chemical and Environmental Engineering, Soochow University, China*
OR-C1-03	11:10~11:30	**Classification of Organic Reaction Mechanisms from Heterogeneous Data Using Transformer Models** **Junu Kim**[*], Muhammad Aarash Abro, Bradford Tuckfield, Shunsei Yayabe *Auxilart Co., Ltd., Japan*
OR-C1-04	11:30~11:50	**Development of a Knowledge Graph-Based RAG System to Support Techno-Economic and Life Cycle Assessment of Chemical Processes** **Juyeon Kim**[1], Minji Kim[2], Jin Ko[2], Youngwon Lee[1], Youlim Chung[1], Junghwan Kim[2], and Jonggeol Na[1,*] [1]*Department of Chemical Engineering & Materials Science, Ewha Womans University, Korea* [2]*Department of Chemical and Biomolecular Engineering, Yonsei University, Korea*
OR-C1-05	11:50~12:10	**A combined Quantum-Chemical-microkinetic-modeling workflow for on-line optimization of an integrated carbon capture and conversion unit** **Supareak Praserthdam**[*] *Department of Chemical Engineering, Chulalongkorn University, Thailand*

Oral Session C2

REGULAR ORAL

Location: Engineering Building D, D403

Chair: Boram Gu (Chonnam National Univ.)

K-C2-01 ● **KEYNOTE**	10:00~10:30	**Automated Physical Modeling in PSE: Literature-to-Model Automation and Multimodal Extensions** **Shota Kato**[*] *Department of Informatics, Kyoto University, Japan*
OR-C2-01	10:30~10:50	**Design of Optimal Lubricants through Computer-Aided Approach** Xian Zhuang Chong, Nishanth G. Chemmangattuvalappil, **Lik Yin Ng**[*] *Faculty of Engineering and Technology, Sunway University, Malaysia*
OR-C2-02	10:50~11:10	**Evaluation of Pre-Combustion CO_2 Capture Processes from High CO_2 Content Gas Sources Using Physical Solvent Absorption and Cryogenic Distillation** **Rendra Panca Anugraha**[*], Renanto Renanto, Juwari Juwari, Raden Ricko Satriyo, Tiara Miratul Zaini and Annisa Maharani *Department of Chemical Engineering, Institut Teknologi Sepuluh Nopember, Indonesia*
OR-C2-03	11:10~11:30	**AI-Augmented Process Systems Engineering for Mixing Design: Constraint-Aware Small-Data Optimization Wrapped Around First-Principles Models** **Richard D. LaRoche**[1,*] and Cenk Feridunoglu[2] [1]*Rwanika-La Roche LLC, USA* [2]*Empower Operations Corp., Canada*
OR-C2-04	11:30~11:50	**Economic-robust optimization of heat load allocation and debottlenecking in heat exchanger networks under multi-source disturbances** **Liwen Zhao**, Guilian Liu[*] *School of Chemical Engineering and Technology, Xi'an Jiaotong University, China*
OR-C2-05	11:50~12:10	**Coupled level-set volume-of-fluid CFD simulation of methane decomposition in molten Ni-Bi, Ni-Bi-Mo, Ni-Bi-Se, and Ga-Bi bubble column reactors for hydrogen production** **Son Ich Ngo**[1,2], Jun-Ho Yang[1], Young-Il Lim[1,*], and Uen-Do Lee[3] [1]*Department of Chemical Engineering, Hankyong National University, Korea* [2]*Faculty of Heat and Refrigeration Engineering, Industrial University of Ho Chi Minh City, Vietnam* [3]*Korea Institute of Industrial Technology (KITECH), Korea*

Oral Session C3

STUDENT ORAL

Location: Engineering Building D, D402

Chair: Moo Sun Hong (Seoul National Univ.)

OS-C3-01	10:00~10:15	**A Temporally Gated Graph Convolutional Model with Dual Dynamic Adjacency for Soft Sensing in Chemical Processes** Zhen-Feng Jiang, **Hsiang-Ting Yuan**, Yuan Yao* *Department of Chemical Engineering, National Tsing Hua University, Taiwan*
OS-C3-02	10:15~10:30	**Process topology-Aware Fault Diagnosis under Operating Conditions Shifts via Domain-Invariant Normal State Alignment** **Hae Rang Roh**, and Jong Min Lee* *Department of Chemical and Biological Engineering, Seoul National University, Korea*
OS-C3-03	10:30~10:45	**Environmental Evaluation of a Cement Clinker Production Process Using Algae-Derived $CaCO_3$** **Hafiz M. Irfan**, and Wei Wu* *Department of Chemical Engineering, National Cheng Kung University, Taiwan*
OS-C3-04	10:45~11:00	**End-to-End Automated Framework for CHO Bioprocess Modeling with Large Language Models** **Han Bit Kim**[1], Young Hyun Cho[1], Dongkyu Kim[1], Janghan Lee[2,3], Seo-Yeon KIM[2,3], Jihoon Kim[2], and Moo Sun Hong[1,*] [1] *Department of Chemical and Biological Engineering, Seoul National University, Korea* [2] *New Drug Development Center, Korea* [3] *College of Pharmacy, Chungbuk National University, Korea*
OS-C3-05	11:00~11:15	**Solving Large-Scale Heat Integration and MINLP Problems via LLM-Driven Adaptive Search** **Hangrui Yang**[1], Xiaodong Hong[1,2,*], Jingdai Wang[1], Yongrong Yang[1], and Zuwei Liao[1,*] [1] *College of Chemical and Biological Engineering, Zhejiang University, China* [2] *Engineering Research Center of Functional Materials Intelligent Manufacturing of Zhejiang Province, China*
OS-C3-06	11:15~11:30	**Development of an energy harvesting sensor device using magnetic phase transition and the accompanying entropy change** **Hikaru Kiyomoto**, Yuka Sakai, and Kansha Yasuki* *Department of Multidisciplinary Sciences, University of Tokyo, Japan*
OS-C3-07	11:30~11:45	**Hierarchical Reinforcement Learning for Sales–Production Coordination: A Stackelberg Game Approach to Manufacturing Scheduling** **Yee Hung Hong** and Zhao Jinsong* *Department of Chemical engineering, Tsinghua University, China*
OS-C3-08	11:45~12:00	**An alternative retrofit strategy for conventional distillation sequences** **Hsiao-Te Liu** and Jeffrey D. Ward* *Department of Chemical Engineering, National Taiwan University, Taiwan*

Oral Session C4

STUDENT ORAL

Location: Engineering Building D, D408

Chair: Ung Lee (KIST)

OS-C4-01	10:00~10:15	**Techno-economic and environmental assessment of SMR-based methanol production: Comparative analysis of biomass and Dac pathways with Aalam cycle integration** **Sungmin Lee**[1], Matthew J. Realff[2,*], and Junghwan Kim[1,*] *[1]Department of Chemical and Biomoleular Engineering, Yonsei University, Korea* *[2]School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, USA*
OS-C4-02	10:15~10:30	**Electrification of Multi-Vessel Batch Distillation** **Surendra Beniwal**, and Sujit S. Jogwar[*] *Department of Chemical Engineering, Indian Institute of Technology Bombay, India*
OS-C4-03	10:30~10:45	**Interpretable Neural Surrogate-Based Flowsheet Optimization under Catalyst Deactivation: Application to CO_2 Methanation** **Teruki Saito**, Osamu Tonomura[*], and Ken-ichiro Sotowa *Kyoto University, Japan*
OS-C4-04	10:45~11:00	**Stable Model-Based Actor-Critic Framework for Continuous Stirred-Tank Reactors Control** **Tiantian Wu**, Jingyi Lu[*] *East China University of Science and Technology, China*
OS-C4-05	11:00~11:15	**Adaptive Physics-Informed Bayesian Optimization for High-Dimensional Material Discovery under Limited Data** **Tomohiro Koji**, Shota Kato, and Manabu Kano[*] *Department of Informatics, Kyoto University, Japan*
OS-C4-06	11:15~11:30	**An Improved Process Configuration for DES-based Carbon Capture Process** **Vaishnavi Gupta**, Soumik Das, Ishan Bajaj[*] *Department of Chemical Engineering, Indian Institute of Technology Kanpur, India*
OS-C4-07	11:30~11:45	**Physics-Informed Active Learning for Cross-Domain Fault Diagnosis in Chemical Processes** **Shaochen Wang** , Wende Tian *, and Zhe Cui *College of Chemical Engineering, Qingdao University of Science and Technology, China*
OS-C4-08	11:45~12:00	**Microscopic Interactions of Multi-component Systems and Energy-Saving Mechanisms in the Mixed Entrainer Distillation Process Title** **Wen Sun**, Shuai Wang[*], Peizhe Cui, Xin Li, Yinglong Wang *College of Chemical Engineering, Qingdao University of Science and Technology, China*

Oral Session D1

REGULAR ORAL

Location: Engineering Building D, D404

Chair: Bor-Yih Yu (National Taiwan Univ.)

K-D1-01 ● **KEYNOTE**	14:30~15:00	**Multi-Scale Advances in CO_2 Capture: From Molecular Solvent Design to Process Intensification** **Yu-Jeng Lin**[1,*] *Department of Chemical Engineering, National Tsing Hua University, HsinChu City, 300 Taiwan*
OR-D1-01	15:00~15:20	**Data-integrated design of organic flow batteries: linking molecular properties, operando response, and predictive engineering** **Soorathep Kheawhom**[*] *Department of Chemical Engineering, Chulalongkorn University, Thailand*
OR-D1-02	15:20~15:40	**Automated Modeling and Optimization of SOFC-CHP Systems via Large Language Models** **Vikram Uday**, Jui-Yuan Lee[*] *Department of Chemical Engineering, National Cheng Kung University, Tainan, Taiwan, R.O.C.*
OR-D1-03	15:40~16:00	**Machine Learning Embedded Superstructure Optimization for Biomethane Production** **Virendra Gunjal**, Ishan Bajaj[*] *Department of Chemical Engineering, Indian Institute of Technology Bombay, India*
OR-D1-04	16:00~16:20	**Safety-by-Design in Chemical Processes: An Ontological Framework for Verifying Critical Sensor Configurations** Chun-yien Chang[1], Ying-ping Chen[1], and **Wei-Jyun Wang**[2,*] *[1]Department of Computer Science, National Yang Ming Chiao Tung University, Taiwan* *[2]Department of Chemical and Materials Engineering, National Central University, Taiwan*
OR-D1-05	16:20~16:40	**Air-to-fuel: direct air capture by aqueous amine solvent and electrochemical CO_2 reduction** **Wonsuk Chung**[1], Hyunyoung Kim[1], Junwoo Park[1], Wonyoung Choi[2], Dae Hyun Lim[1], Da Hye Won[1,3,4], Hyunjoo Lee[1,3,5], and Ung Lee[1,3,6,*] *[1]Clean Energy Research Center, Korea Institute of Science and Technology (KIST), Korea* *[2]Department of Chemical Engineering, Hannam University, Korea* *[3]Division of Energy & Environmental Technology, KIST School, Korea University of Science and Technology (UST), Korea* *[4]KHU-KIST Department of Converging Science and Technology, Kyung Hee University, Korea* *[5]KU-KIST Graduate School of Converging Science and Technology, Korea University, Korea* *[6]Graduate School of Energy and Environment, Korea University, Korea*
OR-D1-06	16:40~17:00	**A new approach to design heat-integrated reactive distillation process** Irvy Ai Xia Teh[1], Yu-Sheng Chen[2], **Zong Yang Kong**[3,*], Yu-Ying Chen[2], Hao-Yeh Lee[2,*], and Jaka Sunarso[1] *[1]Faculty of Engineering, Swinburne University of Technology, Malaysia* *[2]Department of Chemical Engineering, National Taiwan University of Science and Technology, Taiwan* *[3]School of Engineering, Sunway University, Malaysia*

Oral Session D2

REGULAR ORAL

Location: Engineering Building D, D403

Chair: Boreum Lee (Chonnam National Univ.)

OS-D2-01 14:30~14:45

Towards a Near-Zero Carbon Goal: Intensification of Energy- Intensive Distillation Processes Driven by Solar Power

Yan Cheng, Xiao Wang, and Lanyi Sun[*]

State Key Laboratory of Heavy Oil Processing, College of Chemistry and Chemical Engineering, China University of Petroleum (East China), China

OS-D2-02 14:45~15:00

Early-stage Techno-economic and Environmental Assessment Procedure for Emerging Chemical Technologies

Yeonguk Kim, Dami Kim, and Kosan Roh[*]

Department of Chemical Engineering and Applied Chemistry, Chungnam National University, Korea

OS-D2-03 15:00~15:15

Multi-objective optimization of water networks coupled with electrolytic hydrogen production in coal-based chemical industrial parks

Yirui Ge[1], Jing Wang[1,2], Lixia Kang[1,2] and Yongzhong Liu[1,2,*]

[1]*Department of Chemical Engineering, Xi'an Jiaotong University, China*
[2]*University of Shaanxi Province, China*

OS-D2-04 15:15~15:30

Surrogate-Model-Based Optimization of Syngas Distribution–Separation Systems

Yujie Cao, Qiao Zhang[*]

School of Chemical Engineering & Technology, Xi'an Jiaotong University, China

OS-D2-05 15:30~15:45

Techno-Economic Assessment of Perhydro Benzyltoluene as Hydrogen Carrier for an Intercontinental Green Energy Supply Chain

Zhi-Qi Lin[1], Chong-Wei Ong[1], Chun-Cheng Li[1], Wei-Jyun Wang[2], and Cheng-Liang Chen[1,*]

[1]*Department of Chemical Engineering, National Taiwan University, Taiwan*
[2]*Department of Chemical and Materials Engineering, National Central University, Taiwan*

OS-D2-06 15:45~16:00

Research on the Modeling of Multistream Heat Exchangers Based on Equation-Oriented Flash

Zhiyuan Wang, Xijun Wang, Jun Zhao, Lili Wang, Shaohui Tao[*], Xiaoyan Sun[*]

Qingdao University of Science and Technology, China

OS-D2-07 16:00~16:15

A Gate-Based Ensemble of Time Series Foundation Models for Few-Shot Fault Prognosis in Chemical Processes

Zhiyuan Xie[1,2], Jinsong Zhao[1,2]

[1]*Department of Chemical Engineering, Tsinghua University, China*
[2]*State Key Laboratory of Chemical Engineering and Low-carbon Technology, China*

OS-D2-08 16:15~16:30

DFT Study of Support Crystal Face Effects on Ziegler-Natta Catalyzed Olefin Polymerization

KaiQing Sui, XueQin Wei, ZiQi Gao, AiHua He and Xia Yang[*]

College of Chemical Engineering, Qingdao University of Science and Technology, China

OS-D2-09 16:30~16:45

Data-driven mechanism derivation in reaction systems : A hybrid approach integrating mathematical models and machine learning

Sunghun Song, Juhyeon Park, Sungwon Hwang[*]

Program in Energy Process Innovation Convergence, Inha University, Korea

OS-D2-10	16:45~17:00	**Power generation based on combustion and carbon capture strategies for unconverted off-gas from natural gas-based SOFC** **Taehyun Kim**, Jinwoo Park* *Department of Chemical and Biochemical Engineering, Dongguk University, Korea*

Oral Session D3

STUDENT ORAL

Location: Engineering Building D, D402

Chair: Moo Sun Hong (Seoul National Univ.)

OS-D3-01 14:30~14:45

Comparison of control performances of reactive-extractive distillation processes with different reactants

I Gede Pandega Wiratama[1,2], Xuan Liang Choo[3], Zong Yang Kong[1,3,*], Ao Yang[4], Agus Saptoro[5], Jaka Sunarso[1]

[1]Faculty of Engineering, Swinburne University of Technology, Malaysia
[2]Faculty of Engineering Technology, Parahyangan Catholic University, Indonesia
[3]School of Engineering, Sunway University, Malaysia
[4]College of Safety Science and Engineering, Chongqing University of Science & Technology, China
[5]Curtin University, Australia

OS-D3-02 15:45~16:00

Insights into Deep Learning Framework for Molecular Property Prediction Based on Different Tokenization Algorithms

Xiao Wang, Yan Cheng, and Lanyi Sun[*]

State Key Laboratory of Heavy Oil Processing, College of Chemistry and Chemical Engineering, China University of Petroleum (East China), China

OS-D3-03 16:00~16:15

Synergistic mechanism and topological enhancement of mixed entrainer quaternary azeotrope separation: from thermodynamic insights to sequential extraction decoupling

Xiaobin Du, Zhaoyou Zhu, Xin Li, Peizhe Cui, Yinglong Wang[*]

Qingdao University of Science and Technology, China

OS-D3-04 15:15~15:30

Three-stage DMPNN-based prediction model for photodynamic therapy properties of metal complex photosensitizers

Jingxing Gao, Yachao Dong[*], Ran Wang, Wen Sun, Jian Du

School of Chemical Engineering, Dalian University of Technology, China

OS-D3-05 15:30~15:45

Multi-Objective Optimization of Reactive Distillation Column for Silane Production: Impact of Alternative Controllability Criteria and Bidirectional Perturbations

Josué J. Herrera Velázquez[1,3], J. Rafael Alcántara Avila[2], Salvador Hernández[1], and Julián Cabrera Ruiz[1,*]

[1]Universidad de Guanajuato, Mexico
[2]Pontificia Universidad Católica del Perú, Peru
[3]Instituto Tecnológico Superior de Guanajuato, Mexico

OS-D3-06 15:45~16:00

Multiphase computational fluid dynamics of methane pyrolysis in a molten-metal bubble column reactor with carbon coverage

Jun-Ho Yang, Son Ich Ngo, Young-Il Lim[*]

Department of Chemical Engineering, Hankyong National University, Korea

OS-D3-07 16:00~16:15

Dynamic operational planning of modular methanol synthesis via forecast-driven rolling-horizon optimization

Youngkeun Kim[1], Sungmin Lee[1], Jeongdong Kim[2,*], and Junghwan Kim[1,*]

[1]Department of Chemical and Biomoleular Engineering, Yonsei University, Korea
[2]Department of Chemical Engineering, Massachusetts Institute of Technology, USA

OS-D3-08 16:15~16:30

Simplified PID Control for H_2/CO Optimization in Wood Biomass Gasification

Yu Hui Kok, Yuka Sakai and Yasuki Kansha[*]

The University of Tokyo, Japan

OS-D3-09	16:30~16:45	**A non-cooperative game approach to coordinating multiple stakeholders' benefits and carbon emission reduction strategies in coal-based chemical industrial parks** **Kai Li**[1], Jing Wang[1,2] and Yongzhong Liu[1,2,*] *[1]Department of Chemical Engineering, Xi'an Jiarenotong University, China* *[2]University of Shaanxi Province, China*
OS-D3-10	16:45~17:00	**Process Simulation and Technical Feasibility Assessment of CO_2-Based Fischer–Tropsch E-Fuel Production** **Kangyeob Kim**, Jin-Kuk Kim[*] *Department of Chemical Engineering, Hanyang University, Korea*

Oral Session D4

STUDENT ORAL

Location: Engineering Building D, D408

Chair: Kiho Park (Hanyang Univ.)

OS-D4-01	14:30~14:45	**Separation Network Design for Light Olefin Recovery in Plastic Pyrolysis Refineries** **Wen-Yang Lee** and Jeffrey. D. Ward[*] *National Taiwan University, Taiwan*
OS-D4-02	14:45~15:00	**High-Value-Added Byproduct Resource Recycling Feedback Driving Synergistic Optimization of Chemical Process Systems Toward Resource Utilization Efficiency Improvement** **Wenjing Li**, Qiao Zhang[*] *School of Chemical Engineering & Technology, Xi'an Jiaotong University, China*
OS-D4-03	15:00~15:15	**AI-Driven Sustainable ALD Recipe Design Via Multi-Objective Optimization and Process-Level Life Cycle Assessment** **Wonho Lee**, Jeehoon Han[*] *POSTECH, Korea*
OS-D4-04	15:15~15:30	**Selection of entrainers for different separation sequences in extractive distillation of methanol/methyl propionate** **Li Xinying**, Jiang Yangyang, Shang Zewen, Cao Jingxi, Liu Xuhan, Li Xiaohan, Cheng Huanong[*] *College of Chemical Engineering, Qingdao University of Science and Technology, China*
OS-D4-05	15:30~15:45	**Thermodynamic-Guided Computer Aided Molecular Design Framework of Stable Synthetic Ester Lubricants** **Xiao Syuen Lim**, Lik Yin Ng, and Nishanth Chemmangattuvalappil * *School of Engineering, Sunway University, Malaysia*
OS-D4-06	14:45~15:00	**Process Design and 4E Analysis of an Integrated Methane Pyrolysis-Dual Chemical Looping System for Ammonia Production** **Inhye Kim**[1], Minseok Im[1], Sunghyun Cho[1,2,*] *[1]School of Chemical Engineering, Jeonbuk National University, Korea* *[2]Clean Energy Research Center, Jeonbuk National University, Korea*
OS-D4-07	15:00~15:15	**Clean hydrogen production via waste plastic-biomass co-gasification with carbon capture and sequestration: Techno-economic and environmental assessment under policy frameworks** **Minju Jang** and Joonjae Ryu[*] *Department of Chemical Engineering, University of Seoul, Korea*
OS-D4-08	16:15~16:30	**Energy-saving strategies for waste heat recovery in extractive pressure-swing distillation process of chloroform/ethanol/water ternary azeotropic mixture** **Xiaoyan Zhang**, Lulin Sun, Hongbo Xu, Qiyan Yang, Xin Li[*], Yinglong Wang, Peizhe Cui *College of Chemical Engineering, Qingdao University of Science and Technology, China*
OS-D4-09	16:30~16:45	**Theoretical Analysis of Conditions for Negative Transfer in Frustratingly Easy Domain Adaptation with Linear Regression** **Yuki Kobayashi**[1], Sanghong Kim[2], and Manabu Kano[1,*] *[1]Department of Informatics, Kyoto University, Japan* *[2]Department of Applied Physics and Chemical Engineering, Tokyo University of Agriculture and Technology, Japan*

OS-D4-10 16:45~17:00

Predictive Modeling of a renewable methanol synthesis reactor under periodic operations by Kolmogorov-Arnold Networks

Minghui Yu[1], Jing Wang[1,2] and Yongzhong Liu[1,2,*]
[1]Department of Chemical Engineering, Xi'an Jiaotong University, China
[2]University of Shaanxi Province, China

Poster Session P1

Monday, July 6 · Engineering Building D · 55 POSTERS

P-01

Comparative Techno-Economic and Environmental Analysis of Tar Removal and Syngas Upgrading Pathways in SNG Production from Plastic Waste

Doyeong Ahn, and Inkyu Lee[*]

School of Chemical Engineering, Pusan National University, Korea

P-02

Prediction Rationale Based on Occupied Space Information of Three-Dimensional Structures and Molecular Descriptors in Biodegradability Prediction

Atsushi Yoshida[*], Kazuhiro Takeda

Shizuoka University, Japan

P-03

Dynamic Modeling of a Hydrogen-Based Fluidized-Bed Reactor for Iron Ore Reduction

Min Cheol Bae[1], Sang Hwan Son[1,2,*]

[1]School of Chemical Engineering, Pusan National University, Korea
[2]Institute for Environment and Energy, Korea

P-04

Sustainable Integrated Process for Methyl Formate via CO_2 Hydrogenation over Ru-Based Heterogeneous Catalysts

Baejeong Kim, Taeksang Yoon, Minji Kang, Hongjin Park, Sungho Yoon[*] and Chul-Jin Lee[*]

Department of Intelligent Energy and Industry, Chung-Ang University, Korea

P-05

Effect of operating conditions on hydrogen production via non-oxidative polyethylene pyrolysis in a multi-stage molten-tin-based reactor

Bang Thanh Le[1], Son Ich Ngo[1,2], Young-Il Lim[1,*], Young Jae Lee[3], and Uen-Do Lee[3]

[1]Department of Chemical Engineering, Hankyong National University, Korea
[2]Faculty of Heat and Refrigeration Engineering, Industrial University of Ho Chi Minh City, Vietnam
[3]Korea Institute of Industrial Technology (KITECH), Korea

P-06

Upcycling Polymeric Fibrous Waste into Methanol through Carbon Dioxide–Assisted Pyrolysis: A Techno-Economic and Environmental Assessment

Changbeom Shin[1], Taean Go[1], Hyungtae Cho[2], Jaewon Lee[1,*]

[1]Hanyang University ERICA, Korea
[2]Kyung Hee University, Korea

P-07

Novel Energy-Saving Strategies of a Transesterification Reactive Distillation Process with Side-Stream configurations

Yu-Sheng Chen[1] , Irvy Ai Xia Teh[2], Hao-Yeh Lee[1,*], and Zong Yang Kong[3]

[1]Department of Chemical Engineering, National Taiwan University of Science and Technology, Taiwan
[2]Faculty of Engineering, Swinburne University of Technology, Malaysia
[3]School of Engineering, Sunway University, Malaysia

P-08

Criticality Analysis for Redundancy Planning and Preventive Maintenance in Industrial Symbiosis

Yick Eu Chew[1], Bing Shen How[1], Jean Pimentel[2], Petar Sabev Varbanov[2,3], Ferenc Friedler[2], Viknesh Andiappan[1,*]

[1]Faculty of Engineering, Swinburne University of Technology Sarawak, Malaysia
[2]Department of Systems Sciences, Széchenyi István University, Hungary
[3]Faculty of Mechanical Engineering, Brno University of Technology - VUT Brno, Czech Republic

P-09

Comparative Techno-Economic and Life Cycle Assessment of Thermochemical Pathways for Waste Plastic Valorization: Fuel, Hydrogen, and Circular Polyethylene Production

Chanmok Kim, Donghyeon Kim, Heehyun Choi, Hyeonseo Im, and Jiyong Kim[*]

School of Chemical Engineering, Sungkyunkwan University, Korea

P-10 A Dynamic Simulation and Economic Evaluation Framework for Cyclic Distillation of Close-Boiling Mixtures

Cheng-Yen Lai and Jeffrey D. Ward[*]

Department of Chemical Engineering, National Taiwan University, Taiwan

P-11 Process design of ammonia decomposition system for hydrogen and power co-generation with low nitrogen oxide emissions

Seoyeon Cho, and Inkyu Lee[*]

School of Chemical Engineering, Pusan National University, Korea

P-12 Multi-Dataset Sustainable Process Simulation of Food Waste to Biogas system

Mingyo Choi[1], Jaewon Byun[2], Jeehoon Han[1,*]

[1]Department of Chemical Engineering, Pohang University of Science and Technology (POSTECH), Korea
[2]Chonnam National University, Korea

P-13 Learning Temperature-Aware Molecular Representations for Organic Solubility Prediction

Chonghyo Joo and Lauren Ye Seol Lee[*]

Department of Chemical Engineering, University College London, UK

P-14 A Comparative Study of International Renewable Energy Supply Chains Utilizing Green Ammonia as Energy Carrier

Chun-Cheng Li[1], Chong Wei Ong[1,2], Cheng-Liang Chen[1,2,*]

[1]Department of Chemical Engineering, National Taiwan University, Taiwan
[2]Department of Chemical and Environmental Engineering, University of Nottingham Malaysia, Malaysia

P-15 Dynamic Multi-Objective Operational Optimization of the Green Hydrogen Ammonia Synthesis Process under Uncertainty Disturbance

Zijun Wang[1], Shida Gao[2], Kangkang Feng[3], Xiangjian Shi[3], **Cuimei Bo**[1,*]

[1]College of Electrical Engineering and Control Science, Nanjing Tech University, China
[2]Shanghai Jiao Tong University, China
[3]Nanjing Nanrui Jibao Engineering Technology Co., China

P-16 Process Design and Optimization Based on Techno-Economic Evaluation of Green Hydrogen Considering Variations in Cell Number and Operating Conditions of Alkaline Water Electrolysis Stacks

Dong-ha Kim, Joonjae Ryu[*]

Department of Chemical Engineering, Center for Innovative Chemical Processes, Institute of Engineering, University of Seoul,163 Seoulsiripdaero, Dongdaemun-gu, 02504, Seoul, South Korea

P-17 Production of Methanol from Waste Expanded Polystyrene through Pyrolysis-integrated Process: Techno-economic analysis

Dongho Choi, Hyungtae Cho[*]

Department of Chemical Engineering, College of Engineering, Kyung Hee University, Yongin, Republic of Korea

P-18 System Optimization and Techno-Economic Analysis for Renwable Energy-based Green Ammonia Production

Donghyeon Jeon, Jin-Kuk Kim[*]

Department of Chemical Engineering, Hanyang University, Korea

P-19 Energy Management and Optimization of an Off-Grid Wind-Photovoltaic-Hydrogen Storage-Methanol System

Fei Wang, Qiao Zhang[*]

School of Chemical Engineering & Technology, Xi'an Jiaotong University, China

P-20 Sustainable Strategy for Polybutylene Adipate Terephthalate Production Utilizing Biomass-derived Monomers and Lignin Blending

Gihyun Kwon (Underline Presenting Author), and Jeehoon Han[*]

Department of Chemical Engineering, Pohang University of Science and Technology, Korea

P-21 **Structured Surrogate Modeling and Reinforcement Learning for Grade Transition Control in Polypropylene Reactors**

Guyang Liu, Jingyi Lu[*], Wenli Du[*]

East China University of Science and Technology, China

P-22 **Physics Informed Neural Network for Viscoelastic Flows: Application to EPDM Die Swell Prediction**

Gwanghyeon Kwon[1], Hyeong Ro Yoon[1], Seokyoung Hong[1,2], and Jong Min Lee[1,*]

[1]Department of Chemical and Biological Engineering, Seoul National University, Korea
[2]School of Energy and Chemical Engineering, Ulsan National Institute of Science and Technology, Korea

P-23 **Sustainable Design and Economic Analysis of LOHC Dehydrogenation Process using Bayesian Optimization**

Hyungjun Joo, Yeonsoo Kim[*]

Department of Chemical Engineering, Kwangwoon University, Korea

P-24 **Mathematical Modeling and Simulation of an Energiron ZR Shaft Furnace for Hydrogen-Based Direct Reduction**

Halyn Chung[1], and Sang Hwan Son[1,2,*]

[1]School of Chemical Engineering, Pusan National University, Korea
[2]Institute for Environment and Energy, Korea

P-25 **Multi-stage stochastic programming for sustainable syngas injection into blast furnaces via waste plastics valorization**

Heedo Ryou[1], Jinsu Kim[2], and Jeehoon Han[1,*]

[1]Department of Chemical Engineering, Pohang University of Science and Technology, Korea
[2]Department of Petrochemical Materials, Chonnam National University, Korea

P-26 **ML-driven framework for system-level assessment of biomass and waste plastic co-gasification**

Hyeonseo Im, Heehyun Choi, Chanmok Kim, Donghyeon Kim, Jiyong Kim[*]

School of Chemical Engineering, Sungkyunkwan University, Suwon, Republic of Korea

P-27 **Environmental and Economic Feasibility Analysis of Sustainable Aviation Fuel Production via Methanol-to-Jet Pathways Using Bio-methanol**

Heejeong Kim, Jiyun Yoo, Jeehoon Han[*]

Department of Chemical Engineering, Pohang University of Science and Technology, Korea

P-28 **LSTM–Transformer Autoencoder for Anomaly Detection: Application to a Real-World Multimode Industrial Chemical Proces**

Hyeokin Gwon[1], Hyukwon Kwon[2,3], Meng Qi[4], Hyungtae Cho[5,*], Jaewon Lee[2,*]

[1]Department of Materials Science and Chemical Engineering, Hanyang University, Korea
[2]Department of Chemical and Biomolecular Engineering, Yonsei University, Korea
[3]Korea Institute of Industrial Technology, Korea
[4]Department of Chemistry and Bioscience, Aalborg University, Denmark
[5]Department of Chemical Engineering, Kyung Hee University, Korea

P-29 ***Withdrawn***

P-30 **Artificial Photosynthesis-Based Photocatalytic Hydrogen Production: A Techno-Economic and Land-Use Comparison with PV-Electrolysis**

HyunJun Choi, Juyung Byun, Jin Ko and Junghwan Kim[*]

Department of Chemical and Biomolecular Engineering, Yonsei University, Korea

P-31 **Optimization of a Waste Resource Supply Chain Based on Process Modeling of Co-Gasification of Waste Plastics and Biomass**

Juhan Hwang and Joonjae Ryu[*]

Department of Chemical Engineering, University of Seoul, Korea

P-32 Single-Amine Strategy for CO_2 Hydrogenation to Formic Acid: Process Simplification Using NBIM Coupled with Heterogeneous Ru-MACHO-POMP Catalysis

Jaehyeong Choi[1,2], Jiseong Baek[3], Hongjin Park[3], Minsol Kim[1,2], Kibong Lee[2], Ung Lee[1,4,2,*] and Sungho Yoon[3,*]

[1]Clean Energy Research Center, Korea Institute of Science and Technology (KIST), Korea
[2]Department of Chemical and Biological Engineering, Korea University, Korea
[3]Department of Chemistry, Chung-Ang University, Korea
[4]Division of Energy and Environmental Technology, KIST School, Korea

P-33 Deep Reinforcement Learning-Based Thermal Management of Battery Fullpack in Electric Vehicle

Dabin Jeong and Yeonsoo Kim[*]

Department of Chemicl Engineering, Kwangwoon University, Korea

P-34 Integration of Water Electrolysis with Oxy-fuel SMR for Advanced Blue Hydrogen Production

Narin Jeong, Kang Cheongmin[*], Young Woo Chon[*]

Department of Environmental Engineering, Inha University, Korea

P-35 A framework for knowledge-integrated process modeling from natural language using large language models

Jin Ko[1], Minji Kim[1], Juyeon Kim[2], Youngwon Lee[2], Youlim Chung[2], Jonggeol Na[2,*] and Junghwan Kim[1,**]

[1]Department of Chemical and Biomoleular Engineering, Yonsei University, Korea
[2]Department of Chemical Engineering and Materials Science, Ewha Womans University, Korea

P-36 Parallel Computing Strategy of Isotherm Parameters Regression for p-Xylene Simulated Moving Bed Process via Internal Network Approach

Jing-Yang Tseng[1], I-Lung Chien[2], and Hao-Yeh Lee[1,*]

[1]Department of Chemical Engineering, National Taiwan University of Science and Technology, Taiwan
[2]Department of Chemical Engineering, National Taiwan University, Taiwan

P-37 Industrial Plant Implementation and Assessment of Disturbance Observer-Based PID Control for Valve Hysteresis Compensation

Jinki Shoda[*], Masaharu Daiguji

ENEOS Corporation, Japan

P-38 Process Simulation and Economic Evaluation of Converting Mixed Plastic Waste into Methanol and Hydrogen

Jinwoo Gil[1], Dongho Choi[1], Jaewon Lee[2], Hyungtae Cho[1,*]

[1]Department of Chemical Engineering, Kyung Hee University, Korea
[2]Department of materials Science and Chemical Engineering, Hanyang University, Korea

P-39 Integrated Process Evaluation for the Co-Production of Biodiesel and Bio-Lubricants from Biomass: Energy Analysis and Life Cycle Assessment

Jiyun Yoo[1], Yoonjae Lee[1], Seungjun Choi[1], Jaerak Ko[2], Soonho Hwangbo[2], and Jeehoon Han[1,*]

[1]Department of Chemical Engineering, Pohang University of Science and Technology, Korea
[2]Department of Chemical Engineering, Gyeongsang National University, Korea

P-40 Sustainable Integrated Steelmaking through Rotary Hearth Furnace-Based Steel Solid Waste Recycling: A Multi-Objective Optimization Approach

Jongil Bae[1], Myungsuk Son[2], Gayoung Lee[1], Jinsu Kim[3], and Jeehoon Han[1,*].

[1]Department of Chemical Engineering, Pohang University of Science and Technology, Korea
[2]Korea Testing Laboratory, Korea
[3]Department of Petrochemical Materials, Chonnam National University, Korea

P-41 Surrogate Model-Based Optimization of Amine CO_2 Capture Process

Joonyoung Lee[1], Michael John Binns[2], Jin-Kuk Kim[1,*]

[1]Department of Chemical Engineering, Hanyang University, Korea
[2]Department of Chemical Engineering, Dongguk University, Korea

P-42 **Carbon neutral bio-methanol production via catalytic pyrolysis using CO_2**

Junyoung Park, Dongho Choi, Yongsang An, and Hyungtae Cho[*]

Department of Chemical Engineering, Kyung Hee University, Korea

P-43 **Optimization of an Induction Heating-Assisted Ammonia Decomposition Reactor for Efficient Hydrogen Production**

Juyeon Cho, Chul-jin Lee[*]

Department of Chemical Engineering, Chung-Ang University, Korea

P-44 **Temporal fusion transformer–based surrogate modeling for adaptive and energy-efficient operation of hybrid semi-batch/batch reverse osmosis**

Heun Se Kim and Kiho Park[*]

Department of Chemical Engineering, Hanyang University, Korea

P-45 **Quantitative Risk Assessment on Liquid hydrogen receiving Terminal**

Jeong-Hoon Kim, Hak-Tae Lee, Ju-Eon-Bae, Chul-Jin Lee[*]

School of Chemical Engineering & Materials Science, Chung-Ang University, Korea

P-46 **CFD-guided Optimization of Rotationally Driven Slurry Dispersion and Homogeneity**

Taean Ko[1], Changbeom Shin[1], Hyungtae Cho[2], Jaewon Lee[1,*]

[1]Hanyang University ERICA, Korea
[2]Kyung Hee University, Korea

P-47 **Predicting Biodegradation Time Profiles by Leveraging the Effectiveness of Molecular Physicochemical Property–Based Classification**

Kairi Kato[*], Kazuhiro Takeda

Shizuoka University, Japan

P-48 **Explainable AI (XAI) Analysis of Reboiler Heat Duty in a Pilot-Scale MEA CO_2 Capture Process: Identification of Loading- and Thermally-Controlled Regimes**

Yinseo Song, Kiho Park[*]

Department of Chemical Engineering, Hanyang University, Korea

P-49 **Process-Aware Shapley Flow Analysis for Interpretable Fault Diagnosis in Chemical Processes**

Kyojin Jang[1,*], Jeongdong Kim[2]

[1]Samsung Electronics Co., Korea
[2]Massachusetts Institute of Technology, USA

P-50 **Comparison of Energy Efficiency and Remixing Effects among Various Heat-Integrated Distillation Configurations**

Hsin-Hui Liang[1], You-Cheng Jiang[1], Hao-Yeh Lee[1,2,*]

[1]National Taiwan University of Science and Technology, Taiwan
[2]Process Net-Zero Research Center, Taiwan

P-51 **Design and Optimization of a Hydrogen Ventilation System Using Transient CFD Dispersion Analysis in SMR Process**

Sang Won Lee, Yong Woo H wang, Young Woo Chon[*]

Program in Circular Economy & Environmental System, Inha University, Korea

P-52 **Techno-Economic and Life Cycle Assessment of Hydrogen and Methanol Production from Nonwoven Polymer Waste Using CO_2-Assisted Pyrolysis**

Seyeong Lee[1,2], Jaeho Baek[2], Hyungtae Cho[3], Jaewon Lee[4,*]

[1]Korea Institute of Industrial Technology, Korea
[2]Department of Chemical and Biomolecular Engineering, Yonsei University, Korea
[3]Department of Chemical Engineering, Kyung Hee University, Korea
[4]Department of Materials Science and Chemical Engineering, Hanyang University, Korea

P-S1 **Gaussian Process Surrogate Modelling with Electrode Geometry Encoding for Multi-Pollutant Electrocoagulation System using Small Datasets**

Lian See Tan[1,*], Mathias Neufang[2], Antonio Del Rio Chanona[2], Nor Ain Mohd Noor Azli[1], Norhuda Abdul Manaf[1]

[1]Malaysia-Japan International Institute of Technology, Universiti Teknologi Malaysia, Kuala Lumpur, Malaysia
[2]Department of Chemical Engineering, Imperial College London, London, UK

P-S2 **Graphical Approach for Optimal Deployment of Carbon Dioxide Removal (CDR) Methods**

Yu Jian Tan[1], Xue Qin Lim[1], Dominic C. Y. Foo[1], Raymond R. Tan[2]

[1]Department of Chemical and Environmental Engineering/Centre of Excellence for Green Technologies, University of Nottingham Malaysia, Selangor, Malaysia
[2]Department of Chemical Engineering, De La Salle University, Manila, Philippines

P-S3 **Fuzzy-Structured Reinforcement Learning for Nonlinear Process Control under Changing Operating Conditions**

Mohd Fauzi Zanil[1,2], Zainal Ahmad[2,*], Syamsul Rizal Abd Shukor[2], Agus Saptoro[3], Zulfan Adi Putra[4]

[1]School of Engineering, Asia Pacific University of Technology and Innovation, Kuala Lumpur, Malaysia
[2]School of Chemical Engineering, Universiti Sains Malaysia, Penang, Malaysia
[3]Western Australian School of Mines, Curtin University, Kalgoorlie, WA, Australia
[4]Process Engineering Specialist, Exiron Baja Pratama, Bandung, Indonesia

P-S4 **Forecasting-Based Dynamic Dispatch under Process Flexibility Limit Constraints for an Off-Grid Power-to-Methanol System**

Mingqi Bai[1], Pengcheng Wang[1], Meng Qi[2], Yi Liu[2], Zhang Bai[1,*]

[1]College of New Energy, China University of Petroleum (East China), Qingdao, 266580, China
[2]State Key Laboratory of Chemical Safety, College of Chemistry and Chemical Engineering, China University of Petroleum (East China), Qingdao, 266580, China

Poster Session P2

Tuesday, July 7 · Engineering Building D · 56 POSTERS

P-53 **Computational Synthesis and Techno-Economic Optimization of Intensified Cryogenic Distillation Sequences for Olefin Recovery from Diverse Chemical Recycling Feedstocks**

Li-Chin Hsiao and Jeffrey Ward[*]

Department of Chemical Engineering, National Taiwan University, Taiwan

P-54 **Exergy, economic and life cycle assessment of novel cogeneration systems based on chemical heat pumps**

Xijun Wang[1,2], Xiaomeng Jiang[1,2], Xingrui Lan[1,2], Shuguang Xiang[1,2,*], Xiaoyan Sun[1,2], **Lili Wang**[1,2,*], Li Xia[1,2], Shaohui Tao[1,2]

[1]*College of Chemical Engineering, Qingdao University of Science and Technology, China*
[2]*Shandong Key Laboratory of Chemical Process Simulation and Optimization Industrial Software, China*

P-55 **Assessing Feasibility and Consistency in AI-Generated Process Flowsheets**

Margareth[1,2] and Ung Lee[1,2,3,*]

[1]*Clean Energy Research Center, Korea Institute of Science and Technology, Korea*
[2]*Division of Energy and Environmental Technology, University of Science and Technology (UST), Korea*
[3]*Department of Chemical and Biological Engineering, Korea University, Korea*

P-56 ***Withdrawn***

P-57 **GraphSAGE-Based Surrogate Modeling and Optimization of Heating Parameters for Ceramic Firing Process**

Minori Noda, Shota Kato, and Manabu Kano[*]

Department of Informatics, Kyoto University, Japan

P-58 **Chemical Reaction Pathway Synthesis to Recover Value Added Chemicals from Crude Bio-Oil**

Yen Qin Lee[1], Xiao Syuen Lim[2], and **Nishanth Chemmangattuvalappil**[2,*]

[1]*Department of Chemical & Environmental Engineering, University of Nottingham Malaysia, Malaysia*
[2]*School of Engineering, Sunway University, Malaysia*

P-59 **Large Language Model Assisted Workflow Automation for Distillation Process Simulation and Optimization**

Po-Chia Chiu, Yu-Sheng Chen, Hao-Yeh Lee, Yan-Ling Yang[*]

Department of Chemical Engineering, National Taiwan University of Science and Technology, Taiwan

P-60 **An exploratory attempt on integrating anaerobic digestion fundamentals with machine learning concepts in Indian and European Chemical Engineering Academic Classrooms**

Pragya Singh[1], Sara Marchini[2], Asad H. Sahir[1], Markus Schubert[2]

[1]*Indian Institute of Technology Ropar, India*
[2]*Technische Universität Dresden, Germany*

P-61 **Decarbonizing Fluid Catalytic Cracking via Multi-Objective Optimization of a Plant-Calibrated Kinetic Riser Model**

Priyam Nayak[*], Sanjay Mahajani and Kannan Moudgalya

Department of Chemical Engineering, Indian Institute of Technology Bombay, India

P-62 **Machine Learning Surrogate with Cascade Architecture for Wax Hydro-Cracking and -Isomerization**

Pyeong-Gon Jung and Joonjae Ryu[*]

Department of Chemical Engineering, University of Seoul, Korea

P-63 **Advanced Control of Cracking Furnaces in Ethylene Plants Based on Soft Sensing Technology**

Qun Wu[1], Yaoming Wu[2], and Wenli Du[1,*]
[1]*East China University of Science and Technology, China*
[2]*Sinochem Quanzhou Petrochemical Co., China*

P-64 **Multi-Objective Optimization and Integrated Process Intensification for Sustainable and Low-Carbon Methyl Propionate Production**

Ronghua Liang, Ruru Ma, Chunfa Miao, Peizhe Cui, Xin Li, Yinglong Wang[*]
College of Chemical Engineering, Qingdao University of Science and Technology, Qingdao, China

P-65 **Reliability-Aware Plastic Waste-to-Hydrogen Supply Chain Optimisation Considering Spatial Heterogeneity**

Selena Kian Yii Song[1], Jean Pimentel[2], Ákos Orosz[3], Viknesh Andiappan[1], Ferenc Friedler[2], Bing Shen How[1,*]
[1]*Faculty of Engineering, Swinburne University of Technology, Malaysia*
[2]*Department of Systems Science, Széchenyi István University, Hungary*
[3]*Department of Computer Science and Systems Technology, University of Pannonia, Hungary*

P-66 **Spray-reliquefaction using subcooled LH_2 tanks in import hydrogen terminals**

S. W. Park, C. J. Lee[*]
Department of Chemical Engineering, Chung-Ang University, Korea

P-67 **Photothermal Membrane Distillation: Theoretical Analysis of Photothermal Layer Placement Effects in DCMD and SGMD**

Sunyoung Oh, Boram Gu[*]
School of Chemical Engineering, Chonnam National University, Korea

P-68 **Development of a Real-time Detection and Suppression Method for Sequential Alarms in Plant Operations**

Saki Inoue, Masaru Noda[*]
Department of Chemical Engineering, Fukuoka University, Japan

P-69 **Exploration of flexible syngas production pathways via superstructure-based optimization of chemical looping process**

Sang-Hyeok Jeon and Joonjae Ryu[*]
Department of Chemical Engineering, University of Seoul, Korea

P-70 **Life Cycle Assessment-based Optimization of Amine Blends for Blue Hydrogen Production via Carbon Capture from Steam Methane Reforming Flue Gas**

Seungjun Choi[1], Yoonjae Lee[1], Gayoung Lee[1], Shinhyeon Kim[1], Hyunshik Yoon[2], Jaebong Kim[2], Jeehoon Han[1,*]
[1]*Department of Chemical Engineering, Pohang University of Science and Technology, Korea*
[2]*ENIS INC, Korea*

P-71 **Integrated design of ammonia-based solid oxide fuel cell system preventing nickel nitride degradation**

Je-Woo Shim, Dong-Kyoung Shin, Chul-Jin Lee[*]
Department of Chemical Engineering, Chung-Ang University, Korea

P-72 **Neural Network-Based Design of Low-Temperature Selective Catalytic Reduction Catalysts for NOx After-Treatment**

Shinjae Kim and Yeonsoo Kim[*]
Department of Chemical Engineering, Kwangwoon University, Korea

P-73 **Evaluating Circular Economy and Policy Pathways for a Sustainable Transition in the Indian PET Sector**

Shubham Sonkusare, Yogendra Shastri[*]
Department of Chemical Engineering, Indian Institute of Technology Bombay, India

P-74 **Multi-period co-optimization of vertical thermosyphon reboilers for seasonal operation in amine-based carbon capture**

Shuhao Zhang[1], Zekun Yang[2]

[1]School of civil Engineering, Chongqing University, China
[2]Department of Chemical Engineering, University of Manchester, UK

P-75 **Process Design for Fuel-Grade DME production from Biomass**

Songho Lee, Junyoung Park, Dongho Choi and Hyungtae Cho*

Department of Chemical Engineering, Kyung Hee University, Korea

P-76 **Enumeration of Multiperiod Heat Recovery Networks with Integrated Sensible Heat Storage for Energy Intensive Industrial Symbiosis**

Tiffany Jia Ning Ang[1], Jean Pimentel[2], Ákos Orosz[3], Ferenc Friedler[2], Viknesh Andiappan[1], Bing Shen How[1,*]

[1]Faculty of Engineering, Swinburne University of Technology, Malaysia
[2]Department of Systems Science, Széchenyi István University, Hungary
[3]Department of Computer Science and Systems Technology, University of Pannonia, Hungary

P-77 **Large Language Model Assisted Automation for Reactor Process Simulation, Synthesis, and Optimization**

Ting-Yen Chiang, Yu-Sheng Chen, Hao-Yeh Lee, Yan-Ling Yang*

Department of Chemical Engineering, National Taiwan University of Science and Technology, Taiwan

P-78 **Catalyst Performance Prediction Using LLM-Based Feature Selection**

Takahiro Sakashita, Shota Kato, and Manabu Kano*

Kyoto University, Japan

P-79 **Estimation and Attribution Analysis of Alzheimer's Disease Progression Indicators Based on MRI Images Using Deep Learning**

Takumi Sekiya, and Keigo Matsuda*

Nagoya University, Japan

P-80 **Integrating Process Simulation with Large Language Models for Automated Life Cycle Inventory Generation: A Case Study of Reactive Distillation**

Tsai-Wei Wu*, Chun-Wei Chen

Department of Chemical Engineering, National Cheng Kung University, Taiwan

P-81 **Adaptive Organosilicon Optimization via Supervised Contrastive and Condition-Aware Safe Reinforcement Learning**

Jiyang Xiao, Zhongmei Li*, Qinhao Sun, Jionghao Lou, Shiming Wu, Enbo Feng

Key Laboratory of Smart Manufacturing in Energy Chemical Process, East China University of Science and Technology, China

P-82 **Stochastic Robust Optimal Scheduling of Industrial Utility Systems Coupled with Green Ammonia under Multiple Uncertainties**

Xiaoya Cao, Liang Zhao*

Key Laboratory of Smart Manufacturing in Energy Chemical Process, Ministry of Education, East China University of Science and Technology, China

P-83 **Fast data and theory fusion modeling method for dynamic distillation systems based on the Physics-constrained dynamic mode decomposition**

Xing Qian[1], Haotong Wu[1], Yuhui Yin[2,3], Shengkun Jia[2,3], Yiqing Luo[2,3], Xigang Yuan[2,3,*]

[1]College of Information Science and Technology, Beijing University of Chemical Technology, China
[2]School of Chemical Engineering and Technology, Tianjin University, China
[3]State Key Laboratory of Chemical Engineering and Low-carbon Technology, China

P-84 **A Comparative Study of Reinforcement Learning and Model Predictive Control in Isopropanol Dehydration Process**

Yu-Cheng Chao[1], Yan-Ling Yang[2], Hao-Yeh Lee[1,*]

[1]Department of Chemical Engineering, National Taiwan University of Science and Technology, Taiwan
[2]Department of Chemical Engineering, National Taiwan University, Taiwan

P-85 **A comparative analysis of process flexibility for pressure-swing and extractive distillation systems**

Yu-Ying Chen[1], Zong Yang Kong[2], Vincentius Surya Kurnia Adi[3,4], Hao-Yeh Lee[1,*]

[1]Department of Chemical Engineering, National Taiwan University of Science and Technology, Taiwan
[2]School of Engineering, Sunway University, Malaysia
[3]Department of Chemical Engineering, National Chung Hsing University, Taiwan
[4]Department of Chemical Engineering, National Cheng Kung University, Taiwan

P-86 **Process design and multi-objective optimization for the separation of methyl acetate/vinyl acetate/water azeotrope by extractive distillation based on mixed entrainer**

Yang Zhang, Zhaoyou Zhu, Xin Li, Peizhe Cui, Yinglong Wang[*]

Qingdao University of Science and Technology, China

P-87 **Simulation and technoeconomic analysis for low-carbon coal-to-liquids process coupling renewable energy and green hydrogen**

Yao Jiashu, Liu Yurong, and Du Wenli[*]

East China University of Science and Technology, China

P-88 **Techno-Economic Analysis of Amine-Based Carbon Capture for Maritime Liquefied Natural Gas Engines and Solid Oxide Fuel Cells**

Yeji Choi, Jeehoon Han[*]

Department of Chemical Engineering, Pohang University of Science and Technology (POSTECH), Korea

P-89 **Design of an Iron Powder–Based Energy Carrier Supply Chain**

Yi-Hung Lin, Cheng-Liang Chen[*]

Department of Chemical Engineering, National Taiwan University, Taiwan

P-90 **Techno-economic Analysis and Life Cycle Assessment of Sustainable Aviation Fuel Production via CO_2 Fisher-Tropsch Synthesis**

Seonuk Yu, Seungjun Choi, Jeehoon Han[*]

Department of Chemical Engineering, Pohang University of Science and Technology, Korea

P-91 **Investigating the Influences of Electrochemical Kinetic Parameters on the Operating Voltage of PEM Water Electrolysis Cells**

Yu-Da Hsiao[*], Chia-Kai Wang and Shi-Hsuan Lu

Department of Chemical Engineering and Biotechnology, National Taipei University of Technology, Taiwan

P-92 **Numerical Modeling of Ion Transport in Nanofiltration Membranes Using the DSPM-DE Model**

Yunju Kim, and Kiho Park[*]

Department of Chemical Engineering, Hanyang University, Korea

P-93 **Surrogate Model for Joint Prediction of Local Fields and Process-Level KPIs in Ethane Cracking Reactors**

Yunyue Shang, Wenli Du[*], Yichun Li[*]*

State Key Laboratory of Industrial Control Technology, East China University of Science and Technology, China

P-94 **A Parallel Column Generation Algorithm for Two-Dimensional Two-Stage Guillotine Cutting Problem with Multiple Stock Sizes**

Zheng Xinya[1], Liu Changxin[1], Li Zhongmei[1], Li Yichun[1], Yang Minglei[1,2,*]

[1]Key Laboratory of Advanced Control and Optimization for Chemical Processes, East China University of Science and Technology, China
[2]Engineering Research Center of Process Systems Engineering, East China University of Science and Technology, China

P-95 **Multi-Rate Fusion of Acoustic and Vibration Signals for Soft Sensing of Ball Mill Internal States: A Lab-scale Study in Bayer Process**

Xiangyang Zhu, Zhongmei Li[*], Tinghang Zhao, Jingrui Wang, Enbo Feng

Key Laboratory of Smart Manufacturing in Energy Chemical Process, East China University of Science and Technology, China

P-96 **Accelerating Catalyst Discovery for CO_2 hydrogenation via an ML-Driven Cascade Framework and Genetic Algorithm**

Hyunjin Kang[1], Hyundo Park[2], Insoo Ro[3,*], Hyungtae Cho[1,*], Jaewon Lee[4,*]

[1]Department of Chemical Engineering, Kyung Hee University, Korea
[2]Department of Chemistry, Northwestern University, USA
[3]Department of Chemical and Biological Engineering, Korea University, Korea
[4]Department of Materials Science and Chemical Engineering, Hanyang University, Korea

P-97 **Comparative Analysis of CO_2-to-SAF Pathways via Integrated Process Design and Optimization**

Jeongmin Lee and Joonjae Ryu[*]

Department of Chemical Engineering, University of Seoul, Korea

P-98 **Design Optimisation of Baffle Geometry for Mitigating Acceleration-Induced Boil-Off Gas in Liquid Hydrogen Tankers**

Jingyeong Im[1,2], Boram Gu[1,*] and Wangyun Won[2,*]

[1]School of Chemical Engineering, Chonnam National University, Korea
[2]Korea University, Korea

P-99 **Mechanistic-Informed Data-Driven Framework for Generalized Reaction Yield Prediction Across Novel Chemical Spaces**

Zhe Li, and Jingyi Lu[*]

East China University of Science and Technology, China

P-100 **Effects of Photoacid Generator Composition on Proton Transport, Deprotection Kinetics, and Line Edge Roughness in Chemically Amplified Resists: A Reactive Molecular Dynamics Study**

Sangdeok Kim[1], Jaehyun Ryu[1], Seungtae Kim[1], Sangwoo Kwon[1], Claire S. Adjiman[2], and Won Bo Lee[1,*]

[1]School of Chemical and Biological Engineering, Seoul National University, Korea
[2]Department of Chemical Engineering, Imperial College London, UK

P-101 **Multi-Agent Debate for Feasibility-Aware Design of CO_2 Electrolysis Systems from Economic and Environmental Perspectives**

Youngwon Lee[1], Youlim Chung[1], Juyeon Kim, Minji Kim[2], Jin Ko[2], Junghwan Kim[2], and Jonggeol Na[1,*]

[1]Department of Chemical Engineering & Materials Science, Ewha Womans University, Korea
[2]Department of Chemical and Biomolecular Engineering, Yonsei University, Korea

P-102 **Numerical Modeling and Determination of Optimal Catalyst Loading for Ortho-Para Conversion PFHX Reactors in Hydrogen Liquefaction Process**

Changseo Lee[1], Suyeon Kim[1], Sungwon.hwang[1,2,3,*]

[1]Department of Chemistry and Chemical Engineering, Inha University, Korea
[2]Education and Research Center for Smart Energy Materials and Process, Inha University, Korea
[3]3D Convergence Center, Inha University, Korea

P-103 **Dynamic Life Cycle Assessment of Steel Industry Electrification Pathways**

Gayoung Lee[1], Myungsuk Son[2], Jongil Bae[1], Jinsu Kim[3] and Jeehoon Han[1,*]

[1]Department of Chemical Engineering, Pohang University of Science and Technology, Korea
[2]Korea Testing Laboratory, Korea
[3]Department of Petrochemical Materials, Chonnam National University, Korea

P-104 **Uncertainty-Based Cost Optimization of Hydrogen Production Using Dynamic LNG and CEPCI Forecasts**

Dong Guk Kim, Yoo Ri Kim, Seong Bin Ga, Dong Hwi Jeong[*]

Department of Chemical Engineering, University of Ulsan, Korea

P-105 **External Coupling-Based Multi-objective Optimization Framework for DMR Processes in Aspen Plus**

Jeong Cheol Lee, Nguyen Minh Tan, Dong Hwi Jeong[*]

Department of Chemical Engineering, University of Ulsan, Korea

P-106 **A Single Adsorption-Energy Feature for Accurate Prediction of MOF Gas Uptake with a Residual MLP**

Yongsang An[1], Nahyeon An[2], Junyoung Park[1], Hyungtae Cho[1] and Seongbin Ga[3,*]
[1]Department of Chemical Engineering, College of Engineering, Kyung Hee University, Korea
[2]School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, USA
[3]School of Chemical Engineering, University of Ulsan, Korea

P-107 **Spatio-Temporal Techno-Economic Assessment of Power-to-Olefins Production**

Hira Mahmood, Jay Liu[*]
Department of Chemical Engineering, Pukyong National University, Korea

P-108 **xThermoGNN: An Interpretable Multi-Level Graph Neural Network for Predicting the Decomposition Heat of Reactive Chemicals**

Hong Wang[1,2], Meng Qi[1,2], Yi Liu[1,2,*]
[1]State Key Laboratory of Chemical Safety, China University of Petroleum (East China), China
[2]College of Chemistry and Chemical Engineering, China University of Petroleum (East China), China

P-109 **Machine Learning Aided Performance Prediction of Biomass Gasificaiton**

Xin Du[1,2], Junghwan Kim[3,*], Yi Liu[1,2,*]
[1]State Key Laboratory of Chemical Safety, China University of Petroleum (East China), China
[2]College of Chemistry and Chemical Engineering, China University of Petroleum (East China), China
[3]Department of Chemical and Biomolecular Engineering, Yonsei University, Korea

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Abstract Book

12th Asian Symposium on Process Systems Engineering

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PL-01

PLENARY

09:00~10:00 · Plenary · D404

Systems Engineering for Industrial Decarbonization

[1]*Andlinger Center for Energy and the Environment, USA*
[2]*Princeton University, USA*

ABSTRACT

We present a general optimization-based framework for designing chemical and energy systems that experience variability at multiple timescales. Motivated by the need to decarbonize manufacturing, we seek to understand the viability of chemical and energy systems subject to temporal variability in physical and economic conditions. In the first part of the talk, we discuss how systems thinking can enhance our understanding of novel strategies to produce renewable fuels and chemicals and, importantly, identify technological and economic drivers, thereby guiding future research efforts. In the second part of the talk, we outline the proposed framework which can be applied to determine the basic configuration and size of unit operations, associated material and energy flows, and relevant state variables. It is also possible to study optimal design between different cases and identify how optimal design evolves over time. Understanding these behaviors is key to designing processes that successfully operate under multi-scale variability. We apply our framework to study green ammonia synthesis, and identify optimal process designs with distinct operational behavior at hourly, seasonal, and (multi-)yearly timescales. Finally, we discuss how the synthesis of systems based on electricity leads, naturally, to new types of problems for which traditional approaches are insufficient; and outline progress towards the development of methods to address these challenges, including approaches that use AI techniques

PL-02

PLENARY

17:00~18:00 · Plenary · D404

To be announced

Hyundai Motors, Korea

ABSTRACT

Abstract to be provided. Please refer to the official website (pseasia2026.org) for the most up-to-date information.

PL-03

PLENARY

09:00~10:00 · Plenary · D404

Making real-world impacts through modeling – a perspective from Pharma PSE research

University of Tokyo, Japan

ABSTRACT

Recent advances in Pharmaceutical Process Systems Engineering (Pharma PSE) at The University of Tokyo demonstrate the transformative role of model-based approaches in pharmaceutical process design and operation. This plenary lecture highlights key achievements across small molecules, biopharmaceuticals, and regenerative therapy products, emphasizing the critical role of hybrid modeling in addressing industrial challenges.

For small molecule manufacturing, our research focuses on the flow synthesis of drug substances. We proposed novel models for various reaction systems, such as the Grignard reaction, which have been successfully applied to determine design spaces and identify optimal operating conditions. In biopharmaceuticals, we investigated cell cultivation for model development, utilizing an automated bioreactor system to generate experimental datasets. This enabled the creation of a robust hybrid model capable of mapping the design space across a wide range of cultivation conditions for a new cell line. Furthermore, in stem cell and regenerative medicine, we developed models for 2D cell cultivation and cryopreservation, with model-based design spaces and optimal conditions being experimentally validated for real-world applications. Beyond these achievements, our lab conducts social-scale research, including an indicator-based assessment of potential supply risks for pharmaceutical excipients, which successfully identified critical compounds requiring mitigation. Together, these studies illustrate the efficacy of model-based process development and underscore the necessity of close collaborations between experimental and simulation researchers.

Finally, this talk addresses critical open discussions, such as balancing modeling costs against realized benefits as well as the cyclic interactions between reality and modeling. Through these themes, a forward-looking perspective will be provided on the evolving role of PSE in the pharmaceutical industry.

K-A1-01

KEYNOTE

10:00~10:30 · Keynote · Session A1 · D404

Responsible AI for the Future of Process Systems Engineering: From Materials Discovery to Adaptive Operation

Hyeon Yang, **Jiyong Kim***

School of Chemical Engineering, Sungkyunkwan University, Korea

ABSTRACT

Artificial intelligence is rapidly transforming the R&D pipeline in the chemical process industries, with growing impact from early-stage problem defining, precise-solving to instant applications. In process systems engineering, AI is not only improving R&D efficiency but also shortening the traditional scale-up loop of “discovery–validation–modification”, thereby accelerating the translation of research outcomes into industrial practice. At the same time, this acceleration raises an important question: how can we ensure that AI is deployed safely, transparently, fairly, and responsibly in industrial settings? This talk argues that the next stage of AI in process systems engineering must go beyond trustworthy or explainable AI and move toward Responsible AI, where robustness, interpretability, fairness, safety, and governance are treated as essential design principles rather than afterthoughts. I will present examples of AI applications across process systems engineering, including materials discovery, surrogate modeling, process design automation, and autonomous operation. A representative case study on direct non-oxidative methane conversion will be used to illustrate how Responsible AI can support catalyst development, reaction modeling, process synthesis, reverse engineering, and uncertainty quantification in a complex multiscale system. The talk will conclude with a perspective on how Responsible AI can help shape the future of process systems engineering from materials discovery to adaptive operation, while ensuring that industrial innovation remains reliable, transparent, and socially accountable.

KEYWORDS

Responsible AI, Multiscale modeling, Direct non-oxidative methane conversion, AI-driven process design

OR-A1-01

REGULAR ORAL

10:30~10:50 · Session A1 · D404

Digital-Twin-Oriented Pedagogical Integration of BatchSep for Dynamic Modeling and Validation of EtOH/H_2O Batch Distillation

Anawin Ampaipisut, Chayut Chokkhanapitak, Vorravit Saelee, Phongsakon Bangsai, Yuthachai Srivaree, Aknarin Nonbudsri, Patcharapon Saranuttee, Atitaya Naknon, Sureeporn Kromthin, Phavanee Narataruksa, and Piyapong Hunpinyo*

Department of Chemical Engineering, King Mongkut's University of Technology North Bangkok, Thailand

ABSTRACT

Batch distillation is a nonlinear , time-varying separation process whose performance depends strongly on reflux strategy , energy input, and termination criteria. In many undergraduate laboratories, these decisions are made by trial- and- error, limiting student’s exposure to model-based reasoning and control -oriented analysis. This study proposes a digital- twin-oriented pedagogical framework that repurposes Aspen Batch Modeler (BatchSep) as a predictive pre- laboratory and validation tool for EtOH/H 2O batch distillation. A 10-stage column at 1 atm with an initial 6 kg charge (20 wt% EtOH) is simulated using a two- phase sequence: constant -reflux charging followed by controlled distillation. The batch ends at 5 wt% EtOH in the still and 99 wt% EtOH in the distillate, with predicted operation of 45- 60 min and reflux ratio 2.5. Experimental validation in tray and packed columns (as shown in Fig. 1) enabl es structured comparison of temperature dynamic s, composition profiles , reflux sensitivity, and endpoint timing. Novelty lies in integrating phase -based operational sequencing, cross -hardware model validation, structured model experiment comparison, and control -oriented interpretation within laboratory instruction. The pedagogical approach reduces material use, improves safety, and strengthen s dynamic reasoning and systematic model refinement. The framework further cultivates ABET -aligned competencies in engineering design under realistic constraints, collaborative teamwork throughout simulation to laboratory validation activities, and professio nal communication through evidence based technical reporting and reflective analysis of model experiment discrepancies.

KEYWORDS

Chemical engineering education, Batch distillation, digital twin education, Aspen BatchSep pedagogy

ACKNOWLEDGEMENTS

The authors gratefully acknowledge Mr. Veerasak Songsujaritkul and Assoc. Prof. Dr. Chaiwat Prapainainar for their valuable support and contributions to the digital enhancement activities associated with this work. The authors also sincerely thank the Department of Chemical Engineering (ChE), Faculty of Engineering, King Mongkut’s University of Technology North Bangkok, for providing laboratory facilities and apparatus support essential to the experimental implementation.

OR-A1-02

REGULAR ORAL

10:50~11:10 · Session A1 · D404

Pathways to Decarbonization for a Garment Manufacturing Facility: LEAP Modeling & Optimization Analysis

Tin Nok Mak[1], **Charlle Sy**[2,*]

[1] *The Hong Kong University of Science and Technology, Hong Kong*
[2] *Cornell University, USA*

ABSTRACT

The garment manufacturing industry accounts for nearly 10% of global carbon emissions, making decarbonization a critical priority. This study develops a strategic roadmap for a global fashion company's largest facility in Gazipur, Bangladesh, to align with Science Based Targets initiative (SBTi) goals of reducing greenhouse gas emissions by 55% by 2033 and 90% by 2050. Using primary operational data, the Low Emissions Analysis Platform (LEAP) was employed to model baseline and mitigation scenarios, including solar photovoltaic integration, electric vehicle fleet transition, cooling system retrofits, and production adjustments. While combined technical measures achieved only a 50% reduction by 2050, a linear programming optimization framework was introduced to identify the most cost-effective mix of interventions under a hard emissions constraint. Results indicate that maximizing rooftop solar capacity, phasing out R-22 refrigerant systems, and targeted electrification of CNG vehicles can meet the 2033 target without reducing production output. The proposed strategy represents the minimum cost pathway to compliance. Findings underscore the limitations of conventional mitigation approaches and highlight the need for integrated optimization to achieve deep decarbonization in resource-intensive industries.

KEYWORDS

Decarbonization, optimization, sustainability, greenhouse gas emissions

OR-A1-03

REGULAR ORAL

11:10~11:30 · Session A1 · D404

Adaptive Model Predictive Control for Cyclic Distillation Columns

Chengtian Cui[1,2,*], Ali Moradvandi[1], and Anton A. Kiss[1]

[1] *Department of Chemical Engineering, Delft University of Technology, Netherlands*

[2] *Faculty of Science and Engineering, Åbo Akademi University, Finland*

ABSTRACT

Cyclic distillation achieves energy savings of up to 35% and higher throughput compared to conventional continuous distillation, making it a key technology in process intensification. The alternating vapor and liquid flow phases introduce strong nonlinearities and transport delays that cause conventional PID controllers to produce purity violations and prolonged transient responses. This study develops an adaptive MPC framework that maintains top and bottom product purities within specified constraints under feed composition disturbances of up to ± 10% and parametric model uncertainties. The MPC employs an ARMA-based linear model whose parameters are updated online using a recursive least-squares algorithm, which is driven by tray temperature and flow rate measurements to track nonlinear process variations across cyclic phases. This dynamic updating model effectively captures nonlinear process variations and precisely compensates for transport delays inherent in the cyclic phases to achieve superior process control. Simulation studies on a 40-stage cyclic distillation column separating methanol/water demonstrate that the adaptive MPC reduces settling time by 10% and maintains purity above 99% across step changes in feed composition and flow rate. These novel results establish adaptive MPC as a viable control strategy for industrial cyclic distillation columns, directly supporting the scale-up of intensified separation processes.

KEYWORDS

Cyclic distillation, Adaptive control, Model predictive control, Periodic operation, Modeling and control, Process intensification

ACKNOWLEDGEMENTS

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OR-A1-04

REGULAR ORAL

11:30~11:50 · Session A1 · D404

Adaptive Reinforcement Learning–Based Energy Management of Electrolyzer-Coupled District Heating Systems under Uncertainty

Nikita Gupta[1], Vahid Khaligh[1], Jay Liu[2,*]

[1]*Institute of Cleaner Production Technology, Korea*
[2]*Pukyong National University, Korea*

ABSTRACT

The increasing penetration of renewable energy sources and industrial waste heat into district heating networks demands advanced control strategies capable of operating under uncertainty in power availability and electricity markets. To improve efficiency and reduce carbon emissions, these systems are increasingly coupled with power-to-hydrogen technologies, yet their operation remains strongly influenced by variability in renewable generation, electricity prices, and coupled thermal–electrical dynamics. This paper presents a reinforcement learning–based control framework for a district heating network integrated with an electrolyzer operating in a power-to-hydrogen-and-heat mode, aiming to learn adaptive operational strategies through direct interaction with a dynamic environment (Khalid et al., 2023). A compact, physically meaningful state representation captures key operational drivers, including electrolyzer temperature, hydrogen storage level, electricity prices, and stochastic renewable power availability. The learned policy coordinates electrolyzer power allocation, hydrogen production and discharge, waste heat recovery, electricity trading, and discrete operating modes, while explicitly managing on–off cycling, degradation costs, temperature constraints, and conversion efficiency. A physics-informed dynamic electrolyzer model embedded within a Proximal Policy Optimization framework enables robust control without explicit forecasting (Gupta et al., 2023). Simulation results demonstrate effective renewable utilization, meaningful waste heat recovery, and improved operational flexibility under uncertainty. References [1] Khaligh, Vahid, Azam Ghezelbash, Mohammadamin Zarei, Jay Liu, and Wangyun Won. "Efficient integration of alkaline water electrolyzer–A model predictive control approach for a sustainable low-carbon district heating system." Energy conversion and management 292 (2023): 117404. [2] Gupta, Nikita, Shikhar Anand, Tanuja Joshi, Deepak Kumar, Manojkumar Ramteke, and Hariprasad Kodamana. "Process control of mab production using multi-actor proximal policy optimization." Digital Chemical Engineering 8 (2023): 100108.

KEYWORDS

District Heating System, Power to hydrogen, Reinforcement Learning, Proximal Policy Optimization, electrolyzer

ACKNOWLEDGEMENTS

Pukyong National University

OR-A1-05

REGULAR ORAL

11:50~12:10 · Session A1 · D404

Physics-Informed Machine Learning Approaches for Accelerating Chemical Process Development

Seokyoung Hong[1,2] and Jong Min Lee[2,*]

[1]*School of Energy and Chemical Engineering, Ulsan National Institute of Science and Technology, Korea*
[2]*Department of Chemical and Biological Engineering, Seoul National University, Korea*

ABSTRACT

Traditional AI models often struggle in chemical engineering due to data scarcity, black- box nature, and physical inconsistencies. Scientific Machine Learning (SciML) addresses these barriers by integrating domain knowledge such as physical laws and governing equations with data-driven architectures. This talk presents a case study demonstrating SciML in practice. A physics-informed neural ODE framework for chemical process development enables accurate extrapolation from small, sparse data and revealing actionable process insights. By bridging the gap between empirical data and mechanistic understanding, SciML offers a path toward data-efficient, physically consistent, and interpretable AI models for complex engineering systems.

KEYWORDS

Scientific Machine Learning, Domain Knowledge, Physics-informed neural ODE, Sparse data, Interpretable AI

ACKNOWLEDGEMENTS

This work was supported by the InnoCORE program of the Ministry of Science and ICT(1.260005.01)

K-A2-01

KEYNOTE

10:00~10:30 · Keynote · Session A2 · D403

Adaptive Machine Learning Models for Fault Detection and Control of Process Systems

Deepak Kumar[1], Amal Anto[1], Hariprasad Kodamana[1,2,3], and **Manojkumar Ramteke**[1,2,*]

[1] *Department of Chemical Engineering, Indian Institute of Technology Delhi, India*
[2] *Yardi School of Artificial Intelligence, Indian Institute of Technology Delhi, India*
[3] *ANSK School of Information Technology, Indian Institute of Technology Delhi, India*

ABSTRACT

Machine Learning models are shaping the process-system-engineering significantly. However, these often lack the physical basis, interpretability and require a tedious training process. To alleviate these challenges, several interesting algorithms have been developed to incorporate the physics of the problem, eliminating the backpropagation used in neural networks, and improving the accuracy. A forward-learning neural network framework is one such algorithm developed to efficiently update data-driven models in real time for high-frequency data without compromising the accuracy for fault detection in the Tennessee-Eastman dataset, nuclear power flux dataset, and wastewater plant dataset. A Kernel-based Forward Propagating Neural Network (K-FP-NN) is another algorithm developed to eliminate backpropagation, using layer-wise updates for better adaptability for model predictive control of a continuous stirred tank reactor (CSTR) system. Further, a new concept of machine unlearning, which eliminates the impact of faulty data on the trained model with less computational effort than complete retraining, is illustrated on the Tennessee-Eastman dataset and wastewater plant dataset. A unified continual machine learning and unlearning framework for adaptive and corrective model maintenance is developed for Continuous stirred tank reactor (CSTR), Batch Polymerization of Methyl Methacrylate (PMMA) and Gas-Liquid Absorption System (GLAS) exhibiting systemic drift.

KEYWORDS

Forward-learning, Fault detection, Machine unlearning, Systemic drift

ACKNOWLEDGEMENTS

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OR-A2-01 **REGULAR ORAL**
10:30~10:50 · Session A2 · D403

Optimization for the design and operation of flexible Power-to-ammonia systems

Li Zhou[*], Xudong Zhou, Zhang Qingqing, Tian Qiu, Xu Ji

School of Chemical Engineering, Sichuan University, China

ABSTRACT

Decarbonizing chemical industry via renewable hydrogen integration is of strategitic importance for achieving carbon neutrality, yet this transition faces challenges. The inherent intermittent of green hydrogen supply can render the chemical production system accident-prone if not properly addressed. In this context, conventional approaches for system design and operation fall short of practical requirements. To address the challenge, we conducted a series of investigations concerning the Power-to-ammonia system design and operation. Regarding system design, multi-level optimization approaches that integrate system configuration and annual operation scheduling were proposed to address mismatch between intermittent renewable supply and the stable operation requirements of chemial production. Furthermore, high-fidelity models based on reaction mechanisms and Physical-Informed Neural Network were developed to accurately depict the behavior of catalytic reaction systems across a wide operating regime under intermittent renewable feedstocks. Results indicate that enhanced system responsiveness can improve both the economic performance and carbon reduction, though accompanied by an increase in the Average Cumulative Volatility (ACV) of system operation. Our study also reveals that the ammonia synthesis system exhibits notably different behavior across different production loads. Appropriate regulation of purge gas flow rate, reactor inlet temperature, and flash separation temperature is crucial for the system to maintain robust production and improve energy efficiency under varying renewable supply scenarios.

KEYWORDS

Green hydrogen, Power-to-Ammonia, Capacity configuration, Operation optimzation, Modeling and optimization

ACKNOWLEDGEMENTS

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OR-A2-02

REGULAR ORAL

10:50~11:10 · Session A2 · D403

Evaluating Methanol Production Pathways from CO_2 and H_2O via High-Temperature Electrolysis Systems

Edward Egbert[1], Alif Syafiq Zaahir Zaidan Hartono[1], Matthew Putrafael Situmorang[1], **Riezqa Andika**[1,2,*]

[1]*Process Systems Engineering Lab, Department of Chemical Engineering, Universitas Indonesia, Indonesia*
[2]*Center of Excellence for Low Carbon Fuels, Universitas Indonesia, Indonesia*

ABSTRACT

This study presents a techno-economic analysis of methanol production pathways utilizing syngas derived from high-temperature solid oxide co-electrolysis of H2O and CO2. Two process configurations were evaluated: (i) integrated co-electrolysis and CO2 electrolysis, and (ii) standalone co-electrolysis. Process simulations were performed to assess key operational parameters, including current requirements, number of cells, active cell area, and overall power consumption. In addition, feedstock demands for H2O and CO2 were estimated for each configuration to determine material intensity and system efficiency. The economic feasibility of each pathway was examined under multiple scenarios considering reductions in solid oxide electrolysis cell (SOEC) stack investment costs and the implementation of carbon pricing incentives. The analysis focused on the impact of these factors on the overall cost structure and methanol selling price. Results indicate that system configuration significantly influences both energy consumption and economic performance, with co-electrolysis-based pathways generally offering improved efficiency and lower production costs. Overall, this work highlights the importance of process integration and policy support in enhancing the viability of sustainable methanol production from CO2 and H2O.

KEYWORDS

Carbon dioxide utilization, Co-electrolysis, Solid oxide electrolysis cell, Methanol synthesis

OR-A2-03

REGULAR ORAL

11:10~11:30 · Session A2 · D403

A process simulator of cryopreservation for human induced pluripotent stem cells

Maimi Nakano[1], Yusuke Hayashi[1,*], Yuki Uno[2,3], Masahiro Kino-oka[2,3], Hirokazu Sugiyama[1]

[1]*Department of Chemical System Engineering, The University of Tokyo, Japan*
[2]*Department of Biotechnology, The University of Osaka, Japan*
[3]*Research Base for Cell Manufacturability, The University of Osaka, Japan*

ABSTRACT

Human induced pluripotent stem (hiPS) cells have emerged as a promising source for regenerative medicine products. Recently, several clinical studies have been successful (e.g., Parkinson's disease [1]), and the realization of regenerative medicine using hiPS cells is becoming possible. In hiPS cell manufacturing, cryopreservation is one of the most important steps because it is necessary for the transportation and preservation. In general, cryopreservation processes consist of the following three subprocesses: freezing, storage, and thawing.

In the field of process systems engineering, model-based approaches have been applied to stem cell manufacturing processes, e.g., computer-aided exploration of multiobjective optimal temperature profiles in freezing [2] and determination of design spaces for cultivation [3]. However, modeling of cryopreservation processes comprehensively has not been conducted, which leads to difficulty in determining the design parameters reasonably.

This work presents a process simulator of cryopreservation for hiPS cells. The simulator consists of the three subprocess models. Given the operating conditions of the three subprocesses, the simulator can evaluate the cell potential until 24 h after seeding, which can contribute to designing the cryopreservation process reasonably.

References: [1] Sawamoto, et al., Nature (2025); [2] Hayashi, et al., Comput. Chem. Eng. (2021); [3] Hirono, et al., Commun. Biol. (2025).

KEYWORDS

Process design, Operation, Hybrid modeling, Regenerative medicine, Manufacturing, Cold chain

ACKNOWLEDGEMENTS

Y. H. is thankful for the financial support by the Japan Society for the Promotion of Science under grant number 23K13593.

OR-A2-04

REGULAR ORAL

11:30~11:50 · Session A2 · D403

Superstructure-based Optimization for E-fuel Production using Solid Oxide Electrolysis Cells

Meng Qi[1,2,*], Zhengyang Song[2], and Haoshui Yu[2]

[1]*College of Chemistry and Chemical Engineering, China University of Petroleum (East China), China*
[2]*Department of Chemistry and Bioscience, Aalborg University, Denmark*

ABSTRACT

Power-to-X offers a promising route for large-scale, long-term renewable energy storage, but the production of hydrogen (H2)/syngas (H2/CO) for e-fuel synthesis remains the main techno-economic bottleneck in e-fuel synthesis. Solid oxide electrolysis cells (SOECs) provide an efficient platform for generating H2, CO, and syngas, yet the optimal choice among steam electrolysis, co-electrolysis, CO2 electrolysis, and their possible integration with water–gas shift or reverse water–gas shift reactions remains unclear. This study addresses that challenge through surrogate-based superstructure optimization with process integration and techno-economic assessment. The optimization identifies cost-optimal and previously unexplored hybrid SOEC pathways, including configurations that combine steam and CO2 electrolysis as well as routes integrating additional shift reactions to tailor feed composition. Detailed process analysis shows that pathway selection strongly affects feed-gas quality, energy consumption, and overall system efficiency. The proposed framework provides a general methodology for identifying competitive SOEC-based front-end designs for a wide range of e-fuel production pathways.

KEYWORDS

Power-to-X; solid oxide electrolysis cell (SOEC); superstructure; surrogate optimization; process synthesis

ACKNOWLEDGEMENTS

This work was supported by the National Natural Science Foundation of China (No. 22408402), the European Union HORIZON-MSCA-2024-PF-01 (No. 101210608), and the Shandong Provincial Taishan Scholar Program (No. tsqn202507133).

OR-A2-05

REGULAR ORAL

11:50~12:10 · Session A2 · D403

Process development and demonstration for olefin production from steel mill gases

Myung Kyun Lim[1], Cheonwoo Jeong[2], Doowook Kim[3], Kosan Roh[4], Yong-Ki Park[1,*], **Kiwoong Kim**[1,*]

[1]Green Carbon Research Center, Korea Research Institute of Chemical Technology (KRICT), Republic of Korea
[2]Industrial Gas Research Cell, Research Institute of Industrial Science & Technology (RIST), Republic of Korea
[3]Hydrogen Research Department, Korea Institute of Energy Research, Republic of Korea
[4]Department of Chemical Engineering and Applied Chemistry, Chungnam National University, Republic of Korea

ABSTRACT

Blast furnace gas is a byproduct generated during the reduction of iron ore, containing approximately 20–25% CO and 3% H2, with the remainder consisting of CO2 and N2. Due to its high concentrations of CO2 and N2, blast furnace gas is currently utilized as a heat source in power plants, resulting in annual domestic greenhouse gas emissions of 60 million tons. This study aims to discuss the development of low-carbon chemical processes utilizing blast furnace gas, a major source of carbon emissions in the steel industry. To achieve this, low-carbon chemical process technologies were developed using steady-state modeling, dynamic modeling, and a system-level integration approach. To evaluate the developed processes, life cycle assessment (LCA) and economic feasibility analyses were conducted, and global sensitivity analysis was used to identify hotspots associated with high CO2 emissions and high-cost process points. The results confirmed that the VPSA process, which recovers CO from by-product gas, generates significant carbon emissions. To mitigate this, we conducted research on artificial neural network optimization based on integrated process simulation. Based on these results, we designed and constructed a pilot process for the chemical conversion of blast furnace gas, and we intend to discuss the process demonstration process and results from a process system perspective.

KEYWORDS

Blast furnace gas, process development, demonstration, olefin

ACKNOWLEDGEMENTS

This work was supported by the National Research Foundation of Korea(NRF) grant funded by the Korea government(MSIT) (RS-2024-00466475) and by the National Research Council of Science & Technology (NST), grant funded by the Korean government (MSIT) (No. CRC22043-400).

OS-A3-01

STUDENT ORAL
10:00~10:15 · Session A3 · D402

Development of a Cost-Effective Green LH2–NH_3 Hybrid Value Chain via LN2 Circulation and a Heat-Integrated Power Cycle

Yejin Lee, and Inkyu Lee*

School of Chemical Engineering, Pusan National University, Korea

ABSTRACT

Liquid hydrogen (LH2) and ammonia (NH3) are expected to play key roles as hydrogen carriers to address the geographic imbalance in renewable energy generation. However, each process in a standalone value chain has inherent limitations. In conventional LH2 value chains, hydrogen liquefaction consumes substantial power, while cryogenic cold energy is wasted during regasification. In typical NH3 value chains, ammonia synthesis requires significant power for air separation and N2 compression. Meanwhile, medium-grade heat in the flue gas is partially recovered in the NH3 decomposition process. To address these issues across the value chains, we propose a novel hybrid value chain integrating the LH2 and NH3 supply systems. In the hybrid value chain, (1) LN2 is produced by utilizing LH2 cryogenic energy and returned to the export site. It provides cold energy for precooling H2 and is subsequently used as the N2 feedstock for NH3 synthesis. (2) A power cycle is introduced to recover both LH2 cold energy and the waste heat in the flue gas from NH3 decomposition. The proposed value chain was evaluated thermodynamically and economically, demonstrating improved performance under supply–demand balanced conditions.

KEYWORDS

Process design; Liquid hydrogen supply chain; Green ammonia supply chain; Power cycle; Air separation unit

ACKNOWLEDGEMENTS

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (RS-2024-00341380).

OS-A3-02

STUDENT ORAL

10:15~10:30 · Session A3 · D402

Targeting CO_2 emission in a Carbon Capture and Utilisation facility with epistemic uncertainty in the parameters

Abhishek Kumar Pandey*, Santanu Bandyopadhyay

Department of Energy Science and Engineering, Indian Institute of Technology Bombay, India

ABSTRACT

Mitigating CO2 emissions from industries is the 13th Sustainable Development Goal (SDG) set by the United Nations. Carbon capture and utilisation (CCU) is an emerging technology that significantly reduces CO2 emissions from industries by capturing CO2 and utilising it for economic benefits. The CCU facility in industrial parks is designed to maximise CO2 capture with exact parameters using pinch techniques. Lack of system knowledge and unavailability of past data at the design stage introduce epistemic uncertainty in parameters. The existing literature reports incorporation of epistemic uncertainty with pinch technique to minimise resource requirement. This work focuses on minimising CO2 emission from a CCU facility. The mathematical formulation presented in this paper incorporated epistemic uncertainty in parameters using interval numbers. The Best-Worst approach and pinch analysis are used to determine the minimum CO2 emission from a CCU facility. The best-case and the worst-case for CO2 minimisation are identified, and the pinch technique is applied to obtain the solution. The highest and lowest values of minimum CO2 emission are the two extreme solutions and define the interval for CO2 emission from CCU facility. The optimisation approach is demonstrated through an illustrative case study on CCU facility.

KEYWORDS

CCU, Epistemic uncertainty, Pinch Analysis, Interval linear programming

OS-A3-03

STUDENT ORAL

10:30~10:45 · Session A3 · D402

Rigorous and Robust Equation-Oriented Phase Equilibrium Formulation via Phase Stability-Driven Characteristic Variables

Luoyu Zhang[1], Xijun Wang[1], Jun Zhao[1], Jianping Wang[2], Shaohui Tao[1,*], Li Xia[1], Lili Wang[1], Xiaoyan Sun[1,*], and Shuguang Xiang[1]

[1]*Qingdao University of Science and Technology, China*
[2]*Petro-Cyber Works Information Technology Co. Ltd, China*

ABSTRACT

While recent complementarity-based models improve the robustness of equation-oriented (EO) vapor-liquid equilibrium (VLE) calculations, they frequently rely on heuristic simplifications of the cubic equation of state (CEOS). These numerical compromises ensure solver convergence but inherently violate strict thermodynamic phase stability criteria. To resolve this fundamental trade-off, we propose a novel, thermodynamically rigorous, and numerically robust EO flash formulation. First, we reconstruct the simultaneous solution method using phase characteristic variables, formally proving its mathematical equivalence to Gibbs free energy minimization and Tangent Plane Distance (TPD) analysis. Next, to overcome singularities from vanishing physical roots in single-phase regimes, we integrate an analytical pseudo-root method. This preserves the unsimplified CEOS structure while guaranteeing strict continuity and smoothness for all thermodynamic properties and their analytical derivatives across phase boundaries. Implemented in our in-house OPEN simulation platform, extensive PT/PH sweeps and flowsheet validations demonstrate that our model seamlessly navigates phase transitions. By completely eliminating the need for thermodynamic compromises, this work exhibits exceptional initialization efficiency and global convergence, establishing a rigorous new paradigm for large-scale EO optimization.

KEYWORDS

Equation-Oriented;Vapor-Liquid Equilibrium; Cubic Equation of State; Phase Stability

ACKNOWLEDGEMENTS

This work is supported by the Key R&D Program of Shandong Province China (No. 2024CXGC010405) ,National Natural Science Foundation of China (No. 22178190), the National Youth Natural Science Foundation of China (No. 22408195), and Shandong Key Laboratory of Chemical Process Simulation and Optimization Industrial Software (PKL2024F23)

OS-A3-04

STUDENT ORAL

10:45~11:00 · Session A3 · D402

Electrified Reheating of Circulating Sand for Biomass Fast Pyrolysis Toward Low-Carbon Marine Fuels

Aditia Aulia, Daejun Chang*

Department of Mechanical Engineering, Korea Advanced Institute of Science and Technology, Korea

ABSTRACT

The decarbonization of industrial heat and marine fuels is a critical challenge for the maritime sector. While biomass fast pyrolysis offers a pathway to renewable fuels, conventional systems rely on the combustion of process by-products (char and non- condensable gases). This study evaluates the technical feasibility and techno-economic implications of electrifying circulating sand reheating in a circulating fluidized bed reactor to produce upgraded, HFO-range marine biofuels. A kinetic fast pyrolysis model implemented in Aspen Plus was integrated with electrified sand reheating and thermal energy storage to define an operating envelope. Process parameters, including sand temperature and sand-to-biomass ratio (S/B) were varied to quantify riser outlet temperature and reheating duty. Results show that electrified reheating can achieve fast pyrolysis conditions with reheating duties of approximately 3.0–3.5 MW for S/B = 7.5 at target sand temperatures of 600–650 °C. For a representative case, the minimum fuel selling price is estimated at 42.7 $/GJ using grid electricity and 38.7 $/GJ using renewable electricity. Including biochar sequestration credits further reduces MFSP to 32.7 $/GJ at a carbon price of 100 $/tCO2. These results demonstrate that electrified circulating sand reheating provides a viable pathway for low-carbon or potentially carbon-neutral marine fuel production.

KEYWORDS

biomass fast pyrolysis, process electrification, thermal energy storage, marine fuels

OS-A3-05

STUDENT ORAL

11:00~11:15 · Session A3 · D402

Optimization of Methanol Synthesis from Blast Furnace Gas using Surrogate Model

Akihide Wakita[1], Sagar Saren[1], Tomoyuki Yajima[1], Kohei Yoshikawa[2], Yuta Nishikawa[2], Nobuyuki Shigaki[2], and Yoshiaki Kawajiri[1,3,*]

[1]Department of Materials Process Engineering, Nagoya University, Japan
[2]Steel Research Laboratory, Japan
[3]School of Engineering Science, LUT University, Finland

ABSTRACT

The concept of carbon dioxide capture and utilization (CCU) converts CO2 into chemicals and fuels. Among many potential CCUS approaches, producing methanol from captured CO2 is gaining attention; however it remains more costly, largely due to the high costs of CO2 separation and H2 production. CO2 separation by chemical absorption and physical adsorption has been widely explored. Vacuum pressure swing adsorption (VPSA) is attractive because of its operational flexibility and its potential to reduce costs when very high CO2 purity is unnecessary; accordingly, VPSA has been studied for multiple emission sources. To relieve synthesis equilibrium constraints and enable reductions in hydrogen cost, membrane reactors couple reaction with separation; continuous removal of products, especially water, shifts equilibrium and increase conversion. Here we conduct multi-objective optimization of a blast furnace gas CCU flowsheet consisting of a water–gas shift (WGS) reactor, VPSA, and a membrane methanol reactor. These unit operations are modeled using mass and energy balances. Because solving the VPSA model to cycle steady state (CSS) is computationally intensive, we develop a surrogate model over a wide range of operating conditions. The integrated optimization minimizes energy use and maximizes productivity, generating Pareto fronts that elucidate key economic trade-offs.

KEYWORDS

Carbon dioxide Capture and Utilization, Methanol Synthesis, Vacuum Pressure Swing Adsorption, Membrane Reactor, Surrogate modeling

ACKNOWLEDGEMENTS

This research is based on results obtained from a project, JPNP16002, commissioned by the New Energy and Industrial Technology Development Organization (NEDO).

OS-A3-06

STUDENT ORAL

11:15~11:30 · Session A3 · D402

A computer-aided screening of cryoprotective agents for stem cells utilizing transfer learning

Akihiro Kimura[1], Rei Tamaki[1], Yusuke Hayashi[1,*], Yuki Uno[2], Masahiro Kino-oka[2], and Hirokazu Sugiyama[1]

[1]*Department of Chemical System Engineering, The University of Tokyo, Japan*
[2]*Department of Biotechnology, The University of Osaka, Japan*

ABSTRACT

Stem cell therapy has recently emerged as a key player in regenerative medicine. In stem cell manufacturing, freezing processes are one of the most critical steps because the process is necessary to the transportation and preservation. Cryoprotective agents (CPAs) are compounds that protect cells from freezing injuries. Currently, dimethyl sulfoxide (DMSO) is widely used as a CPA, although DMSO has been reported to exhibit cytotoxicity and differentiation-inducing properties [1], making the development of CPAs for stem cells an urgent priority. In the field of process systems engineering, computer-aided large-scale screening has been conducted based on physical properties [2,3]. However, trial-and-error experiments for each cell type are still necessary using these previous methods. This work presents a computer-aided screening of CPAs utilizing transfer learning with different cell types. Freezing injuries were estimated from molecular information using a previously developed freezing process model [4]. As a result, two promising compounds were selected in the computer screening, and it was confirmed a one of them had a cryoprotective effect in a freezing experiment. References: [1] Awan, et al., Regen. Med. (2020); [2] Hayashi, et al., Cryobiology (2021); [3] Tamaki, et al., Digit. Chem. Eng. (2025); [4] Hayashi, et al., Comput. Chem. Eng. (2020).

KEYWORDS

Molecular design, Cryopreservation, Hybrid modeling, Regenerative medicine, Manufacturing, Cold chain

ACKNOWLEDGEMENTS

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OS-A3-07

STUDENT ORAL
11:30~11:45 · Session A3 · D402

Comparative Analysis of Karnopp and He-Based Valve Stiction Models Incorporating Valve Characteristic Transfer Functions for Temperature Control in Deferasirox Purification

Anuchit Wuttitrairat[1], Soottiwan Thamsakona, Wachira Daosud[2] ,Paisan Kittisupakorn[1,*]
[1]*Faculty of Engineering, Chulalongkorn University Bangkok, Thailand*
[2]*Department of Chemical Engineering, Burapha University, Thailand*

ABSTRACT

Valve stiction is an important source of oscillations and performance degradation in chemical process control systems and especially in the temperature-sensitive pharmaceutical production process, and herein pharmaceutical manufacturing processes are considered. In this paper, the valve nonlinear friction effect on temperature control performance in the purification of deferasirox is examined. The purification step of deferasirox demands tight temperature regulation at 55 °C to accomplish total dissolution, ratiocinatedicedation and purity of product. A comparative study of the He and the Karnopp valve stiction models with valve characteristic transfer functions is performed under a simulated jacketed continuous stirred tank reactor (CSTR) for the deferasirox purification process. The criteria to assess the models are their capability to mimic stick–slip behavior and dynamic valve properties that can influence the thermal control quality at the set point of 55 °C. Modeling accuracy and control performance are evaluated using time-domain simulations and Mean Squared Error (MSE) analysis. These results shows the effect of valve stiction on the accuracy of tracking temperature, settling time and, finally, the quality of the product in pharmaceutical crystallization process. The results could help enhance the control reliability and therefore provide a steady operation at 55 °C for reproducible purity in the large scale production of industrial deferasirox.

KEYWORDS

Valve stiction; Karnopp and He models; Temperature control; Deferasirox; Pharmaceutical process control

ACKNOWLEDGEMENTS

We thank Center of Excellence in Intelligent Control Automation of Process Systems, and Department of Chemical Engineering, Faculty of Engineering, Chulalongkorn University Bangkok, 10330 for financial support of this work.

OS-A3-08

STUDENT ORAL

11:45~12:00 · Session A3 · D402

Multi-objective optimization of non-adiabatic reactor configurations for renewable diesel production from waste cooking oil

Bangkit Gotama[1,2], and Hao-Yeh Lee[1,*]

[1]*Department of Chemical Engineering, National Taiwan University and Science and Technology, Taiwan*
[2]*Department of Chemical Engineering, Institut Teknologi Kalimantan, Indonesia*

ABSTRACT

Renewable diesel from waste cooking oil (WCO) offers a low-carbon fuel option for hard- to-abate sectors. Hydroprocessing reactions are highly exothermic and, in adiabatic reactors, can lead to temperature runaway and catalyst deactivation. Although isothermal reactors can maintain reactor temperature, they remain impractical at an industrial scale due to excessive utility demand. Non -adiabatic configurations provide a more viable alternative by enabling controlled heat removal along the reactor length. Despite their relevance, these configurations remain underexplored in WCO hydroprocessing for biofuel production. This study addresses that gap by evaluating co-current and counter- current cooling configurations. An integrated framework combining process simulation, sensitivity analysis, and multi -objective optimization is employed. The optimization simultaneously minimizes total annual cost (TAC), energy consumption, and CO2 emissions. A multi-criteria decision-making approach selects the optimal design from the Pareto-optimal set. The selected designs are then compared across configurations. The results reveal clear trade-offs. The counter-current design achieves a lower TAC (18.8% reduction) and lower energy consumption (52.86% reduction). In contrast, the co-current configuration yields lower CO2 emissions (10.27% reduction). These findings confirm that no single configuration dominates all objective metrics. Integrating process optimization with multi-criteria decision-making is therefore essential for navigating such trade-offs toward more sustainable biofuel production.

KEYWORDS

Renewable diesel, waste cooking oil, non-adiabatic reactors, multi-objective optimization, multi-criteria decision-making.

ACKNOWLEDGEMENTS

The authors thank to National Science and Technology Council (NSTC) of Taiwan for the financial support under the grand of NSTC 113-2221-E-011 - 011 -MY3.

OS-A4-01

STUDENT ORAL

10:00~10:15 · Session A4 · D408

Multiscale Simulation and Mechanism Analysis of R23-R116 Separation by Ionic Liquid Extractive Distillation

Kexin Yin, Chun Deng*

College of Chemical Engineering and Environment, China University of Petroleum, China

ABSTRACT

Electronic-grade trifluoromethane (R23) is an indispensable high-purity etching and cleaning gas in semiconductor and display panel manufacturing. With the rapid development of advanced manufacturing processes such as integrated circuits and OLED in recent years, the demand for high-purity R23 has been increasing. This work focuses on the challenge of difficult efficient separation of the R23-R116 azeotropic system, and proposes an ionic liquid (IL) extraction distillation separation process, aiming to simultaneously achieve the high-purity production of R23 and the resource recovery of R508B refrigerant. Based on the COSMO-RS model, the feasibility of separating R23-R116 using 160 kinds of ILs was predicted. And the melting points and viscosities of these 160 ILs were predicted using the group contribution method. Through quantum chemical calculations and molecular dynamics simulations, the electrostatic potential distribution and interaction mechanism between the IL and R23, R116 molecules. The diffusion behavior of the components to be separated in the IL was clarified, and optimal extractants were determined. Finally, the Aspen Plus simulation verified that this process could purify R23 to the electronic grade standard and achieve the efficient recovery of R116. This work provides a new technical path for fluorine-containing azeotropic refrigerant recovery and low-cost electronic-grade gas preparation.

KEYWORDS

Trifluoromethane, Ionic liquid, Extractive distillation, Molecular simulation

ACKNOWLEDGEMENTS

This work was supported by the National Natural Science Foundation of China (No. 22578490).

OS-A4-02

STUDENT ORAL

10:15~10:30 · Session A4 · D408

Techno-Economic Analysis of Sustainable Aviation Fuel Production Process Incorporating Aromatics from Waste Plastic Pyrolysis

Jeongheon Kim, and Inkyu Lee*

School of Chemical Engineering, Pusan National University, Korea

ABSTRACT

Aromatic compounds are key components for meeting aviation fuel specifications in sustainable aviation fuel (SAF). However, previous studies have primarily focused on addressing the high production cost of SAF, while paying limited attention to the role of aromatics. In 2023, global plastic production reached approximately 414–436 million metric tonnes (Mt), generating about 300–350 Mt of plastic waste. Waste plastics (WP) can generate aromatics at low cost through pyrolysis. This makes them a promising resource for meeting the aromatic requirements specified in American Society for Testing and Materials (ASTM) D7566. Therefore, utilizing WP provides an opportunity to reduce SAF production costs and achieve compliance with ASTM D7566 specifications. In this study, a SAF production process incorporating aromatics derived from WP pyrolysis is proposed while satisfying ASTM D7566 specifications. For comparison, a SAF production process in which aromatics are generated from syngas was also evaluated as a reference process. Energy and techno-economic analyses reveal that the WP–based process exhibits superior energy efficiency and economic performance compared to the syngas-based process. These results demonstrate the potential of WP pyrolysis as an effective strategy for supplying aromatics and enhancing the feasibility of ASTM D7566-compliant SAF production process.

KEYWORDS

Sustainable aviation fuel production; Process design; Waste plastic pyrolysis; ASTM D7566; Techno-economic analysis

ACKNOWLEDGEMENTS

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (RS-2024-00341380).

OS-A4-03

STUDENT ORAL

10:30~10:45 · Session A4 · D408

Behavioral Modelling in Eco-Industrial Parks Using Game Theory and Personality Traits

Leap Wun Yip, and Jui-Yuan Lee*

Department of Chemical Engineering, National Cheng Kung University, Taiwan

ABSTRACT

Despite the circular economy’s critical role in sustainability, the global circularity rate has declined to 7.2% according to the Circularity Gap Report 2024, highlighting a gap between theory and implementation. In the context of Process System Engineering (PSE), techno-economic and environmentally driven models have been effectively optimized, yielding both economically and environmentally beneficial solutions. However, existing frameworks assume seamless collaboration, ignoring the human behavioral constraints that often exist in real-world multi-stakeholder networks. This research proposes a personality-aware optimization framework integrated with a game-theoretic approach for behavioral modelling in decision-making. By incorporating the Big Five personality traits (i.e., openness, conscientiousness, extraversion, agreeableness, and neuroticism) as key decision variables, the cost of behavior is quantified, reflecting collaboration propensity, risk aversion, and bias factors. A case study of a waste-to-product network in hi-tech eco-industrial parks is used to demonstrate the proposed methodology. The optimization adjusts theoretical objectives to perceived objectives, accounting for these behavioral factors. The result shifts the cost-effective, environmentally friendly network toward a more socially robust solution. In essence, the proposed approach offers a rigorous method for designing resilient networks that accounts for the reality of human decision-making.

KEYWORDS

Circular economy, Mathematical programming, Process optimization, Waste management, Waste-to-product, Industrial symbiosis

OS-A4-04

STUDENT ORAL
10:45~11:00 · Session A4 · D408

MPEC-Based Dynamic Optimization of Packed Column Batch Distillation Startup

Na Gyeong Lee and Jong Woo Kim*

Department of Chemical Engineering, Incheon National University, Korea

ABSTRACT

Batch distillation startup from dry initial conditions presents significant computational challenges due to the emergence of degenerate equation systems when liquid holdup approaches zero. While this transient phase is critical in practice, its systematic optimization remains largely unexplored, particularly for packed columns. This work presents a mathematical programming with equilibrium constraints (MPEC) framework for the dynamic optimization of packed column batch distillation startup. The formulation incorporates Billet–Schultes hydraulic correlations to capture the pressure drop and liquid holdup characteristics specific to packed columns. Two distinct types of degeneracy are identified and systematically addressed: formulation-level degeneracy through ε-smoothing of complementarity constraints, and solution-level degeneracy through a δ-continuation strategy with primal–dual warm restarts. A physics-informed initial guess construction procedure is developed, combining equilibrium-based composition profiles, hydraulic pre-calculation, and thermal initialization. The resulting nonlinear program is solved using CasADi with IPOPT and an external continuation loop, avoiding the need for specialized complementarity solvers. The generality of the framework is demonstrated across multiple binary systems exhibiting varying degrees of non-ideality, using modified Raoult's law with NRTL activity coefficients. Results confirm monotonic convergence of complementarity residuals and feasible optimal startup trajectories reaching target specifications across all case studies, validating the robustness of the proposed approach.

KEYWORDS

batch distillation, MPEC, dynamic optimization, packed column, cold startup, complementarity

OS-A4-05

STUDENT ORAL

11:00~11:15 · Session A4 · D408

A Generalized and Robust Initialization Framework for Complex Distillation Columns Using a Pseudo-Transient Hybrid Integration Strategy

Yadi Gao[1], Yiqing Luo[1,2,*], Shengkun Jia[1,2] , Xigang Yuan[1,2]

[1]*School of Chemical Engineering and technology, Tianjin University, China*
[2]*National Engineering Laboratory of Chemical Engineering and Low Carbon Technology (Tianjin University), China*

ABSTRACT

Simulating complex distillation columns with multiple feeds, side draws, and pump-around circuits remains challenging due to the difficulty of reliably initializing large-scale, highly nonlinear models. This work presents a generalized pseudo-transient equilibrium-stage model for full-column simulation, eliminating the need for sectional decomposition. By embedding the steady-state equations within a pseudo-dynamic framework, the proposed method generates high-quality initial guesses through numerical integration, thereby reducing sensitivity to initial conditions. To efficiently solve the resulting large-scale differential–algebraic system, a hybrid integration algorithm is developed that reformulates the tightly coupled interstage mass and energy balance equations into a sequence of flash-type subproblems. This strategy effectively alleviates numerical stiffness and significantly improves computational efficiency. The proposed framework is validated using industrial atmospheric and vacuum crude distillation columns handing wide-boiling mixtures. Compared with the implicit Euler method, the hybrid integrator demonstrates faster convergence and more robust initialization performance under demanding operating conditions. Overall, the proposed approach provides a reliable and efficient strategy for initializing and simulating complex distillation columns, facilitating steady-state convergence in large-scale process models.

KEYWORDS

complex distillation column; pseudo-transient method; robust initialization;; hybrid integration algorithm; large-scale DAE systems

OS-A4-06

STUDENT ORAL

11:15~11:30 · Session A4 · D408

Al-rich Beta Zeolite Acidity Tuning for Enhanced C4 Alkylation Selectivity via Cobalt Modification

Ming Wen, Yijie Ding, Minglei Yang*, Yichun Li, Weizhong Zheng, Weizhen Sun*, and Ling Zhao

School of Chemical Engineering, East China University of Science and Technology, China

ABSTRACT

Beta Zeolite is one of the most promising green catalysts for the isobutane (C4) alkylation with the advantages of eco-friendliness and facile separation. Although Al-rich Beta zeolites are found to exhibit a longer catalytic lifetime in C4 alkylation, they suffer from low selectivity owing to the severe cracking reactions induced by their numerous strong Brønsted acid sites (BAS). In this work, cobalt-modification has been used to modulate the acidity of Al-rich beta zeolite to improve the selectivity of C4 alkylation. The highly dispersed, tetrahedrally coordinated isolated Co(II) species are confirmed to be located at the zeolite cationic sites. These cobalt species exist as Lewis acid sites, with the formation of Co-H species accelerating the hydride transfer rate. Among Co@HB-1 catalysts with various cobalt loadings, the 1.7Co@HB-1 sample exhibits the highest catalytic productivity. Moreover, in the optimization of process conditions, a lower olefin WHSV slows coke accumulation to extend lifetime but intensifies cracking, which in turn reduces RON; a higher I/O ratio accelerates hydride transfer kinetics and thus enhances RON. This study provides fundamental insights into tuning acidity of zeolites for significantly enhanced C4 alkylation selectivity. In future work, we will conduct research on the reaction kinetics modeling of the cobalt-modified Al-rich Beta zeolite catalyzed C4 alkylation system, to further elucidate the reaction mechanism and provide a theoretical basis for the industrial application of this catalyst system.

KEYWORDS

Al-rich beta zeolite, Cobalt loading, Isobutane alkylation, Acidic-modification

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OS-A4-07

STUDENT ORAL

11:30~11:45 · Session A4 · D408

Hydrogen Supply Chain Modeling and Optimization to Decarbonize Steel, Fertilizer, and Steel Sectors

Harsh Bajpai, **Nikhil Sharma**, Ishan Bajaj*

Department of Chemical Engineering, Indian Institute of Technology, India

ABSTRACT

This study develops a linear optimization model based on a resource task network (Fig. 1a) to identify a cost-minimizing hydrogen supply chain to decarbonize refineries, fertilizer, and steel sectors. Specifically, we analyze the roles of grey and blue hydrogen produced at demand zones, alongside green hydrogen (GH2) supplied from designated hubs, in achieving decarbonization goals. The model considers spatiotemporally varying demand and resource availability, green hydrogen share (GH2S), emission reduction targets (ERT), transportation by trucks, and mass and energy balance constraints. We consider three hydrogen hubs and demand zones comprising of steel plants, fertilizer plants, and refineries located throughout India (Fig. 1b). Six scenarios are evaluated based on GH2S and ERT, denoted as GH2S|ERT. Results indicate that increasing GH2S and ERT drives the transition from grey and blue hydrogen toward GH2. However, more than 75% GH2 deployment is constrained by renewable resource availability at hydrogen hubs and transportation-related emissions between hubs and demand zones (Fig. 1c). Hence, the complete substitution of grey hydrogen with low-carbon and renewable hydrogen does not fully eliminate baseline emissions in the current grey-hydrogen system. Finally, we note that higher GH2S and ERT levels lead to increased system costs (Fig. 1d) due to the need for additional renewable energy generation, battery, and hydrogen storage capacity. Consequently, emission reductions plateau at 65-70%, with hydrogen costs ranging from 2.5-10.0 $/kg, depending on the specific ERT and GH2S scenario.

KEYWORDS

Decarbonization, Green Hydrogen, Linear Optimization

ACKNOWLEDGEMENTS

This research received support through Schmidt Sciences, LLC.

OS-A4-08

STUDENT ORAL

11:45~12:00 · Session A4 · D408

Green mixed-solvent extractive distillation for ether-containing azeotropes: Mechanistic insights and energy-saving intensification

Ning Sun, Wenna Liu, and Peizhe Cui*

Qingdao University of Science and Technology, China

ABSTRACT

2-Methoxyethanol recovery from wastewater offers significant environmental and economic benefits. This work employs quantum chemistry methods including electrostatic potential analysis and reduced density gradient calculations to elucidate solvent-azeotrope interactions and guide extractant selection. Process optimization with minimum total annual cost (TAC) as the objective yielded optimal mixed solvent composition: 30% 1-ethyl-3-methylimidazole acetate and 70% N,N-dimethylacetamide. Two energy-saving intensified processes were further investigated. Economic, environmental, and exergy analyses demonstrate that mixed-solvent extractive distillation reduces TAC and gas emissions by 26.79% and 35.45% versus NMP process, and 44.99% and 25.04% versus [EMIM][AC] process, respectively. Heat pump-assisted and heat-integrated configurations achieve additional TAC reductions of 6.77% and 9.93%, with emission decreases of 21.78% and 12.30%. The heat pump configuration excels environmentally, while heat integration offers superior economic performance. This study establishes structure-performance relationships for mixed solvents and provides theoretical foundations for industrial 2-methoxyethanol/water separation.

KEYWORDS

Mixed entrainers, Solvents screening, Ionic liquids, Reinforcement design, Quantum chemistry calculation

K-B1-01

KEYNOTE

14:30~15:00 · Keynote · Session B1 · D404

Enumerating Full Potential of Process Integration using Graph-theoretic Approach

Bing Shen How[1,*], Ákos Orosz[2], Jean Pimentel[3], Ferenc Friedler[3]

[1]Research Centre for Sustainable Technologies, Faculty of Engineering, Computing and Science, Swinburne University of Technology, Malaysia
[2]Department of Computer Science and Systems Technology, University of Pannonia, Hungary
[3]Department of Systems Science, Széchenyi István University, Hungary

ABSTRACT

Conventional optimization techniques in Process Systems Engineering (PSE) often fall short by focusing exclusively on a single mathematically optimal solution. While computationally efficient, this narrow focus frequently overlooks the practical operational constraints critical for real-world commercialization. This work highlights the P-graph framework, a powerful graph-theoretic approach that effectively addresses this critical limitation by simultaneously generating an exhaustive list of n-best solutions alongside the optimum. In a highly dynamic industrial landscape, evaluating these near-optimal alternatives is vital. In fact, this diverse catalog of solutions uncovers invaluable insights typically obscured by rigid conventional methods. To demonstrate the robust capabilities of P-graph methodology, this work explores its successful applications across various PSE problems, ranging from heat recovery network design and resource conservation optimization. Ultimately, the P-graph approach effectively bridges the gap between theoretical optimality and industrial viability, fully enumerating the hidden potential of process integration.

KEYWORDS

Combinatorial optimization, n-best, P-graph, process integration

ACKNOWLEDGEMENTS

The authors would like to acknowledge financial support from SUTS-SZE Research Collaboration Grant (Grant code: 2-4113 Ind.Decarbonization_SZE(09/26)).

OR-B1-01

REGULAR ORAL

15:00~15:20 · Session B1 · D404

Techno-Economic and Life Cycle Assessment of Electrified Naphtha Cracking with Integrated Methane Valorization

Eprillia Intan Fitriasari[1], Hojae Kim[1], Dae Hoon Lee[2], Hohyun Song[2], Minho Jeong[2], Heesoo Lee[2], Jeongan Choi[2], You-Na Kim[2], Chanmi Jung[2], Donghyun Cho[2], Subin Choi[2,3], Tesfalem Aregawi Atsbha[1,4], J. Jay Liu[5], and Chul-Jin Lee[1,*]

[1]Department of Chemical Engineering, Chung-Ang University, Korea
[2]Korea Institute of Machinery and Materials (KIMM), Korea
[3]Department of Mechanical and Design Engineering, Hongik University, Korea
[4]Department of Chemical and Metallurgical Engineering, Aalto University, Finland
[5]Department of Chemical Engineering, Pukyong National University, Korea

ABSTRACT

Electrification of energy-intensive petrochemical processes requires industrial-scale evaluation to capture interactions among reactors, utilities, and downstream separation units. This study presents a comparative process systems analysis of electrified steam cracking and plasma arc cracking of naphtha for ethylene production under multiple electricity supply scenarios and methane valorization routes. Industrial-scale process models were developed to quantify material flows, electricity demand, and co-product integration effects. An integrated framework combining techno-economic analysis, life cycle assessment, and carbon avoidance metrics was applied to evaluate trade-offs among cost, energy consumption, and global warming impact. The results show that overall system performance is governed primarily by electricity intensity and methane valorization rather than cracking performance alone. Using ethylene as the reference product, electrified steam cracking coupled with methane-to-blue-hydrogen conversion achieves the lowest levelized cost of ethylene at \$1.66/kg and the most favorable carbon avoidance performance. In contrast, plasma cracking attains the lowest global warming impact of 0.31 kg CO2-eq/kg ethylene but remains constrained by high electricity demand. Uncertainty analysis further highlights the strong sensitivity of system outcomes to electricity price and carbon intensity. Overall, the results demonstrate the importance of holistic process systems evaluation in guiding electrification strategies for large-scale, low-carbon chemical production.

KEYWORDS

Electrification, Ethylene, Naphtha Cracking, Decarbonization,

ACKNOWLEDGEMENTS

This work(research) was supported by ITECH R&D program of MOTIE/KEIT [project No. RS-2023-00266831, Development of Novel Plasma Process for Hydrocarbon Cracking].

OR-B1-02

REGULAR ORAL

15:20~15:40 · Session B1 · D404

Hybrid Absorption-Adsorption Separation Process using Porous Slurry for Light Hydrocarbon Recovery from Natural Gas

Chun Deng[*], Gao Ninghan, Ruihang Zhang, Kun Li, Bei Liu, Changyu Sun, and Guangjin Chen

College of Chemical Engineering and Environment, China University of Petroleum, China

ABSTRACT

Natural gas will play a key supporting role in China's energy transition under the ‘dual-carbon’ goal. Recovery of ethane and other light hydrocarbons from natural gas can provide high-quality feedstock for ethane cracking to ethylene plants. Low-temperature distillation is currently the mainstream process for natural gas ethane recovery in industry, with high energy consumption and equipment investment costs. Porous slurry absorption-adsorption coupling process is an emerging gas separation technology. Based on the typical metal-organic framework material ZIF-8 and green solvents to prepare porous slurry, using the classical absorption-desorption process flow, it can realize the recovery of light hydrocarbons from natural gas with high yield and low energy consumption. The research team has carried out lab-scale experiments, established the equilibrium stage model of key mass transfer units (absorption-adsorption tower, desorption tower) and the full-flow simulation model of the separation process, carried out sensitivity analysis and parameter optimization, designed and fabricated a 20,000 m3/year continuous separation pilot plant, and carried out three rounds of pilot experiments on the recovery of light hydrocarbons from oilfield associated gas, which verified the feasibility of the separation process. Besides, a process package for the recovery of light hydrocarbons from natural gas is being developed.

KEYWORDS

Natural gas, Low-temperature distillation, Porous slurry, Process modelling

ACKNOWLEDGEMENTS

This work was supported by the National Natural Science Foundation of China (No. 22278429), State Key Laboratory of Heavy Oil Processing, China University of Petroleum, Beijing.

OR-B1-03

REGULAR ORAL

15:40~16:00 · Session B1 · D404

INTHOP: A Second-Order Globally Convergent Method for Nonconvex Optimization

Krishan Kumar[1], Ashutosh Sharma[1], Gauransh Dingwani[2], Nikhil Gupta[1], Vaishnavi Gupta[1] and Ishan Bajaj[1,*]

[1]*Department of Chemical Engineering, Indian Institute of Technology Kanpur, India*
[2]*Department of Chemical Engineering, Indian Institute of Technology Roorkee, India*

ABSTRACT

Second-order Newton-type algorithms are widely used in nonlinear optimization due to their fast convergence. However, their practical application to large-scale nonconvex problems is often restricted by the high computational cost of Hessian evaluations, the expense of matrix inversion, and the difficulty of guaranteeing descent directions when Hessian is indefinite. In this work, we propose INTHOP, an interval Hessian–based optimization algorithm for nonconvex problems. The proposed method constructs a positive-definite approximation of Hessian such that the search direction computed from it is always a descent direction. A key feature of INTHOP is that Hessian approximation and inversion are performed only at selected iterations. When the iterates remain within a prescribed interval, the previously computed approximate Hessian is reused, while gradients are evaluated at every iteration denoted by circle markers in Figure 1. When the iterate exits the interval, Hessian is computed as indicated by square markers in Figure 1. We establish global convergence of INTHOP and apply it to an extensive set of test problems, including high-dimensional cases, and compare its performance with existing methods such as the steepest descent, the limited-memory Broyden-Fletcher-Goldfarb-Shanno (LBFGS) algorithm, and the open-source solver IPOPT . We demonstrate that INTHOP performs competitively with IPOPT and significantly outperforms other methods across all evaluation metrics (see Figure 2).

KEYWORDS

Nonconvex Optimization, Second-Order Methods, Interval Hessian Approximation, Global Convergence, Large-Scale Optimization

ACKNOWLEDGEMENTS

This research received support through Schmidt Sciences, LLC.

OR-B1-04

REGULAR ORAL

16:00~16:20 · Session B1 · D404

Dynamic Life Cycle Assessment with AI and Digital Technologies: Standards-Aligned Pathways for Climate and Regulatory Compliance

Malik Sajawal Akhtar[1], Francesc Romero Gómez[2], Arka Pandit[3], Hira Mahmood[4], Muhammad Ansub Khan[4], Jay Liu[1,4,*]

[1] *Institute of Cleaner Production Technology, Pukyong National University, Korea*
[2] *Cappi Sustainability B.V., Netherlands*
[3] *Dematic, USA*
[4] *Department of Chemical Engineering, Pukyong National University, Korea*

ABSTRACT

Dynamic Life Cycle Assessment (DLCA) is an emerging frontier in sustainability analytics that embeds temporal and spatial dynamics into conventional life cycle assessment frameworks to better represent the evolving nature of environmental impacts. This work synthesizes recent progress in DLCA and illustrates how digital technologies—including the Internet of Things (IoT), artificial intelligence (AI), blockchain, and digital twins—unlock unprecedented granularity and responsiveness in sustainability assessment. At the same time, it underscores that expert judgment remains indispensable to manage uncertainties, validate model outputs, and ensure that results are decision-relevant. This human oversight anchors DLCA in real-world contexts, preserving methodological robustness and stakeholder trust. The synthesis highlights the need to balance automated data acquisition with nuanced interpretation as a prerequisite for credible and actionable DLCA outcomes. It also examines uneven sectoral readiness for digitalization and the implications of data governance, privacy constraints, and regulatory expectations. The study stresses the importance of harmonized standards, flexible methodological frameworks, and targeted capacity building to close implementation gaps and accelerate deployment across industries. By fostering collaboration among researchers, practitioners, and policymakers, DLCA can evolve from a specialized analytical approach into a core instrument for dynamic, transparent, and implementation-ready sustainability management.

KEYWORDS

Dynamic life cycle assessment, Digital transformation, Technology adoption, Automation risks, Data governance, Supply chain transparency

ACKNOWLEDGEMENTS

This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF), funded by the Ministry of Science and ICT (RS-2024-00337129).

OR-B1-05

REGULAR ORAL

16:20~16:40 · Session B1 · D404

Range-specific Sensitivity Analysis with Kolmogorov-Arnold Network

Hyein Jung[1], Suk Hoon Choi[1], Damdae Park[2], TaeUng Lee[3], Hyerim Kim[4], and Kyeongsu Kim[1,5,*]

[1]*Clean Energy Research Center, Korea Institute of Science and Technology, Korea*
[2]*Chungnam National University, Korea*
[3]*Department of Mechanical Engineering, Korea University, Korea*
[4]*Heat Pump Research Center, Korea*
[5]*Division of Energy and Environment Technology, University of Science and Technology, Korea*

ABSTRACT

Optimization problems necessitate sensitivity analysis to identify critical parameters and reduce the number of function evaluation, particularly when physical experiments are required. Although global sensitivity analysis quantifies overall feature importance, it often obscures how sensitivity varies across feature domain in multi-variable systems. To address this limitation, we introduce a range-specific sensitivity analysis framework based on Kolmogorov–Arnold Networks (KANs). By analyzing the second derivatives of the base coefficients learned in KANs, the proposed method identifies critical transitions and inflection points within each feature's domain. This approach determines where a feature exerts dominant influence, characterizing transitions in feature-importance ranking along the feature domain. We validate the framework across optimization problems in diverse domains, including material discovery and chemical process systems. In all cases, the method preserves global predictive accuracy while uncovering fine-grained sensitivity patterns. By bridging global fidelity with local interpretability, this framework establishes sensitivity analysis as a precise diagnostic tool for understanding complex systems and enabling informed decision-making.

KEYWORDS

Sensitivity analysis; Explainable AI.

OR-B2-01

SPECIAL SESSION

13:30~13:55 · Session B2 · D403

Sustainable Hydrogen Production through Dry and Chemical Looping Reforming: Techno-Economic and Environmental Assessment

Jae W. Lee[*]

Department of Chemical and Biomolecular Engineering, Korea Advanced Institute of Science and Technology (KAIST), Korea

ABSTRACT

As hydrogen emerges as a vital clean energy carrier for global carbon neutrality, evaluating the economic and environmental sustainability of its production processes has become critical. This study comprehensively compares dry reforming of methane (DRM) and chemical looping reforming (CLR) as feasible alternatives to the commercially established steam methane reforming (SMR) process. To ensure strict methodological consistency, rigorous process simulations were conducted under identical industrial-scale conditions. Each reforming pathway was integrated with identical downstream units, including consecutive water-gas shift reactors, monoethanolamine (MEA)-based carbon capture, and pressure swing adsorption. Techno-economic assessment reveals that CLR is highly efficient, demonstrating a remarkable 42.6% reduction in specific energy consumption compared to SMR. Furthermore, CLR achieves the lowest levelized cost of hydrogen (LCOH) at $1.79/kg. Although DRM exhibits a slightly higher LCOH of $1.91/kg, sensitivity analyses indicate that its economic competitiveness can be significantly enhanced by optimizing CO2 feedstock supply or in scenarios featuring increased carbon taxes. In terms of environmental impact, DRM and CLR substantially reduce net CO2 emissions by 74.8% and 32.9%, respectively. Ultimately, these findings emphasize that both DRM and CLR present promising, sustainable, and low-carbon alternatives to conventional SMR for future industrial hydrogen production.

KEYWORDS

H2 production, Dry reforming, Chemical looping reforming, Kinetic-based simulation, Economic and environmental sustainability

ACKNOWLEDGEMENTS

This work was supported by the Engineering Research Center (ERC), funded by the National research Foundation of Korea (RS-2022-NR070840).

OR-B2-02

SPECIAL SESSION

13:55~14:20 · Session B2 · D403

Integrated Design of Hydrogen–Electricity Supply Chains: System-Level Insights from Joint Planning Frameworks

Seongmin Heo*

Department of Chemical and Biomolecular Engineering, Korea Advanced Institute of Science and Technology (KAIST), Korea

ABSTRACT

This work presents a system-level framework for the integrated design and operation of hydrogen and renewable electricity supply chains toward carbon-neutral energy systems. The proposed approach is based on a mixed-integer linear programming model that simultaneously determines infrastructure investment and hourly operational strategies across multiple regions, capturing the strong interdependencies between hydrogen production, electricity generation, storage, and transport. Within this framework, both green hydrogen produced via renewable-powered electrolysis and blue hydrogen produced via chemical looping processes are considered, enabling a comparative and synergistic analysis of alternative production pathways. The results show that conventional decoupled planning of hydrogen and electricity systems leads to inefficient infrastructure deployment, whereas joint planning can significantly reduce total system cost and improve operational flexibility. In particular, cogenerative hydrogen production pathways can substantially reduce reliance on electricity transmission and energy storage by simultaneously supplying hydrogen and dispatchable power. Case studies based on national-scale systems demonstrate how technology choices and resource conditions influence optimal system configurations. The findings highlight the importance of integrated planning in achieving cost-effective and resilient hydrogen-based energy systems.

KEYWORDS

Integrated energy systems, Renewable electricity, Clean hydrogen, Planning, Optimization

ACKNOWLEDGEMENTS

This work was supported by the Engineering Research Center (ERC), funded by the National research Foundation of Korea (RS-2022-NR070840).

OR-B2-03

SPECIAL SESSION

14:20~14:45 · Session B2 · D403

Pathways to Net-Zero in Taiwan: Bridging Rigorous Process Modeling and Comprehensive Evaluation with Strategic Planning

Bor-Yih Yu[*]

Department of Chemical Engineering, National Taiwan University, Taiwan

ABSTRACT

Pathways to achieve net-zero vary globally. Given Taiwan's lack of natural energy resources and green electricity, conventional pathways such as widespread electrification and hydrogen-driven CO2 conversion are highly challenging. Additionally, the absence of supporting infrastructure and clear market rules for carbon-based products makes the initiation of Carbon Capture and Utilization (CCU) technologies difficult. To address these issues, it is imperative to develop comprehensive strategies that prudently connect fundamental science, engineering, and societal needs. Under these circumstances, process modeling serves as an essential tool. Through rigorous modeling and multi-aspect evaluation, we can bridge knowledge gaps at both the micro- and macroscopic levels, providing critical process indicators regarding economics, environment, efficiency, and safety. This presentation will provide an overview of current net-zero activities across various sectors in Taiwan. Furthermore, the incorporation of process simulation technologies into CCU-related activities, through both standalone and collaborative efforts, will be introduced.

KEYWORDS

Net Zero, Process modeling, Process Evaluation, CO2 utilization, Carbon capture and utilization (CCU)

OR-B2-04

SPECIAL SESSION

15:15~15:40 · Session B2 · D403

Algorithmic Techno-Economic Optimization of CO_2 Liquefaction Processes for Low-Carbon CCUS Infrastructure

Sung Hyun Ju[1], Jisung Byun[1], Seokjin Yoon[1], Heesung Kim[2], Unpil Hwang[2], Minji Kim[2], Mina Kong[2], **Jong Min Lee**[1,*]

[1]Department of Chemical and Biological Engineering, Seoul National University, Korea
[2]Samsung E&A Co., Korea

ABSTRACT

To achieve global net-zero emissions, establishing cost-competitive CO2 conditioning routes is essential for the large-scale development of carbon capture, utilization, and storage (CCUS). Within these pathways, CO2 liquefaction represents a critical stage; however, its techno-economic performance remains highly sensitive to specific process configurations and delivery specifications. This study presents a rigorous simulation-optimization framework that couples Aspen Plus with Bayesian algorithms to evaluate diverse CO2 liquefaction architectures. We systematically investigate the trade-offs between open-loop, closed-loop, and hybrid configurations, while simultaneously refining structural complexity—including compression stages—and operating parameters. Comparative assessments across varying capacities demonstrate that the optimal process architecture is primarily determined by target product pressure. For low-pressure delivery, open-loop configurations yield the minimum levelized cost of CO2 (LCO2). Conversely, closed-loop systems utilizing refrigerants with high latent heat prove superior for higher-pressure applications due to enhanced thermophysical efficiency. By defining the correlations between process synthesis and economic performance, this research establishes a comprehensive analytical foundation for the strategic deployment of scalable carbon management infrastructure essential for achieving carbon neutrality.

KEYWORDS

Low-carbon infrastructure, CO2 liquefaction, CCUS, Bayesian optimization, Techno-economic analysis, Process synthesis

ACKNOWLEDGEMENTS

This research is financially supported by Samsung E&A Co., Ltd.

OR-B2-05

SPECIAL SESSION

15:40~16:05 · Session B2 · D403

Achieving Net-Negative CO_2 Emissions in Methanol Synthesis via High-Yield Reactive Capture and Conversion

Damdae Park, Margareth, Jaehyung Choi, Chun-Jae Yoo, Kyeongsu Kim, and **Ung Lee***

Clean Energy Research Center, Korea Institute of Science and Technology (KIST), Korea

ABSTRACT

We present the first demonstration of an amine-assisted reactive capture and conversion (RCC) process that directly converts the captured CO2 into methanol, eliminating the need for energy-intensive CO2 regeneration. By employing graph neural network-based material screening framework, we identify optimal amines tailored for target reactions from vast chemical space. This enables a reaction-mechanism-guided process design that optimizes amine selection and process parameters, resulting in an unprecedented single-pass yield of 56%, over twice that of conventional methods (<25%). Rigorous techno-economic analysis and life-cycle assessment indicates up to a 10% reduction in production cost compared to conventional CO2 to methanol processes, along with a carbon abatement of -0.92 kg CO2/kg methanol, approaching nearly 67% of the maximum achievable reduction (-1.37 kg CO2/kg methanol). Comprehensive analyses of catalyst and amine selections, hydrogen supply scenarios, and country-specific assessment demonstrate the economic viability and scalability of the proposed RCC based methanol production. Our findings establish a commercially viable carbon-negative pathway for methanol synthesis, paving the way toward net-negative CO2 emissions.

KEYWORDS

CO2, Hydrogenation, Reactive Capture and Conversion, Process Design

OR-B2-06

SPECIAL SESSION

16:05~16:30 · Session B2 · D403

From Air to Fuel: Process Systems Engineering of Carbon and Water Capture for Scalable Negative Emissions

Jinsu Kim

Department of Petrochemical Materials, Chonnam National University, Korea

ABSTRACT

Atmospheric carbon dioxide and water are ubiquitous resources that are independent of conventional supply chains and particularly valuable in extreme or isolated environments, such as during military operations or in space. This work presents a process systems engineering framework for integrating air-derived carbon and water resources into scalable air-to-fuel pathways. Adsorption-based DAC systems are examined, including specific technological variations such as (i) near-cryogenic and (ii) moisture-swing processes, together with material and process design considerations governing performance under varying climatic conditions. In parallel, AWE using metal–organic frameworks is analyzed through kinetic modeling and climate-informed stochastic optimization to identify optimal operating strategies and site selection. These capture processes are further linked to CO2 utilization pathways for sustainable fuel synthesis, with emphasis on carbon and oxygen recycling strategies and their impact on overall system efficiency and carbon intensity. Various methodologies, including TEA/LCA, ML, and numerical analysis, is integrated to analyze trade-offs across system-level performance metrics. The results highlight the importance of integrated design across capture and conversion steps, demonstrating that coordinated optimization can significantly enhance the feasibility of air-derived resource utilization for negative emissions and sustainable aviation fuel production.

KEYWORDS

Negative Emission Technologies (NETs), Direct air capture, Atmospheric water extraction, Air-to-fuel

OS-B3-01

STUDENT ORAL

14:30~14:45 · Session B3 · D402

Optimization of Reclamation Strategies for Managing MEA Degradation in Rate-Based CO_2 Capture Simulation

Yu-Sheng Chen and Bor-Yih Yu*

National Taiwan University

ABSTRACT

Amine-based chemical absorption is a mature technology for post-combustion CO2 capture; however, solvent degradation remains a critical bottleneck, leading to solvent loss, equipment corrosion, and reduced capture efficiency over time. While commercial process simulators utilizing rate-based models offer high accuracy for mass transfer and thermodynamics, they often lack the capability to directly simulate the dynamic accumulation of degradation products over long operating periods. This limitation has restricted most existing studies to steady-state analyses that do not fully capture the complex interplay between process dynamics and impurity buildup. This study addresses this gap by developing a dynamic simulation framework within Aspen Plus to predict the long-term impact of degradation in Monoethanolamine (MEA) processes. We integrated comprehensive reaction kinetics for both oxidative and thermal degradation, accounting for major byproducts such as HEEDA, HEIA, and heat-stable salts. Since standard rate-based dynamic simulations are computationally restricted for this purpose, our iterative approach successfully mimics the time-dependent accumulation of impurities and their feedback effects on process performance. This work evaluates a hybrid reclamation strategy, focusing on the critical trade-off between purge ratios and solvent makeup costs, which provides a rigorous basis for optimizing reclamation schedules and ensuring the long-term operability of amine-based carbon capture systems. The abstract should be written in 200 words

KEYWORDS

CO2 Capture, MEA Degradation, Rate-based Simulation, Reclamation Strategy, Process Optimization.

OS-B3-02

STUDENT ORAL

14:45~15:00 · Session B3 · D402

Rigorous Process Modeling of Lignin-to-SAF Production via Integrated Hydrothermal Liquefaction and Hydrodeoxygenation

Yi-Ming Chen and Bor-Yih Yu*

National Taiwan University, Taiwan

ABSTRACT

Facing the global 2050 net-zero emission mandate, Sustainable Aviation Fuel (SAF) has emerged as a critical solution for decarbonizing the aviation sector. Lignin, a major aromatic component of lignocellulosic biomass, represents a strategic but recalcitrant feedstock for biorefineries. This study develops a rigorous process simulation framework using Aspen Plus to evaluate the transformation of lignin into SAF-range hydrocarbons via a sequential Hydrothermal Liquefaction (HTL) and Hydrodeoxygenation (HDO) pathway. The proposed model integrates detailed kinetic mechanisms to describe the depolymerization of lignin into oxygenated bio-crude and its subsequent catalytic upgrading to C8–C16 alkanes. To ensure simulation accuracy, advanced thermodynamic packages and property prediction systems are employed to characterize complex lignin-derived intermediates. Preliminary results demonstrate that the integrated HTL-HDO process effectively narrows the carbon distribution toward the aviation fuel fraction while significantly enhancing carbon efficiency. This research provides a systematic evaluation tool for lignin-based biorefineries, offering quantitative insights into the development of resilient green energy supply chains.

KEYWORDS

Lignin, Sustainable Aviation Fuel, Hydrothermal Liquefaction, Hydrodeoxygenation, Process Simulation, Kinetic Modeling.

ACKNOWLEDGEMENTS

The research funding from National Science and Technology Council if R. O. C. (grant number: 114-2221-E-002-199-MY2 and 114-2923-E-006-004) is greatly appreciated.

OS-B3-03

STUDENT ORAL

15:00~15:15 · Session B3 · D402

Real-time Prediction of M2 Monomer Concentration in Organosilicon Synthesis using Near-Infrared Spectroscopy and Enhanced Deep Learning

Chen Zhang, Zhongmei Li, Qinhao Sun, and Enbo Feng*

East China University of Science and Technology, China

ABSTRACT

Organosilicon materials are indispensable in modern industry due to their exceptional thermal stability, dielectric properties, and biocompatibility. As a key monomer in their production, real-time monitoring of dimethyldichlorosilane (M2) concentration is critical for ensuring product quality and yield in organosilicon synthesis. However, the significant time lag inherent in traditional gas chromatography limits its effectiveness for closed- loop control, creating an urgent need for rapid, non-invasive detection methods capable of handling complex reaction dynamics. To bridge this gap, this study proposes a robust and explainable soft-sensing framework utilizing near-infrared (NIR) spectroscopy. Unlike conventional linear models such as Partial Least Squares (PLS), which often fail to capture spectral non-linearities, we introduce an Attention-Augmented One-Dimensional Convolutional Neural Network (1D-CNN). This architecture is specifically tailored to capture deep, non-linear spectral features hidden within noisy industrial data. To enhance robustness, noise injection strategies are integrated during training, effectively mitigating interference from environmental fluctuations. Moreover, the embedded attention mechanism improves model interpretability by dynamically assigning higher weights to characteristic wavelengths, thereby linking learned features to specific chemical functionalities. Experimental results demonstrate that the proposed method achieves a coefficient of determination (R2) of 0.72, significantly outperforming PLS while reducing analysis latency from hours to seconds. This research provides a reliable, high-speed analytical tool for real-time feedback control, contributing to the digital transformation and operational stability of chemical manufacturing.

KEYWORDS

Organosilicon Synthesis; Near-Infrared Spectroscopy (NIR); Deep Learning; Attention mechanism; Real-time monitoring

OS-B3-04

STUDENT ORAL

15:15~15:30 · Session B3 · D402

Modeling of mesenchymal stem cell cultivation processesbased on metabolic flux analysis

Daiki Ikuta, Hiroki Kikukawa, Gaku Shimodaira, Yusuke Hayashi,Masaki Nishikawa and Hirokazu Sugiyama*

Department of Chemical System Engineering, The University of Tokyo, Japan

ABSTRACT

Mesenchymal stem cells (MSCs) are promising cell therapy sources, while balancing quality and productivity during cultivation remains challenging. Although metabolic control has been recognized as a key strategy and investigated experimentally [1], mathematical modeling is essential for quantitative process design. However, conventional modeling approaches have been limited to either macro-level process models [2] or steady-state metabolic flux analysis (MFA) under specific environments [3]. To address these limitations, this study developed an integrated model that couples MFA with a dynamic process model to simulate temporal transitions in intracellular metabolism and growth. The model was validated with experimental data acquired in this study and captured metabolic flexibility in response to varying oxygen levels. The “glycolytic contribution ratio” was newly proposed as a proxy quality indicator, quantifying the balance of ATP production pathways and linking culture conditions to cellular potency. Simulations revealed a productivity-quality trade-off when cultivation time was shortened, whereas hypoxic conditions improved quality without compromising yield. This model-based approach provides a rational basis for process design and supports a shift from empirical optimization to evidence-based MSC manufacturing. References: [1] Burnham et al., Front. Immunol. (2020); [2] Hirono et al., Ind. Eng. Chem. Res. (2022); [3] Fouladiha et al., Cytotechnology (2017).

KEYWORDS

Oxygen condition, Hypoxic culture, Metabolic network, Multiscale modeling, Hybrid modeling, Cell therapy.

ACKNOWLEDGEMENTS

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OS-B3-05

STUDENT ORAL

15:30~15:45 · Session B3 · D402

Literature-Driven Physical Model Building by Graph Neural Network with Context-Embedded Equation Nodes

Ding Yiyang, Shota Kato*, Manabu Kano

Department of Informatics, Kyoto University, Japan

ABSTRACT

In the process industry, physical models grounded in scientific laws are widely used to describe and predict the behavior of target processes. However, building accurate physical models requires high costs because it currently relies heavily on trial and error by experts. Although we have proposed some methods for building physical models from literature, they cannot leverage the contextual information of equations. To address this issue, we propose a Graph Neural Network (GNN)-based method of building physical models from equations with contexts. In the proposed method, each equation is treated as a node, and edges are formed between equation nodes that share variables. For each equation, its contextual information is vectorized by CodeBERT and incorporated as its node feature. The GNN estimates the necessity of each equation and outputs sets of equations with high necessity scores as model candidates. The proposed method was trained and evaluated on cases of a continuous stirred-tank reactor and a biodiesel process. Through the case studies, the proposed method correctly generated model candidates even when symbolic notation was inconsistent. Future work will focus on guaranteeing the solvability of the generated models and refining context selection to improve the precision of the candidates.

KEYWORDS

First-Principles Model, Graph Neural Networks, Automated Model Building.

ACKNOWLEDGEMENTS

This work was supported by JST PRESTO, Japan, Grant Number JPMJPR25T1.

OS-B3-06

STUDENT ORAL

15:45~16:00 · Session B3 · D402

Thermal Conductivity Evaluation of Thermal Interface Materials Using a Hybrid Particle Random Packing Algorithm

Dong-Gi Lee, Boram Gu*

School of Chemical Engineering, Chonnam National University, Korea

ABSTRACT

The rapid growth of electric vehicles has intensified the need for efficient battery thermal management systems. Thermal interface materials (TIMs) play a critical role in facilitating heat dissipation by minimising interfacial thermal resistance between battery cells and heat sinks. To achieve the thermal conductivity required for practical applications, filler volume fractions in TIMs commonly exceed 60 vol%. However, conventional random sequential adsorption methods are limited by a jamming threshold of approximately 40 vol%, limiting their applicability for high-loading composite systems. In this study, a hybrid particle random distribution algorithm integrating Particle size distribution-constrained greedy random sequential (PSD-constrained greedy RSA) algorithm with molecular dynamics is developed to construct high volume fractions up to 80 vol%. The generated microstructures are subsequently employed in heat transfer simulations to evaluate the influence of particle properties on the effective thermal conductivity of the composite. The results indicate that increasing filler volume fraction and the mean particle size markedly enhances thermal conductivity. These findings offer quantitative design guidelines for high-performance TIMs and contribute to the development of advanced thermal management solutions for thermally stable battery operation.

KEYWORDS

Thermal management, thermal interface material, random sequential adsorption methods, molecular dynamics

ACKNOWLEDGEMENTS

This work was supported by the Korea Evaluation Institute of Industrial Technology (KEIT) grant funded by the Korean government (MOTIE) (RS-2024-00412719).

OS-B3-07

STUDENT ORAL

16:00~16:15 · Session B3 · D402

Superstructure-free multi-objective optimization of supercritical CO_2 power cycles: Extensive topology generation and tightened heat exchanger network synthesis

Donghyeon Kim, Chanmok Kim, Heehyun Choi, Hyeonseo Im, and Jiyong Kim*

School of Chemical Engineering, Sungkyunkwan University, Korea

ABSTRACT

Supercritical CO2 (sCO2) power cycles are attractive for waste heat recovery, but their performance is strongly influenced by cycle topology. This study proposes an enhanced superstructure-free optimization framework for the automated synthesis and thermo-economic design of sCO2 cycles. The framework incorporates four main advances: project-level economic evaluation based on levelized cost of electricity (LCOE), a topology control parameter (λt) that continuously spans multiple cycle configurations, heat exchanger network optimization using nonlinear cost functions with three stream-merging strategies, and entropy-weight TOPSIS for systematic selection among Pareto-optimal solutions. A bi-level optimization scheme is employed, combining NSGA-II in the outer loop for topology and operating-variable search with a global MINLP solver in the inner loop for heat exchanger network design. In a case study on internal combustion engine exhaust recovery, the method identifies feasible solutions across nine pressure-level combinations, with net power outputs of 24.9–53.0 kW and LCOE values of 0.119–0.277 $/kWh. The TOPSIS-selected design achieves 35.7 kW at 0.135 $/kWh, demonstrating the framework's effectiveness as a systematic and extensible tool for sCO2 cycle design.

KEYWORDS

Automated flowsheet generation; supercritical CO2 cycle; multi-objective optimization; thermo-economic assessment

OS-B3-08

STUDENT ORAL

16:15~16:30 · Session B3 · D402

Hydrogen network synthesis considering multi-stage separation system and compressor layout

Duankanghui Yang, Linlin Liu*

School of Chemical Engineering, Dalian University of Technology, China

ABSTRACT

As a clean chemical feedstock and versatile energy carrier, hydrogen has emerged as a cornerstone of the global energy transition, experiencing a sustained annual growth in demand [1]. Critical reaction processes in oil refineries—including catalytic reforming, hydrotreating, and hydrocracking—involve extensive hydrogen consumption and recycling, presenting substantial potential for hydrogen conservation. Hydrogen Network (HN) synthesis integrating process unit simulation serves as a core technical approach to reducing hydrogen consumption in refineries, enabling synchronous optimization of process units and hydrogen allocation system [2]. In HN, the purification unit is used to recycle low purity hydrogen and is an important unit to reduce fresh hydrogen consumption and to decrease the correlative cost. Furthermore, the compressor unit is an essential process unit to ensure that hydrogen is transported between nodes at different pressures. Therefore, to address the incomplete and insufficient integration of the above two important process units with HN, it is necessary to carry out a comprehensive study of the HN considering multistage and multi-technology purification unit and compressor arrangement in order to achieve the simultaneous optimization of the hydrogen distribution and process units in the refinery. Firstly, Pressure Swing Adsorption (PSA) and Membrane Separation (MS) technologies are extensively utilized for hydrogen purification. The integration of these two purification technologies has been demonstrated to enhance the performance of the purification system, thereby reducing large quantity of fresh hydrogen. To determine the optimal HN, a superstructure model is proposed, which is embedded with a purification system of multistage PSA and multistage MS units. The operating pressure of the purification unit is used as a decision variable. This allows the HN structure and the operating parameters of the purification units to be optimized simultaneously. Case studies demonstrate that this HN model includes broader spectrum of refinery scenarios. And the total cost of the optimal solution is reduced by 2% to 22% in comparison with the HN model employing just single purification unit. Secondly, the compressor costs significantly contribute to the overall expense of HN. Consequently, an essential objective in the optimization of HN is to identify an optimal compressor layout that reduce power consumption and the overall cost. Therefore, a Group Cascade Compressor - Hydrogen Network (GCC-HN) model is constructed to optimize hydrogen distribution and compressor arrangement simultaneously. The model divides the compressors in the compressor system into three groups: centralized hydrogen source compressors, centralized hydrogen sink compressors, and individual stream compressors. This enables full consideration of shared and cascaded compressors in HN. The inlet and outlet pressures of the compressors are continuous optimization variables, the model solution results include the optimal intermediate pressures of the cascaded compressors. The forementioned mathematical model usually contains a large number of nonlinear terms and optimization variables, leading to a challenging solving problem. A two-stage synthesis approach is proposed to address this issue. In the initial phase, a pre-synthesized hydrogen network model is employed to optimize the hydrogen distribution. In the subsequent phase, the optimization results from the preceding stage are utilized as inputs to rebuild the hydrogen network and the compressor system by the GCC-HN model. In comparison with recent studies, the present method is time-efficient and results in further savings of 2%-3% in the compressor-related costs. Moreover, the two-stage synthesis method can be applied not only to the hydrogen network synthesis problem where both the hydrogen source and the hydrogen sink pressures are fixed, but also to the hydrogen network synthesis problem involving the optimization of process unit pressures. [1] DE J, AZKONA-BEDIA I, CORNEJO-JIMENEZ C, et al. Assessment of levelized costs for green hydrogen production for the national refineries system in Mexico[J/OL]. International Journal of Hydrogen Energy, 2025, 108: 121-132.

DOI:10.1016/j.ijhydene.2024.03.316. [2] CHEN S, SHEN F, ZHONG W, et al. Synchronous adjustment framework for the integrated hydrogen network and production system: A concurrent optimization strategy of the system based on multi-model ensemble method[J/OL]. Applied Energy, 2024, 36: 122636. DOI:10.1016/j.apenergy.2024.122636.

KEYWORDS

refinery; hydrogen; hydrogen network; purification unit; compressor; optimization

OS-B3-09

STUDENT ORAL

16:30~16:45 · Session B3 · D402

Meta-Learning for Dementia-Related Disease Prediction with Limited Brain MRI Data

K. Fujii, K. Matsuda*

Nagoya University, Japan

ABSTRACT

Machine learning has achieved significant results in medical image diagnosis, but insufficient clinical data remains a major challenge. To address this, this study aimed to predict dementia-related diseases using numerical and image data from brain MRI scans. We employed Prototypical Networks, a meta-learning method capable of adapting to new tasks with limited training data. For classifying Alzheimer's disease, Lewy body dementia, and healthy controls, we compared our numerical data approach against Multi-Layer Perceptrons (MLP), Random Forests (RF), and Support Vector Machines (SVM), and our image data approach against standard Convolutional Neural Networks (CNN). Results showed that the proposed method achieved an F1 score of 0.87 using numerical data, surpassing conventional methods (MLP: 0.83, RF: 0.83, SVM: 0.85). Furthermore, it demonstrated high generalization performance, maintaining an F1 score of 0.79 on unseen diseases (Mild Cognitive Impairment and Frontotemporal Dementia). The image-based approach also achieved an F1 score of 0.73, surpassing the CNN (0.71). However, performance on unseen diseases dropped to 0.52. This study demonstrates the potential effectiveness of meta-learning in addressing the challenge of insufficient data for diagnosing dementia-related diseases.

KEYWORDS

Machine Learning, Meta-Learning, Medical Data, Dementia-related diseases, Brain MRI

ACKNOWLEDGEMENTS

This research was supported by Health and Labour Sciences Research Grants (JP23GB1003).

OS-B3-10

STUDENT ORAL

16:45~17:00 · Session B3 · D402

Effects of a Third Component on CO_2 Absorption in Tetrabutylammonium Bromide-Based Deep Eutectic Solvents

Guilin Wen, Zhaoyou Zhu*

College of Chemical Engineering, Qingdao University of Science and Technology, China

ABSTRACT

Deep eutectic solvents (DESs) represent promising absorbents for CO2 capture. Experimental measurements and theoretical calculations were employed to investigate the regulatory effects of third-component incorporation on the CO2 absorption performance of TBAB-based DESs. 3-Aminopropanol (AP) and monoethanolamine (MEA) served as the hydrogen bond donors (HBDs). Piperazine (PZ) was combined with TBAB-AP/MEA to prepare ternary DESs, and the the variation in CO2 absorption performance after PZ introduction was studied. The characteristics of system viscosity and CO2 absorption performance with the addition of water and methanol were examined respectively. Experimental results showed that TBAB-MEA(1:7) exhibited a superior CO2 absorption capacity toTBAB-AP(1:4). The addition of PZ to binary DESs could effectively enhance their CO2 solubility, yet it caused a significant increase in system viscosity at the later stage of absorption. The incorporation of water or methanol into the DES systems can effectively reduce the absorbent viscosity, which improves the CO2 mass transfer rate and thus enhances the overall CO2 absorption performance of the DESs. This study clarified the regulatory rules of different third components on the physicochemical properties and CO2 absorption behaviors of TBAB-based DESs, confirming that high-performance CO2-capturing DES absorbent system can be designed by introducing functional third-components.

KEYWORDS

Deep eutectic solvents; CO2 absorption; Molecular dynamics simulations; Third-component

OS-B4-01

STUDENT ORAL

14:30~14:45 · Session B4 · D408

A Hybrid Modelling Framework: Integrating Machine learning Models for anaerobic digestion of rice straw

Pragya Singh, Asad Hasan Sahir*

Indian Institute of Technology Ropar, India

ABSTRACT

Rice-based agricultural systems in India, South Korea, and China generate substantial straw residues, presenting environmental challenges and opportunities for renewable energy transition. Anaerobic digestion of rice straw offers a pathway to reduce emissions, strengthen decentralized rural energy systems, and recycle nutrients through digestate application, advancing circular bioeconomy goals across Asia. However, feedstock heterogeneity, fluctuating operating conditions, and sensor uncertainties hinder predictive reliability and large-scale adoption. The Anaerobic Digestion Model No. 1 (ADM1), developed by the International Water Association, provides a mechanistic description of methane production but is computationally intensive for real -time use in decentralized systems. To address this, a hybrid di gital framework integrating ADM1 simulations with machine learning is proposed. Synthetic datasets were generated to represent rice residue digestion scenarios, with controlled noise mimicking sensor disturbances. Principal Component Analysis retained 85 –90% of variance, identifying stability indicators such as pH, hydrogen, volatile fatty acids, microbial biomass, and methane concentration. Random Forest regression achieved strong predictive accuracy (test R2 ≈ 0.98), while ongoing work with Long Short-Term Memory networks captures temporal dynamics. The hybrid approach is expected to assist in strategies leading to enhanced methane production, strengthen biogas plant operational reliability, and support sustainable residue valorisation.

KEYWORDS

Bioenergy, Machine learning, Circular bioeconomy, Anaerobic Digestion

OS-B4-02

STUDENT ORAL

14:45~15:00 · Session B4 · D408

PINN-driven modeling and optimization of green ammonia reactors across wide operating regimes under intermittent renewable feedstocks

Qingqing Zhang, Jiaming Wang, Xudong Zhou, Li Zhou*, Xu Ji

School of Chemical Engineering, Sichuan University, China

ABSTRACT

Volatile renewable energy necessitates robust green ammonia synthesis, yet autothermal reactor complexity challenges online optimization. To adress the prohibitive computational cost of rigorous simulations, This study proposes a Residual-Attention Physics-Informed Neural Network (PINN) surrogate. Trained on high-fidelity Aspen Plus data, the model incorporates explicit flow reciprocal features (1/Fin) to capture non-linear residence time sensitivities and employs a residual-attention architecture to resolve stiff reaction hotspots. The proposed surrogate yields prediction errors of less than 1% for both temperature and conversion metrics, while accelerating inference speed by approximately three orders of magnitude relative to traditional numerical solvers. Leveraging this surrogate, This study compares traditional quench, series indirect, and series-parallel split configurations. Results demonstrate that the series-parallel split configuration achieves superior performance. Particularly under low loads (10%-50%), it effectively prevents extinction and thermal runaway via adaptive split ratios. T-X phase diagram analysis reveals its operating trajectory closely approximates the thermodynamic equilibrium curve, maximizing the reaction driving force.This study provides a theoretical basis for flexible reactor design, demonstrating how feature-augmented deep learning can solve complex operational bottlenecks in decarbonized chemical processes.

KEYWORDS

Green Ammonia; Physics-Informed Neural Networks (PINN); Autothermal Reactor; Process Intensification

ACKNOWLEDGEMENTS

The financial support provided by the National Natural Science Foundation of China (No. 22478260 and 22108178) is gratefully acknowledged.

OS-B4-03

STUDENT ORAL

15:00~15:15 · Session B4 · D408

Capacity Configuration of Power-to-Methanol Systems: A Bi-level Optimization Approach Based on Bayesian and Clustering Algorithms

Yi Wang[1], **Tian Qiu**[2], Miao Yang[1], Qingqing Zhang[2], Xu Ji[2], Li Zhou[2,*]

[1]*China Petroleum Engineering & Construction Co. Ltd. southwest branch, China*
[2]*School of Chemical Engineering, Sichuan University, China*

ABSTRACT

Decarbonizing methanol production via renewable integration is crucial for achieving carbon neutrality, yet this transition faces a fundamental challenge. The inherent intermittent of renewables can render the process cost-prohibitive if not properly addressed. This study proposes a Bayesian-enhanced, interactive bi-level optimization approach for the capacity configuration of off-grid wind-solar-driven methanol systems. The uppler level optimizes the capacities of key components (renewable power, electrolyzer, hydrogen storage, and methanol synthesis), while the lower level evaluates the annual economic performance of each configuration through a scenario-based stochastic programming model for operation scheduling. To reduce computational burden, K-means clustering is applied to abstract representative scenarios with occurence probabilities from the annual renewable profile of the targeted location. These scenarios enable rapid estimation of key opertional performance indicators (annual methanol yield and operational cost) for various configurations. These estimated indicators are then fed into a Bayesian optimization algorithm, guided by a Gaussian process surrogate model on the upper level, to efficiently map the configuration-economic response surface and navigate the non-convex design space. Applied to a case study in Northeast China targeting 300,000 tons of annual green methanol production from captured CO2, the method proves effective in optimizing system capacities while enhancing both economic performance and computational efficiency. Findings reveal that while wind-solar hybrids smooth operational fluctuations, they do not necessarily minimize the levelized cost of methanol (LCOM) due to substantially higher capital costs. In certain cases, configurations dominated by a single renewable source may offer superior economic outcomes.

KEYWORDS

Green Methanol; Capacity Configuration; Bi-level Optimization; Bayesian Optimization; K-means Clustering; Mixed-Integer Linear Programming (MILP)

ACKNOWLEDGEMENTS

The financial support provided by the National Natural Science Foundation of China (No. 22478260, No. 22108178) is gratefully acknowledged.

OS-B4-04

STUDENT ORAL

15:15~15:30 · Session B4 · D408

Hybrid Auxiliary Heating Optimization for Solar Thermal Integration in Industrial Processes: A Screening Curve Approach

Rohit K. Yadav[1,2,*], Santanu Bandyopadhyay[1], Andrew Hoadley[2] and Roger Dargaville[2]

[1]*Department of Energy Science and Engineering, Indian Institute of Technology Bombay, India*
[2]*Department of Chemical and Biological Engineering, Monash University, Australia*

ABSTRACT

Industrial process heating contributes significantly to greenhouse gas emissions. Solar thermal energy can supply heat at temperatures matching industrial requirements, but its intermittent nature necessitates auxiliary heating for continuous operation. This paper combines Pinch Analysis with screening curve analysis from power systems economics to co-optimize solar thermal system sizing and hybrid auxiliary heating technology selection. The screening curve determines the economically optimal capacity split between a heat pump and a resistive heater by identifying the crossover operating hours beyond which the heat pump becomes more economical. This crossover is mapped onto the auxiliary load duration curve, unique to each candidate design, to size both devices optimally. The methodology is applied to a dairy processing plant using evacuated tube collectors with thermal storage. A two-stage grid search over collector area and storage volume minimizes the Total Annualized Cost over 8,760 hourly timesteps with cyclic steady-state convergence. The optimal design achieves a solar fraction of 51.2%. The total annualized cost is $837,476/year with an LCOH of $57.04/MWh. Sensitivity analysis identifies electricity tariff, heat pump COP, and discount rate as the primary economic drivers, each shifting TAC by more than 14%.

KEYWORDS

Solar Thermal, Modelling and Simulations, Pinch Analysis, Heat Exchanger Network, Renewable and Sustainable Energy

OS-B4-05

STUDENT ORAL

15:30~15:45 · Session B4 · D408

Prospective Life Cycle Assessment of Succinic Acid Production from Cyanobacteria

Roja K, and Yogendra Shastri*

Department of Chemical Engineering, Indian Institute of Technology Bombay, India

ABSTRACT

This work performs a cradle-to-gate prospective life cycle assessment (pLCA) of the cyanobacterial system producing succinic acid (SA). Prospective life cycle inventory (pLCI) databases were generated using the tool “premise” by modifying the ecoinvent® v3.9 database. Upstream experimental data on cyanobacteria cultivation producing disodium succinate, as well as downstream experimental and simulation data on SA recovery and purification, were used with pLCI databases for impact analysis. The climate change impact was 35.18 kg CO2 eq/kg SA. As 95% of the total impact was contributed by the gas-fired boiler, the 100% grid-electricity-powered electric boiler and the 100% solar-operated SA plant were considered as potential options. Comparative pLCA was conducted for all the cases with the conventional SA production process. pLCA studies showed a 5-6% reduction in natural gas usage, an 87% reduction with a 100% grid-electricity-operated electric boiler, a 62% reduction with a 100% solar-operated SA plant, and a 19% reduction with the conventional SA process by 2050. A carbon credit of 1.49 kg CO2/kg SA was accounted for, and the study concluded that 100% solar-operated SA production plant will be environmentally beneficial by 2040 (moderate mitigation strategies) and 2050 (minimal mitigation strategies) compared with the conventional SA production process.

KEYWORDS

cyanobacteria, prospective life cycle assessment, succinic acid, integrated assessment models

ACKNOWLEDGEMENTS

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OS-B4-06

STUDENT ORAL

15:45~16:00 · Session B4 · D408

Spatiotemporal Data Analysis for the Development of Physics-informed Machine Learning Models to Design Pre-Swelling Processes for Green Peptide Synthesis

Rui Tsukui, Thossaporn Wijakmatee, Hideyuki Matsumoto*

Department of Chemical Science and Engineering, Institute of Science Tokyo, Japan

ABSTRACT

Resin swelling level profoundly influences reaction efficiency in solid-phase peptide synthesis. Although extensive research has addressed the equilibrium swelling ratio, the lack of focus on dynamic swelling behavior hinders the shortening of pre-swelling processes and the substitution of alternative green solvents. Predicting dynamic swelling behavior is challenging due to complex and multi-parameter interactions, necessitating advanced modeling methods such as machine learning. Specifically, physics-informed machine learning (PIML), incorporating the molecular information, can be applied to enhance model's interpretability and flexibility. In this study, an in-situ monitoring system was developed and utilized to acquire dynamic swelling profiles across various resins (Rink amide, Rink amide PEG and Wang) and solvents (DMF, NMP and anisole), resulting in a dataset with 816 data points. PIML models, including neural network, traditional and ensemble learning, were developed by integrating experimentally dynamic data with thermodynamic properties obtained from COSMO-RS and Flory-Rehner calculations. Five inputs consist of initial resin diameter, chemical potential change, resin molar density, solvent molar volume, and operation time, while swelling ratio defined as the output. The ensemble models exhibit superior performance (R2 > 0.986), where green solvent screening can be flexibly conducted with reducing experimental time and cost to promote sustainable green peptide synthesis.

KEYWORDS

Resin Swelling, Solid-Phase Peptide Synthesis, In situ monitoring, COSMO-RS method, Physics-informed Machine Learning, Green Solvent

OS-B4-07

STUDENT ORAL

16:00~16:15 · Session B4 · D408

Achieving Sustainable Ammonia by Multiple Hydrogen Production Technologies: From A Comparative Techno-Economic-Environmental Perspective

Ruiyang Duan[1], Lixia Kang[1,2,*], Le Wu[3], Yongzhong Liu[1,2]

[1] *Department of Chemical Engineering, Xi'an Jiaotong University, China*
[2] *University of Shaanxi Province, China*
[3] *Department of Chemical Engineering, Northwest University, China*

ABSTRACT

Ammonia synthesis is a core chemical product underpinning global food security and industrial systems. Yet conventional production remains heavily dependent on fossil-based hydrogen, resulting in high energy consumption and substantial greenhouse gas emissions, making ammonia a pivotal target for industrial decarbonization. Although the categories of grey, blue and green ammonia have emerged, existing studies largely focus on optimizing individual process routes. Standardized cross-comparisons among alternative feedstock pathways remain scarce, and the synergistic effects and substitution boundaries within multi-process integrated systems are insufficiently understood. This study establishes a unified benchmark of 0.5 million tons of ammonia per year to systematically evaluate four standalone production routes – coal-to-ammonia (CtA), natural gas-to-ammonia (MtA), biomass-to-ammonia (BtA), and power-to-ammonia via water electrolysis (PtA), together with 43 multi-process integrated configurations. By integrating techno-economic analysis (TEA) with life-cycle assessment (LCA), we quantify differences in energy efficiency, production cost and carbon emissions across pathways. Our analysis spans scales from unit-level optimization within process systems to industry-level transition trajectories from fossil-based production to green ammonia, providing across-scale decision support for the low-carbon transformation of the ammonia sector.

KEYWORDS

ammonia production; techno-economic analysis; LCA; process integration

ACKNOWLEDGEMENTS

The research is supported by National Natural Science Foundation of China (under grant No. U24B6016 and No. 22378323)

OS-B4-08

STUDENT ORAL

16:15~16:30 · Session B4 · D408

Comprehensive Analysis and Life Cycle Assessment of Combined Cycle Power Generation and Cogeneration Systems

Ruru Ma, Wenwu Xu, Lili Yang, Zhaoyou Zhu, Yinglong Wang, Peizhe Cui*

Qingdao University of Science and Technology, China

ABSTRACT

The global energy industry is undergoing a significant transformation driven by the advent of renewable energy sources. This study proposes a polygeneration system that utilizes waste plastics and biomass to produce green methanol in a low-carbon and efficient manner through plasma gasification, and combines supercritical carbon dioxide brayton cycle (SCBC) and organic rankine cycle (ORC) for joint power generation. The system's thermodynamic performance and economic benefits were explored through energy, exergy, and economic analyses, and a carbon footprint (CF) analysis based on the entire life cycle was conducted. The results demonstrate that the energy and exergy efficiencies of the system are 71.70 and 58.10%, respectively. Furthermore, the system can achieve cost recovery and generate a profit within 6.25 years, with a net present value of up to 9655.35 thousand U.S. dollars, representing a substantial economic benefit. Across the entire methanol (MeOH) production process, the CF is only 2.1252 kg CO2-eq/MJ MeOH, indicating low CO2 emissions. This study offers a novel approach to the utilization of organic solid waste, providing a valuable reference point for the future production of MeOH in an environmentally sustainable manner.

KEYWORDS

organic solid waste, plasma gasification, green methanol, life cycle assessment

OS-B4-09

STUDENT ORAL

16:30~16:45 · Session B4 · D408

Integrated Modeling and Evaluation of a Green Dimethyl Ether–Based Energy Supply Chain

S.-C. Lien, C.-W. Ong, C.-C. Li, Z.-Q. Lin, and C.-L. Chen*

Department of Chemical Engineering, National Taiwan University, Taiwan

ABSTRACT

Long-distance transport of renewable electricity remains challenging when supply and demand are geographically separated. Hydrogen is widely recognized as a low-carbon carrier; however, its low volumetric energy density complicates large-scale storage and shipping. This study develops and evaluates a closed-carbon-loop international supply chain in which renewable electricity is converted to green dimethyl ether (DME) in exporting countries and reconverted to electricity in importing grids. On the exporting side, water electrolysis produces hydrogen for DME synthesis. On the importing side, DME undergoes steam reforming followed by H2/CO2 separation, CO2 liquefaction for return transport and recycling, followed by fuel-cell power generation. Aspen Plus–based simulations were performed for DME synthesis, reforming, separation, and CO2 liquefaction, while electrolysis, marine transport, and fuel cells were evaluated using system-level models. For the base case, 44.99 MWh_e per t-H2 of renewable electricity yields 14.29 MWh_e per t-H2 delivered to importing grids, corresponding to a round-trip efficiency of 31.8%. At USD 30/MWh_e renewable electricity, the delivered electricity cost is USD 271.8/MWh_e, and a screening life-cycle assessment estimates global warming potential.

KEYWORDS

green DME; renewable energy supply chain; DNE synthesis; DME steam reforming; CO2 capture; CO2 liquefaction

OS-B4-10

STUDENT ORAL

16:45~17:00 · Session B4 · D408

Uncertainty Quantification and Reliability Evaluation Approaches for Multiscale Complex Systems

Yang Sun[1], Zhe Cui[1], Wei Wang[2], and Wende Tian[1,*]

[1] *College of Chemical Engineering, Qingdao University of Science & Technology, China*
[2] *Department of Mechanical Engineering, City University of Hong Kong, China*

ABSTRACT

The subjects of Process Systems Engineering (PSE) are Process Safety. Key parameters of multiscale complex systems exhibit inherent uncertainties, and the excessive computational cost of multiscale high-fidelity models renders the accurate characterization, efficient propagation of uncertainties and quantitative reliability assessment of such systems a core challenge. Accordingly, a unified theoretical framework is proposed for uncertainty quantification and reliability analysis tailored to multiscale complex systems, which integrates multiscale coupled modeling, surrogate model-assisted dimensionality reduction, and multifidelity efficient sampling techniques. The framework employs polynomial chaos expansion (PCE) as an alternative model to overcome the computational bottleneck of high-fidelity multi-scale models, achieving the screening and dimensionality reduction of key parameters in high-dimensional systems, and alleviating the dilemma of imbalance between computational efficiency and accuracy. Furthermore, a Multilevel Monte Carlo (MLMC) hierarchical sampling strategy is adopted to enable high-precision uncertainty propagation and quantitative evaluation of system reliability. The proposed framework is validated using a multiscale catalytic flow reactor as a typical case, through which accurate uncertainty quantification, key parameter identification and system reliability assessment are accomplished. The results demonstrate that the framework possesses favorable practicality and scalability, providing a practical support for uncertainty quantification and reliability evaluation of multiscale complex process systems.

KEYWORDS

Multiscale systems; Uncertainty quantification; MLMC; Reliability analysis

ACKNOWLEDGEMENTS

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K-C1-01

KEYNOTE

10:00~10:30 · Keynote · Session C1 · D404

AI-Driven Design and Optimization for Complex Chemical Processes

Xiaodong Hong, **Zuwei Liao***

State Key Laboratory of Chemical Engineering and Low-Carbon Technology, College of Chemical and Biological Engineering, Zhejiang University, China

ABSTRACT

This talk presents two key research advances in process systems engineering. First, an adaptive sampling Bayesian optimization algorithm is developed for constrained black-box optimization, alongside a two-stage reverse design framework for HEN-ORC systems. Combining group contribution-artificial neural network models, we screen high-performance, low-GWP hydrofluoroolefin working fluids from a massive molecular library, effectively cutting total annual cost and boosting power output. Second, a two-stage expert-guided deep reinforcement learning (DRL) strategy is proposed for large time-delay process control. Taking PID as the expert, the method realizes learning and surpassing the expert via staged reward design, achieving superior control performance in industrial polyethylene fluidized bed reactors with a 264.8 s time delay. The proposed AI-driven methods show great potential for complex industrial process design and optimization.

KEYWORDS

Reinforcement Learning, Process Optimization, Molecular Design, Time-delay System

ACKNOWLEDGEMENTS

The financial support provided by the Project of the National Natural Science Foundation of China (22308314, U22A20415)

OR-C1-01

REGULAR ORAL

10:30~10:50 · Session C1 · D404

AI Chemical Process Designer Using LLM Agents and the Model Context Protocol: From Aspen Plus Flowsheet Generation to Heat Exchanger Design

Jia-Lin Kang[1,*], Yuan Yao[2], and David Shan Hill Wong[2]

[1]Department of Chemical Engineering, National Chung Cheng University, Taiwan
[2]Department of Chemical Engineering, National Tsing Hua University, Taiwan

ABSTRACT

This study presents an LLM-based chemical process design framework that integrates the Model Context Protocol (MCP) with Aspen Plus to convert natural language and scientific literature into executable simulation workflows. The core capability of the framework is semantic process modeling, including flowsheet generation, specification assignment, simulation convergence, and iterative design adjustment. In binary distillation, pressure-swing distillation, and isopropanol process reconstruction, the system accurately interpreted engineering intent, extracted key process data from multimodal literature sources, and generated converged rigorous simulations. To further examine extensibility beyond flowsheet construction, a heat exchanger optimization module was incorporated using MCP-guided interaction with Aspen EDR and skill-based learning. Rather than replacing the main Aspen Plus workflow, this module serves as a representative downstream design task, showing that the same LLM-MCP architecture can optimize pre-designed heat exchangers under engineering constraints while improving robustness through adaptive error-correction skills. Overall, the results demonstrate that MCP enables LLMs to move from conversational assistance toward reliable engineering action, supporting both process simulation automation and targeted equipment-level optimization in computer-aided process engineering.

KEYWORDS

Large Language Models, Model Context Protocol, Aspen Plus, Process Simulation, Heat Exchanger Optimization, AI-Assisted Design

ACKNOWLEDGEMENTS

The authors acknowledged the financial support provided by Ministry of Science and Technology, R.O.C through the grants of NSTC 113-2221-E-194 -045 -MY3 and NSTC 114-2218-E-007 -018.

OR-C1-02

REGULAR ORAL

10:50~11:10 · Session C1 · D404

What Chemical Engineers can Learn from the Digestive System: Multiscale Modeling for Knowledge Discovery and Engineering Innovation

Jie Xiao*

School of Chemical and Environmental Engineering, Soochow University, China

ABSTRACT

Human digestive system consists of multiple organs that work collaboratively and highly efficiently for food digestion and nutrient absorption. Understanding the phenomena taken place in these organs is of great importance for human health. More importantly, those fundamental understandings may lead to novel process intensification strategies. Through collaboration with researchers in biomedical, food and nutrition sciences, chemical engineers are believed to be able to make unique contributions to this field by offering scientific discoveries and technological innovations. In this talk, we will share with the audience our ongoing efforts on multiscale modeling and simulation for the digestive system, i.e., a complex system under biological neural control. At the microscale, we quantitatively evaluated the influence of villi movement on absorption and mass transfer in the vicinity of the intestinal wall. At the individual organ scale, we revealed the mixing and absorption intensification mechanisms by the multiscale structures on the inner surface of stomach and intestine. At the macroscopic system scale, we coupled the digestive system model with the insulin regulation model to realize blood sugar prediction under different diet conditions. Moreover, inspirations from the digestive system motivated us to develop the soft elastic reactor (SER), which will be briefly introduced.

KEYWORDS

Multiscale modeling and simulation; Process intensification; Digestive system; Mass transfer; Mixing; Biological neural control

OR-C1-03

REGULAR ORAL

11:10~11:30 · Session C1 · D404

Classification of Organic Reaction Mechanisms from Heterogeneous Data Using Transformer Models

Junu Kim*, Muhammad Aarash Abro, Bradford Tuckfield, Shunsei Yayabe

Auxilart Co., Ltd., Japan

ABSTRACT

Elucidating reaction mechanisms is fundamental to constructing mechanistic models for process design and optimization. Kinetic studies offer deep insights into reaction pathways while enabling the estimation of system-specific parameters. Traditionally, however, these studies are resource-intensive, requiring iterative cycles of data acquisition and model refinement. While machine learning (ML) has been proposed to automate mechanism classification, existing methods often assume idealized conditions, such as uniform time intervals and complete feature sets. In practice, experimental data are irregular: sampling intervals vary, and measured species differ across systems, limiting the applicability of conventional ML approaches.

In this work, we present a Transformer-based framework for mechanism classification in organic reactions that directly addresses these limitations. By employing a Transformer encoder, our approach leverages self-attention to associate informative time points across uneven intervals, effectively handling variable-length inputs and irregular sampling. To adapt to incomplete or inconsistent features, we integrate randomized feature masking to ensure robust representations even under missing measurements. Training data were generated via ODE-based simulations with diverse parameter combinations and uneven timesteps to mimic real-world experimental variability. Our results demonstrate that this architecture, combined with a multi-sample inference strategy, significantly improves classification accuracy and generalizability across heterogeneous kinetic datasets.

KEYWORDS

Transformer, Reaction mechanism, Machine learning, Chemical reaction

ACKNOWLEDGEMENTS

N/A

OR-C1-04

REGULAR ORAL

11:30~11:50 · Session C1 · D404

Development of a Knowledge Graph-Based RAG System to Support Techno-Economic and Life Cycle Assessment of Chemical Processes

Juyeon Kim[1], Minji Kim[2], Jin Ko[2], Youngwon Lee[1], Youlim Chung[1], Junghwan Kim[2], and Jonggeol Na[1,*]

[1]*Department of Chemical Engineering & Materials Science, Ewha Womans University, Korea*
[2]*Department of Chemical and Biomolecular Engineering, Yonsei University, Korea*

ABSTRACT

Techno-economic assessment (TEA) and life cycle assessment (LCA) are widely used to evaluate the feasibility and sustainability of chemical processes. These analyses require information on feed and product compositions, operating conditions, reactor and separation performance, utility consumption, mass and energy balances, and economic and environmental indicators. However, such information is often scattered across journal articles, technical reports, and supplementary materials, and is presented not only in text but also in tables, figures, and equations. In this study, we developed a knowledge graph-based retrieval-augmented generation (RAG) system to support TEA and LCA of chemical processes. The system combines vector retrieval and knowledge graph retrieval so that both semantic similarity and process relationships can be considered during information search. Two graph structures were used: a process-specific knowledge graph describing chemical engineering entities such as unit operations, process streams, utilities, operating variables, and assessment metrics, and a general knowledge graph for broader background knowledge. The system was also designed to handle multimodal documents containing text, images, tables, and mathematical expressions. This approach is intended to help users find relevant information more efficiently and organize dispersed evidence for TEA/LCA and process evaluation.

KEYWORDS

Techno-economic assessment (TEA), Life cycle assessment (LCA), Chemical process evaluation, Knowledge graph, Retrieval-augmented generation (RAG)

ACKNOWLEDGEMENTS

This research was supported by the BK21 FOUR (Fostering Outstanding Universities for Research) funded by the Ministry of Education(MOE, Korea) and National Research Foundation of Korea(NRF-5199990614253)

OR-C1-05

REGULAR ORAL

11:50~12:10 · Session C1 · D404

A combined Quantum-Chemical-microkinetic-modeling workflow for on-line optimization of an integrated carbon capture and conversion unit

Supareak Praserthdam*

Department of Chemical Engineering, Chulalongkorn University, Thailand

ABSTRACT

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 feed-forward control loop calculations. Acknowledgments We acknowledged (1) 111th Anniversary Engineering Research Catalyst Fund Towards U Top 100, (2) TSRI Fund, (IND_FF_69_054_2100_009), (3) N42A670295, NRCT, and RCAD (B41G690089) References [1] S. Praserthdam, P.B. Balbuena, Reaction Kinetics, Mechanisms and Catalysis, 122 (2017) 53–68. [2] S. Praserthdam, P.B. Balbuena, Catal Today, 312 (2018) 23–34. [3] S. Praserthdam, S. Somdee, M. Rittiruam, P.B. Balbuena, Energy Fuels, 34 (2020) 4855–4864. [4] J. Noppakhun, M. Rittiruam, T. Saelee, J.S. Shaikh, P. Khajondetchairit, S. Praserthdam, P. Praserthdam, Chemcatchem, 15 (2023).

KEYWORDS

Dry Reforming; CCUS; Catalyst Screening

K-C2-01

KEYNOTE

10:00~10:30 · Keynote · Session C2 · D403

Automated Physical Modeling in PSE: Literature-to-Model Automation and Multimodal Extensions

Shota Kato*

Department of Informatics, Kyoto University, Japan

ABSTRACT

Physical models are central to process design and control, yet building and maintaining them remains labor-intensive because experts must repeatedly survey the literature, decide how to combine equations into useful models, and evaluate where the models succeed or fail. To systematize this end-to-end procedure, we proposed the concept of an automated physical model builder (AutoPMoB) and have been developing methods to realize it. AutoPMoB is designed to retrieve relevant documents, extract variables and equations, normalize notation by judging equivalence of definitions and expressions, and build and rank candidate models by selecting consistent equation sets. We developed information extraction and equivalence judgment methods based on natural language processing (NLP) and combined computer algebra systems (CAS) with process systems engineering (PSE) knowledge to design algorithms tailored to physical model building from literature information. This keynote presents the AutoPMoB roadmap and progress on each component, then outlines recent directions motivated by advances in large language models (LLMs) and vision language models (VLMs): using LLM-encoded constraints to narrow symbolic-regression search spaces and supporting model evaluation with plots and VLMs. The talk closes by discussing how AI-assisted workflows can make physical modeling in PSE more systematic, reproducible, and scalable.

KEYWORDS

physical modeling, literature mining, information extraction, notation normalization, large language models, model evaluation

ACKNOWLEDGEMENTS

This work was partially supported by JST PRESTO Grant Number JPMJPR25T1.

OR-C2-01

REGULAR ORAL

10:30~10:50 · Session C2 · D403

Design of Optimal Lubricants through Computer-Aided Approach

Xian Zhuang Chong, Nishanth G. Chemmangattuvalappil, **Lik Yin Ng***

Faculty of Engineering and Technology, Sunway University, Malaysia

ABSTRACT

The depletion of fossil fuel reserves and increasing environmental concerns have necessitated the transition towards sustainable, biodegradable lubrication alternatives. However, natural vegetable oils often exhibit physicochemical limitations, such as poor low-temperature fluidity and oxidative instability, which restrict their industrial application. This study aims to address these limitations by developing an integrated Computer-Aided Molecular Design framework to identify optimal biolubricant from vegetable oil feedstocks. The framework utilizes Rough Set Machine Learning to analyze 31 vegetable oils. The generated predictive rules were used to identify critical property targets, specifically dynamic viscosity and pour point. Five molecules were generated and verified using Kappa indices (k1, k2) to quantify the relationship between molecular architecture and performance. The results demonstrated that all candidates met the dynamic viscosity target, but their thermal stability varied based on structural topology. Solution 1 was identified as the optimal design, achieving an exceptional Viscosity Index of 501.83. This significantly surpasses conventional mineral oils, due to its compact topological profile (k2 = 37.8) and a balanced degree of unsaturation, which maintains hydrodynamic stability without excessive polarity observed in lower-performing candidate. The proposed framework effectively translates target physicochemical properties into feasible molecular designs, offering a promising pathway for developing high-performance, sustainable biolubricants.

KEYWORDS

Biolubricant oil; Computer-aided molecular design (CAMD); Rough Set Machine Learning (ROSE 2); Kappa Indices; Pour Point; Viscosity Index

ACKNOWLEDGEMENTS

The professional guidance provided by Dr. Micky Lee Fu Xiang and Dr. Chong Yen Yee from Oleon Port Klang Sdn Bhd are gratefully appreciated.

OR-C2-02

REGULAR ORAL

10:50~11:10 · Session C2 · D403

Evaluation of Pre-Combustion CO_2 Capture Processes from High CO_2 Content Gas Sources Using Physical Solvent Absorption and Cryogenic Distillation

Rendra Panca Anugraha[*], Renanto Renanto, Juwari Juwari, Raden Ricko Satriyo, Tiara Miratul Zaini and Annisa Maharani

Department of Chemical Engineering, Institut Teknologi Sepuluh Nopember, Indonesia

ABSTRACT

Responses to the urgency of greenhouse gas emissions focus on CO2 capture technologies, especially for high-CO2 content gas that requires separation to meet product specifications. This study assesses the feasibility of applying two CO2 capture technologies: Physical Solvent Absorption and Cryogenic Distillation. The evaluation was conducted using process simulation, where both capture schemes were modeled and benchmarked using key performance indicators such as CO2 capture efficiency and economic performance. Compared to post-combustion capture, pre-combustion CO2 capture offers advantages due to higher CO2 partial pressure, providing separation driving forces and improved capture efficiency. Physical solvent absorption removes CO2 primarily through pressure-driven dissolution in the solvent, making it favorable for gas streams due to solubility. For this route, the process achieves 95.8% CO2 removal, and the economic assessment identifies Purisol as the most cost-effective option, delivering a 29.9% lower TAC than Selexol and a 37.7% lower TAC than Rectisol. In contrast, cryogenic distillation separates CO2 by cooling the gas to induce phase separation, enabling high-purity CO2 production suitable for transport, storage, or utilization. For the cryogenic route, CFZ distillation produces high CO2 quality with 98.72% CO2 purity, while reporting a CO2 capture cost of 7.9 USD/tonne CO2 in the Natuna case study.

KEYWORDS

CO2 Capture, Pre-Combustion, Physical Solvents, Cryogenic Distillation

ACKNOWLEDGEMENTS

This research was funded by Institut Teknologi Sepuluh Nopember under research grant scheme “Strategic Research Grant”

OR-C2-03

REGULAR ORAL

11:10~11:30 · Session C2 · D403

AI-Augmented Process Systems Engineering for Mixing Design: Constraint-Aware Small-Data Optimization Wrapped Around First-Principles Models

Richard D. LaRoche[1,*] and Cenk Feridunoglu[2]

[1]*Rwanika-La Roche LLC, USA*

[2]*Empower Operations Corp., Canada*

ABSTRACT

We present an AI-augmented Process Systems Engineering workflow for mixing design that addresses a common industrial bottleneck: rapid, defensible exploration of large, constrained design spaces with a limited budget of evaluations. The workflow couples a first-principles mixing simulator (KaeMix) as the physics engine with a small-data, constraint-aware optimization layer (OASIS.AI) that sequentially proposes candidate designs to evaluate. Here, “AI” denotes learning-guided search and constraint handling; it does not replace mechanistic modeling, and engineers remain in the loop by defining objectives, constraints, and permissible variables . A bioprocess case study illustrates aerobic, shear-sensitive bioreactor design. The search spans impeller configuration and operating policies (agitation and gassing) subject to a mass-transfer requirement (kLa constraint), power limits, and operability bounds, while minimizing a turbulence-based shear proxy. Compared with manual tuning or coarse parametric sweeps, the AI-augmented workflow converges faster to feasible designs and reveals non-obvious alternatives that satisfy kLa at materially reduced power and lower predicted shear exposure. Outputs are delivered as a constraint-filtered Pareto set that makes trade-offs explicit and supports robustness and operability review. The approach generalizes to other unit operations where iteration cost dominates progress, aligning with PSE ASIA themes of AI/ML, optimization, safety/operability, and energy efficiency.

KEYWORDS

AI-augmented modeling, mixing design, constrained optimization, bioreactors, design-space exploration

ACKNOWLEDGEMENTS

The authors thank André Bakker (KaeMix LLC) for technical discussions and guidance on mixing modeling using KaeMix.

OR-C2-04

REGULAR ORAL

11:30~11:50 · Session C2 · D403

Economic-robust optimization of heat load allocation and debottlenecking in heat exchanger networks under multi-source disturbances

Liwen Zhao, Guilian Liu*

School of Chemical Engineering and Technology, Xi'an Jiaotong University, China

ABSTRACT

Heat exchanger networks are prone to heat load imbalance and local bottlenecks under multi-source disturbances, which reduce system energy efficiency and stability. An economically robust optimization method is proposed to determine optimal heat load allocation and cost-efficient debottlenecking solutions under disturbances. Based on information flow graphs and equipment/system heat balance analysis, disturbance propagation paths are identified, and quantitative relationships among equipment heat load variations, dynamic heat transfer capacity requirements, and uncertain disturbances are established. By treating manipulated-variable heat load allocation weights as decision variables, a comprehensive cost model that accounts for both control adjustment expenses and bottleneck elimination costs is developed. Robust optimization is used to determine the load allocation strategy that minimizes total annual cost across multiple disturbance scenarios. Key bottlenecks are identified, and targeted debottlenecking measures that do not require topological modifications are proposed. A case study on benzene alkylation validates the method. By regulating heat load and eliminating bottlenecks, system feasibility is maintained, and the total annual cost is reduced by 8.7% compared with the baseline solution. This research provides an implementable, cost-effective technical pathway for enhancing the resilience and energy-saving retrofit of complex industrial energy systems.

KEYWORDS

Heat exchanger network; Disturbance; Bottleneck; Optimization; Economic

ACKNOWLEDGEMENTS

Financial support provided by the National Natural Science Foundation of China (U24B6016), the Higher Education Institution Academic Discipline Innovation and Talent Introduction Plan ("111 Plan") (No. B23025), and the Key Research and Development Program of Shaanxi (Program No. 2025PT-ZCK-09) are gratefully acknowledged.

OR-C2-05

REGULAR ORAL

11:50~12:10 · Session C2 · D403

Coupled level-set volume-of-fluid CFD simulation of methane decomposition in molten Ni-Bi, Ni-Bi-Mo, Ni-Bi-Se, and Ga-Bi bubble column reactors for hydrogen production

Son Ich Ngo[1,2], Jun-Ho Yang[1], Young-Il Lim[1,*], and Uen-Do Lee[3]

[1]*Department of Chemical Engineering, Hankyong National University, Korea*
[2]*Faculty of Heat and Refrigeration Engineering, Industrial University of Ho Chi Minh City, Vietnam*
[3]*Korea Institute of Industrial Technology (KITECH), Korea*

ABSTRACT

Catalytic decomposition of methane (CDM) in molten-metal bubble column reactors (MMBCRs) for hydrogen production is governed by complex hydrodynamics and bubble surface reactions. Quantifying these processes is challenging owing to complex bubble dynamics, the low optical transparency of the molten medium, and the harsh operating conditions. This study employed a coupled level-set volume-of-fluid (LS-VOF) computational fluid dynamics (CFD) framework, integrated with pricewise linear interface calculation (PLIC) method, to simulate the decomposition of a single methane bubble in various molten alloy catalyts, including Ni-Bi, Ni-Bi-Mo, Ni-Bi-Se, and Ga-Bi. Multiphase turbulence was resolved using large-eddy simulation (LES) with the WALE subgrid-scale model. Inert carbon particles were artificially introduced at the bubble surface as a surrogate for the solid carbon product formed during the reaction. Pronounced variations in bubble size, shape, and residence time were observed across the different alloys. Particle tracking revealed distinct circulation patterns of solid carbon within the MMBCR. These findings elucidate the coupled interplay among hydrodynamics, bubble dynamics, and reaction kinetics in MMBCRs. The present study provides critical insights to guide the optimization of reactor configuration and catalyst selection for enhanced hydrogen production efficiency.

KEYWORDS

Hydrogen production, Catalytic decomposition of methane, Molten metal bubble column reactor, Hydrodynamics, Coupled level-set volume-of-fluid (LS-VOF).

ACKNOWLEDGEMENTS

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OS-C3-01

STUDENT ORAL

10:00~10:15 · Session C3 · D402

A Temporally Gated Graph Convolutional Model with Dual Dynamic Adjacency for Soft Sensing in Chemical Processes

Zhen-Feng Jiang, **Hsiang-Ting Yuan**, Yuan Yao*

Department of Chemical Engineering, National Tsing Hua University, Taiwan

ABSTRACT

This paper proposes an industrial multivariate time-series forecasting model for soft sensing of quality-relevant variables in chemical processes by integrating graph convolution with temporal gating mechanisms, termed the Temporally Gated Graph Convolutional Model with Dual Dynamic Adjacency (TGGC-DA), to characterize the nonlinear and multi-time-scale dynamics of chemical reactors. The model employs dynamic feature-adjacency learning to capture causal relationships among process variables, while temporal adjacency learning is incorporated to model horizon-dependent dependencies on historical information. Through this design, TGGC-DA simultaneously learns dynamic dependency structures at both the feature and temporal levels. A parameter-efficient Time Gated Unit (TGU) is adopted as the recurrent core, enabling reduced model complexity while preserving predictive capability. This architecture addresses the limitations of conventional sequence-to-sequence (StS) models, which rely on implicit variable-independence assumptions and often struggle with long-delay quality-variable prediction. When applied to a simulated continuous stirred-tank reactor, multi-step forecasting results for reactor pressure, hydrogen-to-ethylene ratio, and melt index demonstrate that TGGC-DDAL consistently outperforms standard StS and memory-layer StS (ML-StS) baselines in terms of RMSE, MAE, and R2. Notably, without introducing gain-consistency or explicit physical constraints, the model delivers predictions that are both accurate and interpretable, highlighting its potential for industrial digital-twin applications.

KEYWORDS

soft sensing; chemical process prediction; graph convolutional network; dynamic adjacency learning; sequence-to-sequence models

OS-C3-02

STUDENT ORAL

10:15~10:30 · Session C3 · D402

Process topology-Aware Fault Diagnosis under Operating Conditions Shifts via Domain-Invariant Normal State Alignment

Hae Rang Roh, and Jong Min Lee*

Department of Chemical and Biological Engineering, Seoul National University, Korea

ABSTRACT

Fault diagnosis in complex chemical plants with various operating conditions is highly challenging, making it impractical to collect exhaustive fault data for every operational state. These varying conditions act as distinct domains, inducing severe domain shifts that hinder the generalization of deep learning models. Under the realistic assumption that normal operating data is readily available across all conditions, we propose a novel graph neural network-based framework for cross-domain fault diagnosis. The feature extraction module of the proposed framework extracts domain-invariant latent representations of normal states from both source and target domains via unsupervised alignment, using topological relationships reflected in an adjacency matrix from the process flow diagram. In the subsequent fault classification module, features extracted from the source domain are fused with the shared normal representations via multi-head attention. By contextualizing the input features against this domain-invariant normal baseline, the attention mechanism effectively isolates fault-specific deviations from domain-induced shifts. Consequently, the proposed approach enables accurate fault classification in the target domain during test time, even in the complete absence of target domain fault data during training.

KEYWORDS

Cross-domain Fault Diagnosis, Domain Generalization, Process Topology, Graph Neural Networks, Multi-head Attention

ACKNOWLEDGEMENTS

This work was supported by Samsung Electronics Co., Ltd.

OS-C3-03

STUDENT ORAL

10:30~10:45 · Session C3 · D402

Environmental Evaluation of a Cement Clinker Production Process Using Algae-Derived CaCO3

Hafiz M. Irfan, and Wei Wu*

Department of Chemical Engineering, National Cheng Kung University, Taiwan

ABSTRACT

Traditional cement manufacturing is a major source of greenhouse gas emissions; therefore, the incorporation of calcareous green algae and fly ash as partial cement replacements offers a promising pathway toward near-zero carbon cement production. As a calcareous green alga, Halimeda macroloba is a significant producer of biogenic calcium carbonate (CaCO3), sequestering approximately 440 kg of carbon dioxide (CO2) per 1000 kg of CaCO3, with CaCO3 production reported in relation to algal biomass. To assess the new low-carbon/low-waste cement production process, the proposed scenarios (2 and 3) are validated via Python-based modeling (Python 3.12) and Aspen Plus® simulation (Aspen V14). The core technology is the pre-calcination of algae-derived CaCO3 and fly ash from coal combustion, which are added to a rotary kiln to enhance the proportions of tricalcium silicate (C3S) and dicalcium silicate (C2S) for forming the desired silicate phases in clinker. Through the lifecycle assessment (LCA) of all scenarios using SimaPro® (SimaPro 10.2.0.3), the proposed Scenario 2 achieves the GWP at approximately 0.906 kg CO2-eq/kg clinker, lower than the conventional cement production process (Scenario 1) by 47%. If coal combustion is replaced by natural gas combustion, the fly ash additive is reduced by 74.5% in the cement replacement materials. However, the proposed Scenario 3 achieves a GWP of approximately 0.753 kg CO2-eq/kg clinker, which is lower than Scenario 2 by 16.9%. Moreover, the LCA indicators show that Scenario 3 has lower environmental impacts on human health, ecosystem, and resources than Scenario 1 by 24.5%, 60.0%, and 68.6%, respectively.

KEYWORDS

Process simulation; cement production; calcareous green algae; life cycle assessment; waste recovery

OS-C3-04

STUDENT ORAL

10:45~11:00 · Session C3 · D402

End-to-End Automated Framework for CHO Bioprocess Modeling with Large Language Models

Han Bit Kim[1], Young Hyun Cho[1], Dongkyu Kim[1], Janghan Lee[2,3], Seo-Yeon KIM[2,3], Jihoon Kim[2], and Moo Sun Hong[1,*]

[1] *Department of Chemical and Biological Engineering, Seoul National University, Korea*
[2] *New Drug Development Center, Korea*
[3] *College of Pharmacy, Chungbuk National University, Korea*

ABSTRACT

Accurate modeling of Chinese Hamster Ovary (CHO) cell bioreactors is essential for understanding process dynamics and supporting model-based design and control in biopharmaceutical manufacturing. However, constructing predictive models that capture both macroscopic metabolic behaviors and dynamic cultivation strategies requires extensive data preprocessing, model structuring, and domain expertise. These steps remain a major bottleneck in practical deployment, particularly when adapting models across diverse experimental conditions. To address this challenge, an end-to-end framework is developed that integrates large language models (LLMs) into bioprocess modeling workflows. The framework translates high-level user specifications into executable modeling pipelines, including data preprocessing, model formulation, and parameterization. By systematically incorporating bioprocess knowledge, the LLM interprets heterogeneous cultivation data and guides consistent and adaptable model construction. The proposed system supports multiple modeling approaches, including mechanistic, data-driven, and hybrid ODE-based formulations. It dynamically configures model structures, kinetic expressions, and parameter estimation settings based on user-defined objectives. This modular architecture allows flexible adaptation without manual reconfiguration. By automating key decision-making steps in bioprocess modeling, the framework reduces the need for manual expert input while improving scalability and reproducibility. This work demonstrates the potential of LLM-based systems as a unified interface for advanced bioprocess systems engineering applications in biomanufacturing.

KEYWORDS

Chinese Hamster Ovary (CHO) cells; Bioprocess modeling, Large Language Models (LLMs); Process automation

ACKNOWLEDGEMENTS

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OS-C3-05

STUDENT ORAL

11:00~11:15 · Session C3 · D402

Solving Large-Scale Heat Integration and MINLP Problems via LLM-Driven Adaptive Search

Hangrui Yang[1], Xiaodong Hong[1,2,*], Jingdai Wang[1], Yongrong Yang[1], and Zuwei Liao[1,*]

[1]*College of Chemical and Biological Engineering, Zhejiang University, China*
[2]*Engineering Research Center of Functional Materials Intelligent Manufacturing of Zhejiang Province, China*

ABSTRACT

Solving large-scale heat integration and Mixed-Integer Nonlinear Programming (MINLP) problems is of paramount importance in Process Systems Engineering (PSE), while is highly challenging due to non-convexities and discrete-continuous coupling. Large Neighborhood Search (LNS) is a promising heuristic, but its neighborhood selection lacks adaptability for complex structures. We propose LELMIN, a Large Language Model (LLM)-Enhanced LNS for MINLP, where an adaptive search framework for automated heuristic design is proposed. LELMIN translates complex MINLP structures into LLM-comprehensible text priors via nonlinear profiling. It evaluates strategy health using dynamic iterative feedback and employs a multi-agent collaborative mechanism for precise, noise-resistant code evolution. Evaluated on Heat Exchanger Network (HEN) synthesis and standard MINLP benchmarks, our LLM-driven strategies demonstrate exceptional efficiency. Within given time limits, LELMIN significantly outperforms state-of-the-art solvers (SCIP, BARON) and LLM-based baselines, discovering new best-known solutions for large-scale industrial instances.

KEYWORDS

MINLP, HENS, LLM, LNS.

ACKNOWLEDGEMENTS

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OS-C3-06

STUDENT ORAL

11:15~11:30 · Session C3 · D402

Development of an energy harvesting sensor device using magnetic phase transition and the accompanying entropy change

Hikaru Kiyomoto, Yuka Sakai, and Kansha Yasuki*

Department of Multidisciplinary Sciences, University of Tokyo, Japan

ABSTRACT

As interest in digitalization of industry and society is on the rise, so is the demand for novel data collection devices that make such digitalization possible. With concepts such as Industry 4.0 and, in the case of the Japanese movement for digitalization, Society 5.0 becoming more prevalent, it is clear that there is an urge for societal and industrial transition towards digitalization. A key component in Society 5.0 are devices for data collection, processing, and communication. Such devices need to be capable of these tasks in a large-scale, real-time, and crucially in an energy-smart way. The authors have proposed a novel energy harvesting temperature sensor device that utilizes the entropy change in magnetic materials that accompanies magnetic phase transitions. By combining this with electromagnetic induction, the device can collect temperature data while generating a small amount of electricity, thereby showing potential for application as an energy-smart sensor device. Here, the device is evaluated as an energy harvester by assessing energy efficiency from a thermodynamic perspective. The development and social application of the proposed device have the potential to greatly contribute not only to the recent push towards digitalization in industries, but also a greener energy transition on a societal level.

KEYWORDS

Energy harvester, magnetic phase transition, sensor, digitalization

ACKNOWLEDGEMENTS

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OS-C3-07

STUDENT ORAL

11:30~11:45 · Session C3 · D402

Hierarchical Reinforcement Learning for Sales–Production Coordination: A Stackelberg Game Approach to Manufacturing Scheduling

Yee Hung Hong and Zhao Jinsong*

Department of Chemical engineering, Tsinghua University, China

ABSTRACT

In make-to-order manufacturing systems, sales and production departments often pursue different objectives, leading to coordination inefficiencies that affect both operational and financial performance. Sales departments tend to accept more orders to increase revenue, whereas production departments must generate feasible schedules under limited capacity, machine availability, and due-date constraints. This mismatch may result in production congestion, delayed deliveries, and reduced overall profitability. To address this issue, this paper proposes a hierarchical reinforcement learning framework for sales–production coordination from a Stackelberg game perspective. In the proposed framework, the sales department is modeled as the leader that determines order acceptance decisions, while the production department is modeled as the follower that responds through production scheduling and resource allocation. The objective is to maximize long-term system profit while balancing key operational measures, including tardiness, schedule feasibility, and machine utilization. By explicitly modeling the hierarchical interaction between order acceptance and shop-floor scheduling, the proposed approach provides a practical method for integrated sales–production decision-making in dynamic manufacturing environments.

KEYWORDS

Intelligent manufacturing; Sales–production coordination; Hierarchical reinforcement learning; Stackelberg game; Flexible manufacturing systems

ACKNOWLEDGEMENTS

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OS-C3-08

STUDENT ORAL

11:45~12:00 · Session C3 · D402

An alternative retrofit strategy for conventional distillation sequences

Hsiao-Te Liu and Jeffrey D. Ward*

Department of Chemical Engineering, National Taiwan University, Taiwan

ABSTRACT

Distillation is the most energy-intensive unit operation employed in chemical manufacturing worldwide. Nonetheless, it remains the dominant method for separating liquid mixtures. Many researchers have recently been looking for alternative solutions with lower energy consumption and lower costs. For existing distillation systems, retrofit strategies are generally more realistic than complete reconstruction. Dividing-wall columns (DWCs) are often suggested as a retrofit option. This study uses a conventional dual-column direct distillation sequence (CS) as the case study for separating the ternary mixture of MCM (methylcyclopentane, cyclohexane, and methylcyclohexane).1 The feed conditions are 1 atm and 80.95°C, with a total flowrate of 1300 kg/h. The mass fractions of methylcyclopentane, cyclohexane, and methylcyclohexane are 24%, 54.7%, and 21.3%, respectively.2 The product purity is specified as 99.9 wt% for all components. In this work an alternative retrofit configuration is proposed: stacked side-stream sequences (SSSs).3 The CS is first optimized through simulated annealing algorithm (SAA), followed by retrofitting into both SSSs and DWCs. Energy consumption and cost performances are then systematically compared. The results show that retrofitting into SSSs leads to the greatest reductions, with energy consumption and total annual cost (TAC) decreasing by approximately 42.75% and 40.91%, respectively.

KEYWORDS

Distillation; Retrofit; Process Intensification; Process Optimization

ACKNOWLEDGEMENTS

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OS-C4-01

STUDENT ORAL

10:00~10:15 · Session C4 · D408

Techno-economic and environmental assessment of SMR-based methanol production: Comparative analysis of biomass and Dac pathways with Aalam cycle integration

Sungmin Lee[1], Matthew J. Realff[2,*], and Junghwan Kim[1,*]

[1] *Department of Chemical and Biomoleular Engineering, Yonsei University, Korea*
[2] *School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, USA*

ABSTRACT

This study evaluates four Small Modular Reactor (SMR)-based methanol production pathways (approximately 100 kt MeOH/yr) to address the cost-carbon trade-off in deep decarbonization. We compare biomass gasification and Direct Air Capture (DAC) as carbon sources, both with and without Allam cycle integration. The assessment utilizes multidimensional indicators: energy and exergy efficiency, Levelized Cost of Methanol (LCOM), carbon and water footprints, and the required carbon price (Cp*). Results show that LCOM ranges from \$762/ton for the lowest-cost biomass pathway to \$1,167/ton for the highest-cost DAC pathway. While all pathways significantly reduce carbon footprints (65.0% to 96.2%) compared to the fossil baseline, the DAC pathways achieve carbon negativity, reaching as low as -2.429 tCO2/tMeOH in Case 3. Interestingly, this high mitigation depth reverses the Cp* ranking; Case 3 requires the lowest carbon price at \$251/tCO2, a figure further reduced to \$155/tCO2 by 45Q tax credits—well within the IEA NZE 2050 benchmark of \$250/tCO2. However, a critical water-carbon nexus is identified, as nuclear life-cycle water consumption accounts for 51% to 69% of the total water footprint across the pathways. Sensitivity analysis reveals that SOEC/Co-SOEC stack lifetime is the most critical variable across all cases. This study provides a decision-making framework for optimizing carbon source selection and policy incentives to enhance the competitiveness of nuclear-based e-fuel production.

KEYWORDS

Small modular reactor, Direct air capture, Carbon-negative methanol, Water-carbon nexus, Techno-economic analysis

ACKNOWLEDGEMENTS

This research was supported by Korea Institute for Advancement of Technology(KIAT) grant funded by the Ministry of Trade, Industry & Energy(MOTIE), Korea Government (RS-2024-00436106, Human Resource Development Program for Industrial Innovation)

OS-C4-02

STUDENT ORAL

10:15~10:30 · Session C4 · D408

Electrification of Multi-Vessel Batch Distillation

Surendra Beniwal, and Sujit S. Jogwar*

Department of Chemical Engineering, Indian Institute of Technology Bombay, India

ABSTRACT

The electrification of distillation, given its widespread industrial use, high energy consumption, and low energy efficiency, offers promising pathway towards decarbonization and sustainable operation. Multi-vessel batch distillation (MVBD), an energy-efficient configuration for multicomponent separation, improves both energy and economic performance under total reflux operation by enabling simultaneous separation without off-cut generation. As shown in Figure 1(a), the MVBD column is divided into multiple sections by holdup vessels, with heat supplied at the bottom reboiler. Additionally, the intermediate vessels can act as reboilers, reducing vaporization temperature requirements and providing extra degrees of freedom. Heat-pump-assisted electrification of distillation offers significant carbon reduction potential. Accordingly, this work proposes the electrified MVBD configuration shown in Figure 1(b), a multi-stage compression scheme utilizing energy from overhead vapour to supply heat to both bottom and intermediate reboilers. The lower heating temperature requirement at intermediate reboilers reduces compression power, resulting in overall performance improvement and carbon emission reduction. In this work, the role of intermediate reboilers in electrified MVBD is systematically evaluated in terms of separation, energy consumption, and carbon emissions. Lastly, the effectiveness of the proposed framework is demonstrated through a simulation study of quaternary mixture separation. (a) MVBD (b) VR-MVBD Figure 1: Multi-vessel batch distillation

KEYWORDS

Decarbonization, Electrification of distillation, Process systems engineering, Multi-vessel batch distillation

OS-C4-03

STUDENT ORAL
10:30~10:45 · Session C4 · D408

Interpretable Neural Surrogate-Based Flowsheet Optimization under Catalyst Deactivation: Application to CO_2 Methanation

Teruki Saito, Osamu Tonomura*, and Ken-ichiro Sotowa

Kyoto University, Japan

ABSTRACT

Realizing a decarbonized society requires effective CO2 utilization technologies, among which CO2 methanation is a promising candidate. While extensive research has focused on catalyst development and reactor design, holistic flowsheet optimization over large design spaces and under process uncertainties, particularly catalyst degradation, remains computationally demanding. This study proposes an interpretable machine learning-based framework for comprehensive process design and optimization. The framework was applied to a CO2 methanation process consisting of multi-stage adiabatic reactors with internal recycling. By automating Aspen Plus v14 using Python, approximately 20,000 steady-state simulation data points were generated to train a differentiable neural network surrogate model. The surrogate enabled gradient-based optimization and reduced computational time by a factor of 3,500 compared to direct simulation. SHAP (SHapley Additive exPlanations) analysis identified feed composition, rather than reaction conditions, as the primary driver of cost efficiency and CO2 reduction. Furthermore, sequential optimization accounting for catalyst deactivation minimized replacement frequency. Under an identical annual cost constraint, the adaptive strategy reduced annual costs by 6 million JPY and achieved an additional 2,500 kmol/year CO2 reduction. The proposed framework provides a computationally efficient and explainable approach for robust process design and operational decision-making.

KEYWORDS

4-6 words (Font: Times New Roman, 12pt, Italic) CO2 methanation, surrogate modeling, flowsheet optimization, interpretability, catalyst deactivation

OS-C4-04

STUDENT ORAL

10:45~11:00 · Session C4 · D408

Stable Model-Based Actor-Critic Framework for Continuous Stirred-Tank Reactors Control

Tiantian Wu, Jingyi Lu*

East China University of Science and Technology, China

ABSTRACT

The severe nonlinearity inherent in continuous stirred-tank reactors (CSTRs) complicates high-performance control design. While model predictive control explicitly optimizes performance, its reliance on accurate analytical models and intensive online computation limits practical applicability. Reinforcement learning (RL) provides a viable data-driven alternative for deriving feedback policies directly from interaction data. However, standard neural-network-based RL lacks closed-loop stability guarantees and frequently yields oscillatory or overly aggressive control actions during deployment. To address this limitation, we propose a stable model-based actor-critic framework for CSTR systems. By integrating nominal mechanistic knowledge, we propose a Lyapunov-based stability-preserving structure for policy optimization. Constraining policy updates within a theoretically admissible set guarantees uniform ultimate boundedness of the closed-loop system and ensures safe exploration. To mitigate plant-model mismatch, an adaptive conformal inference method is introduced for model uncertainty quantification. This yields an uncertainty-aware mechanism that dynamically adjusts the model rollout horizon, optimally trading off the sample efficiency of synthetic rollouts against prediction bias accumulation. Simulation studies on a CSTR system demonstrate the effectiveness of the proposed approach. The derived policy not only ensures stable and sample-efficient optimization but also achieves precise setpoint tracking performance.

KEYWORDS

Continuous stirred-tank reactor; model-based reinforcement learning; stable control; adaptive rollout

OS-C4-05

STUDENT ORAL

11:00~11:15 · Session C4 · D408

Adaptive Physics-Informed Bayesian Optimization for High-Dimensional Material Discovery under Limited Data

Tomohiro Koji, Shota Kato, and Manabu Kano*

Department of Informatics, Kyoto University, Japan

ABSTRACT

High-dimensional material discovery requires finding optimal solutions under severely restricted evaluation budgets due to high experimental costs. This challenge is compounded by extremely limited data. While Trust Region Bayesian Optimization (TuRBO) remains a representative approach to high-dimensional Bayesian optimization, it typically requires hundreds to thousands of evaluations and fails under highly constrained conditions. To address this issue, we propose Adaptive Physics-Informed BO, which extends the TuRBO framework for catalyst discovery by integrating physical knowledge. Specifically, we model the relationship between electronegativity and catalytic activity using a Sabatier-based volcano plot. This physical model is incorporated as an adaptively updated bias into the acquisition function. We validated the proposed method using the Open Catalyst Project (OC20) dataset with 55-dimensional composition vectors. The proposed method achieved earlier discovery of highly active catalysts compared to TuRBO, particularly when starting with a single initial observation. By utilizing electronegativity, this physical model narrows down promising regions and excludes unlikely areas. This mechanism allows the algorithm to concentrate on high-potential subspaces early in the search and accelerates the discovery of optimal catalysts. Consequently, these findings indicate that integrating domain knowledge reduces the required experimental costs for high-dimensional optimization. (191 words) The abstract should be written in 200 words

KEYWORDS

Material Discovery, Bayesian Optimization, Catalyst Design, Physics-Informed Optimization, High-Dimensional Optimization, Data Efficiency

OS-C4-06

STUDENT ORAL

11:15~11:30 · Session C4 · D408

An Improved Process Configuration for DES-based Carbon Capture Process

Vaishnavi Gupta, Soumik Das, Ishan Bajaj*

Department of Chemical Engineering, Indian Institute of Technology Kanpur, India

ABSTRACT

Post-combustion carbon capture is essential for decarbonizing fossil-fuel-based power plants. However, conventional solvents such as monoethanolamine (MEA) have high volatility and energy-intensive regeneration. Deep eutectic solvents (DES), formed by combining hydrogen-bond donors and acceptors in specific ratios, have tunable thermophysical properties and are promising alternatives. Previous system-level studies on DES-based carbon capture have explored limited process configurations. In this work, we explore flue gas compression and lean gas expansion (FCLE) configuration (Figure 1a), wherein a turbine recovers energy from the high-pressure N2-rich stream leaving the absorption column. The process employs multi-stage compression with intercooling and turbine expansion with intermediate heating. We also perform heat integration by utilizing compressor outlet streams to preheat the turbine inlets. The resulting formulation is a mixed-integer nonlinear programming (MINLP) model that minimizes the annualized carbon capture cost. The model is applied to assess the performance of choline chloride (1:2) DES in natural gas combined-cycle (NGCC), coal-based power, and cement plants. In the NGCC plant, the FCLE configuration reduces capture costs from $226/tCO2 to $153/tCO2, whereas it reduces from $69.14/tCO2 to $52/tCO2 and from $34.52/tCO2 to $29.46/tCO2 for coal-based power and cement plants, respectively. Importantly, DES-based FCLE configuration exhibits lower heating and cooling requirements than the MEA-based process but requires more electricity because of compression. Figure 1. a) Process flowsheet of the proposed post-combustion carbon capture system, and b) Cost breakdown ($/tCO2 captured) for the NGCC, coal, and cement plants.

KEYWORDS

Carbon capture, deep eutectic solvents, process optimization, energy recovery

ACKNOWLEDGEMENTS

This research received support through Schmidt Sciences, LLC.

OS-C4-07

STUDENT ORAL

11:30~11:45 · Session C4 · D408

Physics-Informed Active Learning for Cross-Domain Fault Diagnosis in Chemical Processes

Shaochen Wang , Wende Tian *, and Zhe Cui

College of Chemical Engineering, Qingdao University of Science and Technology, China

ABSTRACT

Fault diagnosis in complex chemical processes faces severe data imbalance and cross-domain distribution shifts: real industrial fault samples are scarce, while simulation data, though abundant, differ significantly from real operations. To address this issue, a physics-constrained domain-aware active learning framework is proposed. First, simulation data generated from mechanism-based dynamic modeling are used for supervised pretraining to capture fault priors. Then, correlation alignment is applied to reduce distribution discrepancies between simulation and real data. To efficiently utilize limited labeling budgets, a domain-aware active learning strategy is introduced, integrating uncertainty, diversity, and a physics consistency metric derived from mass balance, energy balance, and mass transfer principles, ensuring physically plausible sample selection. Furthermore, pseudo-label-based adaptation enhances target domain learning, and a residual correction model is designed in the logits space to compensate for systematic biases between domains. The proposed framework follows a progressive paradigm of “simulation pretraining–active learning adaptation–residual correction,” enabling effective knowledge transfer under limited labeled data. Experimental results demonstrate improved diagnostic accuracy, robustness, and cross-domain generalization, highlighting its potential for real-world industrial applications.

KEYWORDS

Fault diagnosis; Active learning; Physics modeling; Chemical process systems

ACKNOWLEDGEMENTS

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OS-C4-08

STUDENT ORAL

11:45~12:00 · Session C4 · D408

Microscopic Interactions of Multi-component Systems and Energy-Saving Mechanisms in the Mixed Entrainer Distillation Process Title

Wen Sun, Shuai Wang*, Peizhe Cui, Xin Li, Yinglong Wang

College of Chemical Engineering, Qingdao University of Science and Technology, China

ABSTRACT

To realize the high-purity separation of methanol (MeOH)/tert-amyl methyl ether (TAME)/water azeotropic system, a novel mixed entrainer extractive distillation process was developed. Combined with a multi-objective genetic algorithm optimization, mixed entrainers and corresponding process schemes were identified. It is found that the optimal entrainer for each of the MeOH-TAME and TAME-Water azeotropes are not the best combination for the mixed entrainers. Therefore, quantum chemical and intermolecular interaction analysis, combining the mixed entrainer distillation process, were investigated to clarify the reasons for this phenomenon. To further study the separation processes with efficient performance, single entrainer extractive distillation (SEED), single entrainer extractive pressure-swing distillation (SEEPSD), mixed entrainer extractive distillation (MEED), mixed entrainer extractive pressure-swing distillation (MEEPSD), and MEEPSD with heat-integration (HI-MEEPSD) and heat-pump technology (HPI-MEEPSD) were explored. Compared with the SEED process, the MEEPSD process using DMSO-EG as the mixed entrainer decreases the total annual cost (TAC) by 8.74% and the gas emissions by 16.59%. The emission reduction rates of the aforementioned indicators were further raised to 11.41% and 34.52%, respectively, by implementing the heat-integrating and heat-pump technologies. The findings demonstrate that the developed HPI-MEEPSD process using DMSO+EG as entrainer exhibits efficient separation performance and can achieve sustainable separation of the MeOH/TAME/water system.

KEYWORDS

Extractive distillation; Electrostatic potential analysis; Mixed entrainer; Intensification design; Multi-objective optimization;

K-D1-01

KEYNOTE

14:30~15:00 · Keynote · Session D1 · D404

Multi-Scale Advances in CO_2 Capture: From Molecular Solvent Design to Process Intensification

Yu-Jeng Lin[1,*]

Department of Chemical Engineering, National Tsing Hua University, HsinChu City, 300 Taiwan

ABSTRACT

Industrial decarbonization demands a paradigm shift toward high-efficiency CO2 capture. This keynote presentation addresses these challenges via a multi-scale approach combining experiments and simulations to develop advanced solvents, introduce innovative process configurations, and elucidate their design synergies. To overcome the kinetics–capacity trade-off, we demonstrate a novel hybrid configuration utilizing two independent solvent loops. Operating each loop with solvents selected within their optimal performance windows significantly reduces energy requirements. In parallel, we develop advanced water-lean solvents by introducing a novel carbamate-to-alkyl carbonate pathway. This approach simultaneously enhances absorption kinetics and capacity by integrating protic solvents with sterically hindered amines. Furthermore, uncovering the mechanistic role of latent heat shuttling on temperature-induced mass transfer pinches enables optimized water-lean solvent design. In the deep decarbonization of steelmaking, a self-sustained process is achieved via an electricity-driven CO2 capture integrated with blast furnace gas-fired cogeneration. This approach maximizes energy utilization efficiency and eliminates external energy dependency. Finally, to bridge these molecular and process scales, we present a first-principles framework to predict amine-CO2 chemistries without empirical data, facilitating rapid solvent design based on system-level performance.

KEYWORDS

Water-lean solvent, deep decarbonization, process electrification, quantum chemical calculation

OR-D1-01

REGULAR ORAL

15:00~15:20 · Session D1 · D404

Data-integrated design of organic flow batteries: linking molecular properties, operando response, and predictive engineering

Soorathep Kheawhom*

Department of Chemical Engineering, Chulalongkorn University, Thailand

ABSTRACT

Organic flow batteries offer molecular tunability, flexible architecture, and the potential use of earth-abundant materials for sustainable energy storage. However, their development often remains fragmented across molecular design, electrochemical testing, and engineering evaluation, limiting predictive understanding of performance and durability. This presentation introduces a data-integrated framework that combines molecular descriptors, operando and electrochemical measurements, and process-level operating variables to support mechanism-informed design decisions. Organic flow battery behavior arises from coupled interactions among molecular structure, electrolyte properties, transport, flow conditions, and degradation pathways. By translating these heterogeneous data into interpretable engineering descriptors, the framework identifies dominant factors governing voltage efficiency, capacity utilization, reversibility, and cycling stability. A representative organic flow battery system is used to show how linked data layers reveal performance-loss mechanisms and guide choices in molecule selection, electrolyte formulation, and operating strategy. The framework provides a pathway from empirical screening to predictive systems engineering.

KEYWORDS

Organic flow batteries; Data-integrated design; Operando characterization; Predictive engineering; Process systems engineering

OR-D1-02

REGULAR ORAL

15:20~15:40 · Session D1 · D404

Automated Modeling and Optimization of SOFC-CHP Systems via Large Language Models

Vikram Uday, Jui-Yuan Lee*

Department of Chemical Engineering, National Cheng Kung University, Tainan, Taiwan, R.O.C.

ABSTRACT

Solid oxide fuel cell (SOFC)-based combined heat and power (CHP) systems are pivotal for high-efficiency stationary power generation, especially using biogas. However, developing reliable SOFC-CHP models remains challenging due to the complex coupling of electrochemical kinetics, reforming reactions (i.e., steam methane reforming/water-gas shift), and heat transfer. Conventional modeling requires manual equation derivation and programming, often taking weeks and hindering rapid performance analysis. This study proposes a large language model (LLM)-assisted framework to streamline SOFC-CHP model development. By leveraging LLMs via structured commands, the framework automatically generates governing equations and executable Python code for the SOFC, reformer, and combustor units. A baseline configuration is established to evaluate net electrical efficiency, followed by sensitivity-based optimization of key design parameters, including fuel utilization, operating temperatures, and active cell area. The generated models are validated against Aspen Plus, showing excellent agreement with literature data. Results demonstrate that the proposed workflow significantly reduces development time while maintaining high fidelity. Finally, a case study on biogas-fueled systems illustrates the framework's utility for sustainable process systems engineering.

KEYWORDS

Biogas; Python-based simulation; Distributed power generation; Electrochemical kinetics

ACKNOWLEDGEMENTS

This research was funded by the National Science and Technology Council (NSTC), Taiwan, R.O.C. (Project Nos. 114-2221-E-006-033; 114-2811-E-006-034).

OR-D1-03

REGULAR ORAL

15:40~16:00 · Session D1 · D404

Machine Learning Embedded Superstructure Optimization for Biomethane Production

Virendra Gunjal, Ishan Bajaj*

Department of Chemical Engineering, Indian Institute of Technology Bombay, India

ABSTRACT

We develop a superstructure-based optimization framework (Figure 1a) that integrates machine learning (ML) models, simultaneously optimizing process design, operating conditions, and discrete technology choices for biomethane production. We adopt a detailed Aspen Plus (AP) model for biogas production via anaerobic digestion [1] and develop biogas upgradation AP models, including water and monoethanolamine (MEA) scrubbing with detailed rate-based models for the absorption and stripping columns, and methanation via the Sabatier process, modeled as a fixed-bed reactor. We train ML models on data generated using Latin hypercube sampling and AP simulations to predict stream compositions and energy consumption. ML models efficiently approximate complex process models, as shown in Figure 1b and substantially accelerate the optimization. During data generation, insufficient solvent flowrates often resulted in infeasible simulations with invalid stream composition outputs. To address this, we trained a classification model to identify feasible and infeasible solvent flow regimes (Figure 1c). The ML models are embedded within an optimization model resulting in MINLP and solved to global optimality using Gurobi. The results suggest that water scrubbing is the optimal technology, achieving a levelized cost of biomethane of €0.83/kg. Cost and revenue contributions are shown in Figure 1d. Figure 1e shows that profitability is driven mainly by biomethane price, while carbon credit price has a smaller effect. Figure 1: a) Superstructure for biomethane production, b) Sample parity plot of Random Forest model (for methane), c) Confusion matrix showing the accuracy of the classification model on test data, d) Cost & Revenue breakdown in optimal purification technology, e) Heatmap showing the effect of biomethane and carbon credit price on net profit

KEYWORDS

Anaerobic Digestion, Biogas Upgradation, Process Optimization

OR-D1-04

REGULAR ORAL

16:00~16:20 · Session D1 · D404

Safety-by-Design in Chemical Processes: An Ontological Framework for Verifying Critical Sensor Configurations

Chun-yien Chang[1], Ying-ping Chen[1], and **Wei-Jyun Wang**[2,*]

[1] *Department of Computer Science, National Yang Ming Chiao Tung University, Taiwan*
[2] *Department of Chemical and Materials Engineering, National Central University, Taiwan*

ABSTRACT

Conventional Hazard and Operability (HAZOP) analyses rely primarily on manual examination of documentation, making it difficult to systematically verify whether complex chemical process designs incorporate adequate sensing capabilities to support essential protection layers, notably Basic Process Control Systems (BPCS) and Safety Instrumented Systems (SIS). To address this issue, this work introduces a standards-based, ontology-driven framework that enables scalable verification of safety-critical sensor configurations by integrating formalized process semantics with steady-state process models. Departing from traditional node-by-node worksheet approaches, this framework utilizes semantic causal reasoning to trace catastrophic hazards, such as explosions and runaway reactions, back to the critical process variables that require monitoring. Through rule-based logic, the ontology methodically analyzes the process topology to determine if the existing sensor configuration ensures sufficient observability of these key parameters to activate the necessary BPCS and SIS interventions. The practical applicability of this methodology is demonstrated through a case study involving a vinyl acetate monomer (VAM) process, in which it effectively identifies critical sensor omissions. Ultimately, this approach provides a rigorous Safety-by-Design verification tool that significantly strengthens design-time assurance of critical protection layers in complex chemical plants.

KEYWORDS

Process Safety, Ontology, Semantic Reasoning, Sensor Validation, and Safety-by-Design

ACKNOWLEDGEMENTS

The work was supported in part by the National Science and Technology Council of Taiwan under Grants NSTC 114-2221-E-A49-094.

OR-D1-05

REGULAR ORAL

16:20~16:40 · Session D1 · D404

Air-to-fuel: direct air capture by aqueous amine solvent and electrochemical CO_2 reduction

Wonsuk Chung[1], Hyunyoung Kim[1], Junwoo Park[1], Wonyoung Choi[2], Dae Hyun Lim[1], Da Hye Won[1,3,4], Hyunjoo Lee[1,3,5], and Ung Lee[1,3,6,*]

[1]Clean Energy Research Center, Korea Institute of Science and Technology (KIST), Korea
[2]Department of Chemical Engineering, Hannam University, Korea
[3]Division of Energy & Environmental Technology, KIST School, Korea University of Science and Technology (UST), Korea
[4]KHU-KIST Department of Converging Science and Technology, Kyung Hee University, Korea
[5]KU-KIST Graduate School of Converging Science and Technology, Korea University, Korea
[6]Graduate School of Energy and Environment, Korea University, Korea

ABSTRACT

The 1.5°C climate tipping point is projected to be exceeded within the decade. A cost-effective direct air capture and utilization (DACU) process could stimulate atmospheric CO2 removal at a gigaton scale, thereby mitigating the rate of global climate change beyond the tipping point. Herein, we report a high-performance reactive carbon capture (RCC) strategy integrating air solvent scrubbing with electrochemical CO2 reduction of the dissolved CO2 to CO. This streamlined chemistry avoids the redundant energy and costs associated with conventional carbon regeneration and reduction approaches. In our pilot test, an aqueous amine solution demonstrated an excellent direct air capture (DAC) rate (>90%) and 33% CO Faradaic efficiency using the DAC outlet catholyte. This resulted in a sufficient H2:CO ratio (2:1) for fuel production (e.g., methanol). Furthermore, we performed comprehensive modeling of the direct air contactor and evaluated the DACU process under various conditions, identifying its energy consumption, carbon reduction potential, and CO2 avoidance cost. Sensitivity analysis was conducted to investigate technology-relevant parameters and the impact of climatic and regional factors on DACU performance. The results highlight the competitiveness of our RCC process compared to conventional DACU pathways.

KEYWORDS

direct air capture, amine based carbon capture, electrochemical reactive carbon capture, pilot-test, process evaluation (Font: Times New Roman, 12pt, Italic)

OR-D1-06

REGULAR ORAL

16:40~17:00 · Session D1 · D404

A new approach to design heat-integrated reactive distillation process

Irvy Ai Xia Teh[1], Yu-Sheng Chen[2], **Zong Yang Kong**[3,*], Yu-Ying Chen[2], Hao-Yeh Lee[2,*], and Jaka Sunarso[1]

[1] Faculty of Engineering, Swinburne University of Technology, Malaysia
[2] Department of Chemical Engineering, National Taiwan University of Science and Technology, Taiwan
[3] School of Engineering, Sunway University, Malaysia

ABSTRACT

Reactive distillation (RD) has attracted considerable attention as a process intensification strategy because it combines chemical reaction and separation in a single unit, offering the potential for improved energy efficiency. Despite these advantages, RD systems are still energy intensive in industrial practice. To further reduce energy consumption, heat integration is often introduced to enhance overall energy performance. In most existing studies, however, the typical workflow is to first optimize the overall process by minimizing energy consumption or total annual cost and only then implement heat integration. Because HI requires detailed stream information and adds design complexity, it is usually treated as a post-optimization step. Here we show that this conventional approach does not necessarily lead to the best energy recovery after heat integration. Instead, we propose an alternative strategy in which the reactive distillation column is optimized first, prior to applying heat integration. Our results demonstrate that this new approach consistently delivers greater energy savings compared to the conventional design sequence. Overall, the findings challenge common design practices and provide a practical alternative for achieving improved energy efficiency in heat-integrated reactive distillation systems.

KEYWORDS

Energy conservation; Process Intensification; Process Integration; Process simulation; Separations

ACKNOWLEDGEMENTS

Z. Kong gratefully acknowledge the support from Sunway University, Malaysia for the conference support funding.

OS-D2-01

STUDENT ORAL
14:30~14:45 · Session D2 · D403

Towards a Near-Zero Carbon Goal: Intensification of Energy- Intensive Distillation Processes Driven by Solar Power

Yan Cheng, Xiao Wang, and Lanyi Sun*

State Key Laboratory of Heavy Oil Processing, College of Chemistry and Chemical Engineering, China University of Petroleum (East China), China

ABSTRACT

Methyl tert-butyl ether (MTBE) is an important chemical feedstock and fuel additive with significant applications in the chemical and petrochemical industries. However, the MTBE production process often forms an MTBE/ methanol (MeOH) azeotrope, making separation challenging. In previous work, we proposed an effective extractive distillation separation process. This work aims to develop an alternative, highly efficient pressure-swing distillation (PSD) process. First, based on thermodynamic analysis, two conventional PSD processes were proposed and optimized to minimize the total annual cost (TAC) and CO2 emissions while maximizing thermodynamic efficiency. Subsequently, eight intensified separation processes incorporating heat integration, vapor recompression heat pump, and solar energy were designed. Finally, the comprehensive performance of all schemes was evaluated from economic, environmental, energy, and exergy (4E) perspectives. Results indicate that PSD2 outperforms PSD1, with the dual heat pump-solar energy intensified sequence (PSD2- HP-SE) being the optimal scheme, achieving reductions in TAC, CO2 emissions, total energy consumption, and exergy loss by 49.34 %, 100 %, 100 %, and 72.61 %, respectively, and an increase in thermodynamic efficiency by 68.17 %.

KEYWORDS

Pressure-swing distillation; Vapor recompressed heat pump; Solar energy; Multi-objective optimization; 4E analysis

ACKNOWLEDGEMENTS

We acknowledge the National Natural Science Foundation of China (No. 22278437 and No. 22578499).

OS-D2-02

STUDENT ORAL
14:45~15:00 · Session D2 · D403

Early-stage Techno-economic and Environmental Assessment Procedure for Emerging Chemical Technologies

Yeonguk Kim, Dami Kim, and Kosan Roh*

Department of Chemical Engineering and Applied Chemistry, Chungnam National University, Korea

ABSTRACT

Emerging chemical technologies require reliable early-stage economic and environmental assessments to support their research prioritization and investment decisions. However, such evaluations remain uncertain and challenging at low technology readiness levels (TRLs) because technical knowledge is limited and large-scale process data are scarce. In this study, we propose a more refined TRL-based early-stage evaluation procedure using a back-casting approach and illustrate its use with a case study of methanol production via natural gas reforming. The process was evaluated at three maturity levels, including Theoretical level, Intermediate level, and Engineering level, to examine how techno-economic and environmental indicators shift as process knowledge increases. The Theoretical level (TRL 1-2) is based on stoichiometric and thermodynamic bounds, the Intermediate level (TRL 3-5) uses experiment-informed short-cut process designs, and the Engineering level (TRL > 5) represents a detailed benchmark based on rigorous process design. The results show a clear stage-dependent bias. Theoretical-level assessments systematically underestimate production cost and climate change impact, whereas Intermediate-level assessments tend to overestimate them because the process remains insufficiently optimized. Process-concept uncertainty was considered at the Theoretical level, while operating-condition uncertainty was analyzed at the Intermediate level. These analyses improve the interpretation of early-stage results by accounting for stage-specific sources of uncertainty. By quantifying these systematic shifts, the proposed framework clarifies when and why early-stage assessments deviate from mature process performance. This approach improves the interpretability of early-stage assessments and supports more reliable decision-making for emerging chemical technologies.

KEYWORDS

early-stage assessment, Backcasting, TEA, LCA, Methanol synthesis

ACKNOWLEDGEMENTS

This work is supported by the Development of next-generation biorefinery platform technologies for leading bio-based chemicals industry project (2022M3J5A1056072) and by Development of platform technologies of microbial cell factories for the next-generation biorefineries project (2022M3J5A1056117) from National Research Foundation supported by the Korean Ministry of Science and ICT

OS-D2-03

STUDENT ORAL

15:00~15:15 · Session D2 · D403

Multi-objective optimization of water networks coupled with electrolytic hydrogen production in coal-based chemical industrial parks

Yirui Ge[1], Jing Wang[1,2], Lixia Kang[1,2] and Yongzhong Liu[1,2,*]

[1]*Department of Chemical Engineering, Xi'an Jiaotong University, China*
[2]*University of Shaanxi Province, China*

ABSTRACT

Utilizing wastewater electrolysis for hydrogen production in coal-based chemical industrial parks (CCIPs) not only reduces freshwater consumption but also becomes an important pathway for CO2 emissions reduction in coal chemical systems. However, the high water quality requirement of water electrolysis for hydrogen production poses new challenges to traditional water reuse network optimization, which primarily focuses on meeting the demands of process units. To address this issue, an optimization design method for wastewater regeneration and reuse networks oriented toward wastewater-to-hydrogen is proposed, targeting water networks coupled with centralized alkaline electrolytic hydrogen production in CCIPs. A superstructure model of the water network, encompassing freshwater deep treatment, multi-stage wastewater regeneration treatment, and water usage of electrolytic hydrogen production, is constructed to describe the distribution relationships of different water sources among various treatment units and reuse pathways in the CCIP. A multi-objective water network optimization model is established, aiming to minimize both the total annualized cost and freshwater consumption. Constraints are imposed to restrict the applicable water quality ranges for different regeneration treatment technologies, providing a foundation for the rational matching of water streams with treatment units. In the case study, the results indicate that, under the premise of meeting the water quality requirements for electrolytic hydrogen production, the proposed method can significantly reduce freshwater intake in the CCIP. The coordination characteristics between the wastewater regeneration and reuse and the water demands of electrolytic hydrogen production are further investigated. These findings not only provide an analytical tool for wastewater-to-hydrogen and water network optimization in CCIPs but also offer a decision-making basis for transitioning water reuse systems from mere waste resource recovery towards value creation for water resources in CCIPs .

KEYWORDS

Coal-based chemical industrial park; Wastewater reuse network; Electrolytic hydrogen production; Superstructure; Multi-objective optimization

ACKNOWLEDGEMENTS

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OS-D2-04

STUDENT ORAL

15:15~15:30 · Session D2 · D403

Surrogate-Model-Based Optimization of Syngas Distribution–Separation Systems

Yujie Cao, Qiao Zhang*

School of Chemical Engineering & Technology, Xi'an Jiaotong University, China

ABSTRACT

To address the issues of inefficient gas allocation and low resource utilization in syngas utilization, this study proposes a surrogate model-based optimization method for syngas distribution and separation systems. A mixed-integer linear programming (MILP) gas allocation model is developed to optimize the selection of multi-component pathways, gas flow rates, and component distributions under product yield constraints. Simultaneously, surrogate models for PSA hydrogen purification, MEA CO2 capture, and cryogenic H2/CO separation are established to rapidly predict separation performance and infer optimal operating parameters. The results show that the R2 of all surrogate models exceeds 0.95, confirming their high predictive reliability. Under product yield constraints, the optimized system achieves a synergistic minimization of feedstock consumption and carbon emissions, increasing hydrogen recovery to 99.9%, which is significantly higher than the approximately 80% reported for conventional syngas utilization systems. Moreover, the surrogate models provide optimal operating parameters that satisfy all constraints, enabling direct guidance for practical separation operations. This study offers a new approach for the efficient utilization of syngas and demonstrates potential practical applicability.

KEYWORDS

syngas; Surrogate model; gas distribution Network Optimization; mixed-integer linear programming (MILP); Energy Saving and Emission Reduction

ACKNOWLEDGEMENTS

The financial support from the National Natural Science Foundation of China under grant 21736008 is gratefully acknowledged.

OS-D2-05

STUDENT ORAL

15:30~15:45 · Session D2 · D403

Techno-Economic Assessment of Perhydro Benzyltoluene as Hydrogen Carrier for an Intercontinental Green Energy Supply Chain

Zhi-Qi Lin[1], Chong-Wei Ong[1], Chun-Cheng Li[1], Wei-Jyun Wang[2], and Cheng-Liang Chen[1,*]

[1]*Department of Chemical Engineering, National Taiwan University, Taiwan*
[2]*Department of Chemical and Materials Engineering, National Central University, Taiwan*

ABSTRACT

Long-distance hydrogen energy transport remains constrained by low volumetric density and high energy penalties with compression and liquefaction. Meanwhile, existing liquid organic hydrogen carrier (LOHC) studies often overlook rigorous heat integration. Herein, a techno-economic assessment of a benzyltoluene (BT)/perhydro benzyltoluene (H12-BT) system is developed for an integrated power-to-x-to-power international energy supply chain. Aspen Plus® models incorporating validated reaction kinetics, separation design and catalyst deactivation are coupled with solid oxide electrolysis/fuel cells (SOEC/SOFC) and green-methanol-fueled shipping. The hydrogenation reactor achieves >99% conversion while dehydrogenation maintains >94% single-pass conversion over one catalyst half-life using temperature-ramping control. Normalized to one tonne of hydrogen, the system delivers 18.78 MWh of electricity, with a round-trip efficiency (RTE) of 42.01%. Using Australia-to-Taiwan route as a case study transporting 85,440 t-H2/y, the analysis yields a levelized cost of hydrogen (LCOH) of 5.19 USD/kg. Sensitivity analysis reveals SOEC efficiency as the primary cost driver, followed by the exporter's electricity price. The results identify that coupling exothermic hydrogenation with SOEC and SOFC with endothermic dehydrogenation reduces external energy demand. This work demonstrates that BT-based LOHC, when designed with rigorous process and thermal integration, constitutes a technically viable and scalable pathway for low-carbon international hydrogen and electricity transport.

KEYWORDS

Power-to-x-to-power (PtXtP) system, techno-economic assessment (TEA), benzyltoluene (BT)/perhydro benzyltoluene (H12-BT), hydrogenation, dehydrogenation.

OS-D2-06

STUDENT ORAL

15:45~16:00 · Session D2 · D403

Research on the Modeling of Multistream Heat Exchangers Based on Equation-Oriented Flash

Zhiyuan Wang, Xijun Wang, Jun Zhao, Lili Wang, Shaohui Tao*, Xiaoyan Sun*

Qingdao University of Science and Technology, China

ABSTRACT

Equation-oriented (EO) modeling of multistream heat exchangers (MHEXs) under cryogenic phase-change conditions often encounters solution bottlenecks due to the discrete logic of phase switching. This paper proposes a general parameterized MHEX model incorporating a smoothing complementarity-based EO flash algorithm, which enables the construction of a globally continuously differentiable system of equations without pre-defined phase sequences. Furthermore, algebraic constraints to prevent temperature crosses, grounded in rigorous enthalpy calculations, are directly embedded into the residual vector to fundamentally eliminate non-physical intermediate solutions. Validations using air separation, LNG production, and ethylene cold box cases demonstrate that the fully coupled simultaneous solution strategy significantly enhances computational efficiency by eliminating the outer-loop tearing iterations typical of traditional sequential modular (SM) methods. This study provides a flexible and robust computational unit for the global simultaneous optimization of complex chemical processes and heat exchanger networks.

KEYWORDS

Multistream heat exchangers; Equation-oriented modeling; EO flash; Complementarity constraints; Phase equilibrium; Process simulation

ACKNOWLEDGEMENTS

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OS-D2-07

STUDENT ORAL

16:00~16:15 · Session D2 · D403

A Gate-Based Ensemble of Time Series Foundation Models for Few-Shot Fault Prognosis in Chemical Processes

Zhiyuan Xie[1,2], Jinsong Zhao[1,2]

[1] *Department of Chemical Engineering, Tsinghua University, China*
[2] *State Key Laboratory of Chemical Engineering and Low-carbon Technology, China*

ABSTRACT

Fault prognosis is essential for maintaining operational safety and reliability in chemical processes. However, most existing data-driven prognosis approaches require substantial labeled fault data, while few-shot fault prognosis remains largely underexplored. The capability to achieve accurate prognosis under limited fault samples is crucial for industrial applications, as it enables rapid model deployment and adaptation to newly emerging faults. To address this challenge, this study proposes a Time Series Foundation Model (TSFM) framework for few-shot fault prognosis in chemical processes. By leveraging transferable representations learned from large-scale time-series data, the proposed model enhances feature generalization and temporal pattern extraction under data-scarce conditions. The effectiveness of the framework is validated on the Tennessee Eastman Process (TEP) benchmark. Experimental results demonstrate that the proposed approach achieves reliable fault prognosis with only a small number of labeled samples, highlighting its potential for practical implementation in process industries.

KEYWORDS

Fault Prognosis, Prediction, Time series forecasting, Time series foundation model, Process Safety

ACKNOWLEDGEMENTS

This work was supported by the National Key Research and Development Program of China (2024YFC3013601).

OS-D2-08

STUDENT ORAL

16:15~16:30 · Session D2 · D403

DFT Study of Support Crystal Face Effects on Ziegler-Natta Catalyzed Olefin Polymerization

KaiQing Sui, XueQin Wei, ZiQi Gao, AiHua He and Xia Yang*

College of Chemical Engineering, Qingdao University of Science and Technology, China

ABSTRACT

TiCl4/MgCl2-supported Ziegler–Natta catalysts are the most widely used system in modern polyolefin industry. Their activity, selectivity, and polymer structure strongly depend on the surface structure of MgCl2 support. Although experiments have confirmed that different MgCl2 surfaces significantly affect olefin polymerization, the microscopic mechanism of surface-regulated coordination, insertion, and chain growth remains unclear, especially the kinetic and thermodynamic analysis based on quantum chemistry calculations. In this work, density functional theory (DFT) was employed to establish Ti active site models on MgCl2 (110) and (104) surfaces. Using ethylene, propylene, and isoprene as model monomers, we systematically studied the coordination–insertion pathways, calculated key energetic and structural parameters, and compared the effects of different surfaces on catalytic activity and stereoselectivity.

KEYWORDS

Ziegler-Natta catalyst, MgCl2 crystal surface, Olefin polymerization, Density functional theory

ACKNOWLEDGEMENTS

This work was financially supported by the National Key Research and Development Program of China (2022YFB3704700 (2022YFB3704702)), the Major Scientific and Technological Innovation Project of Shandong Province (2021CXGC010901) and the Taishan Scholar Program. And we are grateful to National Supercomputing Center in ShenZhen for the support of high performance computing resources.

OS-D2-09

STUDENT ORAL

16:30~16:45 · Session D2 · D403

Data-driven mechanism derivation in reaction systems : A hybrid approach integrating mathematical models and machine learning

Sunghun Song, Juhyeon Park, Sungwon Hwang*

Program in Energy Process Innovation Convergence, Inha University, Korea

ABSTRACT

This study presents a hybrid framework that combines a black-box surrogate model with an equation-based mechanism verification model to identify the reactants responsible for side reactions in hydrogenation systems and to derive their mechanisms. Because hydrogenation involves complex reaction networks, exhaustive analysis and prediction of all side reactions are impractical, and such uncertainty can reduce product quality and cause economic loss. To address this, a reliable dataset was built from real operating data through preprocessing to remove missing values and outliers, and an Artificial Neural Network (ANN) with a Multi-Layer Perceptron (MLP) architecture was developed. By applying data transformation based on reaction rate expressions to reflect domain knowledge, model generalization improved, achieving an R2 of 0.97 and an RMSE of 0.04. In addition, SHAP and Partial Dependence Plot (PDP) analyses were used to quantify and visualize the influence of each reactant on ANN predictions, enabling prioritization of species for candidate mechanism construction. Candidate mechanisms were then evaluated using Langmuir–Hinshelwood and Power Law rate expressions with a Monte Carlo-based mathematical model. Validation showed excellent performance for all products (R2 > 0.98, MAPE < 2.31%), confirming convergence to the global optimum through kinetic parameter sensitivity analysis.

KEYWORDS

Hybrid Reactor Modeling, Hydrogenation reaction, Reaction network, Artificial neural network, Explainable AI, Monte Carlo

OS-D2-10

STUDENT ORAL

16:45~17:00 · Session D2 · D403

Power generation based on combustion and carbon capture strategies for unconverted off-gas from natural gas-based SOFC

Taehyun Kim, Jinwoo Park*

Department of Chemical and Biochemical Engineering, Dongguk University, Korea

ABSTRACT

In this study, the design and comparison of power generation processes for combusting unconverted off-gas from a solid oxide fuel cell (SOFC) are presented. Air combustion and oxy-fuel combustion were compared, and a CO2 based thermodynamic cycle was introduced for additional waste heat recovery. For air combustion, two pressure conditions (1 and 15 atm) were considered, followed by carbon capture using either cryogenic capture or chemical absorption. For oxy-fuel combustion, three cases were investigated: 1 atm, 297 atm, and chemical looping combustion (CLC) using metal oxides. Because oxy-fuel combustion does not require a additional carbon capture unit, CO2 was assumed to be compressed directly to storage pressure. Based on the lower heating value, the energy efficiencies were 60.35% and 60.61% for air combustion at 1 and 15 atm, respectively. With carbon capture, the efficiencies decreased to 53.86–56.51%. Oxyfuel-combustion resulted in efficiencies of 53.01–56.29%.

KEYWORDS

Solid oxide fuel cell, Oxy-fuel combustion, Air combustion, Carbon capture, Waste heat recovery

ACKNOWLEDGEMENTS

This work was supported by National Research Foundation of Korea (NRF) grants funded by the Korean Government (MSIT) (No. RS-2025-25397244)

OS-D3-01

STUDENT ORAL

14:30~14:45 · Session D3 · D402

Comparison of control performances of reactive-extractive distillation processes with different reactants

I Gede Pandega Wiratama[1,2], Xuan Liang Choo[3], Zong Yang Kong[1,3,*], Ao Yang[4], Agus Saptoro[5], Jaka Sunarso[1]

[1] *Faculty of Engineering, Swinburne University of Technology, Malaysia*
[2] *Faculty of Engineering Technology, Parahyangan Catholic University, Indonesia*
[3] *School of Engineering, Sunway University, Malaysia*
[4] *College of Safety Science and Engineering, Chongqing University of Science & Technology, China*
[5] *Curtin University, Australia*

ABSTRACT

Reactive-extractive distillation (RED) is a promising process for separating water-containing ternary azeotropic mixtures. Most existing studies employ ethylene oxide (EO) as the reactant in RED (EO-based RED), while only a limited number of recent studies have investigated the use of glycidol (GD) as the reactant (GD-based RED). Previous studies on GD-based RED have focused on steady-state performance in terms of economic, energy, and environmental aspects. However, to the best of the authors' knowledge, no study has yet investigated the dynamic behavior and control of GD-based RED, nor compared it with EO-based RED. This research addresses this gap by conducting dynamic and control simulations of both GD-based and EO-based RED for the separation of tetrahydrofuran (THF)/methanol (MeOH)/water mixtures. The proposed control structure employs temperature-based inferential control, in which the stage temperatures are selected based on sensitivity analyses of reboiler duty and reflux ratio with respect to the column temperature profile. The purpose is to compare the controllability between GD-based RED and EO-based RED under the same control structure.

KEYWORDS

Azeotropic separation; Inferential control; Process intensification; Hydration reaction;

ACKNOWLEDGEMENTS

I Gede Pandega Wiratama would like to acknowledge the support from Swinburne University of Technology Sarawak Campus in the form of Full Fee-Waiver Studentship for his Doctor of Philosophy.

OS-D3-02

STUDENT ORAL

15:45~16:00 · Session D3 · D402

Insights into Deep Learning Framework for Molecular Property Prediction Based on Different Tokenization Algorithms

Xiao Wang, Yan Cheng, and Lanyi Sun*

State Key Laboratory of Heavy Oil Processing, College of Chemistry and Chemical Engineering, China University of Petroleum (East China), China

ABSTRACT

With the rapid development of deep learning, research on quantitative structure– property relationships based on deep learning has received widespread attention. The deep learning architecture combining Bidirectional Encoder Representation from Transformers (BERT) and Feedforward Neural Networks (FNN) is proposed to compare the performance of different tokenization algorithms. And t-distributed stochastic neighbor embedding reveals valuable information about the mechanism of structure– property relationships. Additionally, a deep learning framework, BERT-Convolutional Neural Network (CNN)-FNN, is developed based on the optimal tokenization algorithm to accurately predict the σ-profile and VCOSMO. The molecular structures are vectorized with the BERT model capturing local and global features of the entire molecule. And the CNN model enhances the latent representation associated with molecular properties, while the FNN model establishes the correlation. The deep learning frameworks predict σ-profile and VCOSMO properties with R2 greater than 0.9703, making it a promising intelligent tool for guiding solvent design and screening.

KEYWORDS

Deep learning; Molecular latent representation; Tokenization algorithm; QSPR; COSMO-SAC

ACKNOWLEDGEMENTS

We acknowledge the National Natural Science Foundation of China (No. 22278437 and No. 22578499).

OS-D3-03

STUDENT ORAL

16:00~16:15 · Session D3 · D402

Synergistic mechanism and topological enhancement of mixed entrainer quaternary azeotrope separation: from thermodynamic insights to sequential extraction decoupling

Xiaobin Du, Zhaoyou Zhu, Xin Li, Peizhe Cui, Yinglong Wang*

Qingdao University of Science and Technology, China

ABSTRACT

Separating the highly non-ideal quaternary azeotropic mixture of ethyl acetate, ethanol, acetonitrile, and water presents significant thermodynamic challenges. First, an entrainer screening framework based on system characteristics is established, evolving from single-solvent benchmarking to a synergistic mixed entrainer (ethylene glycol/1,3-propanediol) guided by COSMO-RS molecular insights. Crucially, based on this optimal entrainer, a systematic synthesis of separation sequences is conducted. Driven by NSGA-II multi-objective optimization, various sequence topologies are thoroughly evaluated. A novel "light-first decoupling" topology is identified as the techno-economic optimum, effectively mitigating the cumulative thermal penalty of high-latent-heat components through strategic sequential extraction. Finally, process intensification strategies combining internal heat integration and mechanical vapor recompression are implemented. Comprehensive performance evaluation confirms that this hybrid design drastically minimizes utility consumption, providing a highly sustainable paradigm for complex separations.

KEYWORDS

Thermomechanical analysis; Extractive distillation; Mixed entrainer; Multi-objective optimization; Internal heat integration.

OS-D3-04

STUDENT ORAL

15:15~15:30 · Session D3 · D402

Three-stage DMPNN-based prediction model for photodynamic therapy properties of metal complex photosensitizers

Jingxing Gao, Yachao Dong*, Ran Wang, Wen Sun, Jian Du

School of Chemical Engineering, Dalian University of Technology, China

ABSTRACT

Photodynamic therapy is a noninvasive clinical treatment for cancers using photosensitizers and light. While most research has focused on organic molecules such as porphyrins as photosensitizers, there is emerging interest in the utilization of transition metal complexes, which can display intense absorptions in the visible region, and many also possess high two-photon absorption cross-sections, enabling two-photon excitation with NIR light [1]. Machine learning and deep learning method has gained popularity and proved to be a powerful tool in various areas of sciences and technologies, which uses algorithms to learn from data, detect patterns, and make fast and accurate prediction [2]. In our previous work, hybrid machine learning models with density functional theory (DFT)-based descriptors and other descriptors are constructed to predict the singlet oxygen quantum yield of transition metal complex (TMC) photosensitizers [3]. However, the high computational cost of DFT restricts its application in high-throughput screening processes. Therefore, it is critical to develop a fast and accurate end-to-end prediction model for the absorption wavelength and singlet oxygen quantum yield of TMC photosensitizers as a pre-screening tool. In this presentation, a three-stage-model consisting of pre-training, fine-tuning and downstream prediction is proposed for the quantitative structure-property relationship (QSPR) of photosensitizers. During the first stage, the encoder based on the directed message passing neural network (DMPNN) was pre-trained on over 12,000 TMCs to learn their structural features, converting molecular graph data into a 128-dimensional graph embedding. In the second stage, the absorption wavelengths of the top 10 excited states of over 4,000 TMCs calculated by DFT were used to fine-tune the pre-trained encoder. The aim of this stage was to make the encoder more capable of learning the relationship between the complex structure and the excited state properties by using optical properties that are less sensitive to the structure. In the third stage, the focus will be on combining the pre-trained graph embeddings of structural information with the fine-tuned graph embeddings that emphasize excited-state information. These, along with external conditions such as excitation wavelength and solvent environment, will be used as input for the downstream prediction model to predict the highly nonlinear excited-state oscillator strength and singlet oxygen quantum yield that are sensitive to minor structural changes. The former determines whether the absorption wavelength of this excited state matches the absorption peak in the experimental spectrum, while the latter is the key property that determines the efficacy of type II photodynamic therapy. The results of the fine-tuning stage indicate that the pre-training - fine-tuning model based on DMPNN has a good predictive effect on the absorption wavelength of TMC. The R2 value of the training set, validation set and test set for the first 10 excited states is 0.970±0.005, 0.873±0.027, and 0.877±0.018. The results of the downstream prediction indicate that the three-stage model also has a relatively high accuracy in predicting complex properties. The R2 value of the training set, validation set and test set for the singlet oxygen quantum yield are 0.955, 0.928 and 0.815 while the accuracy that the strongest oscillation strength excited state prediction error within 2 excited states of the training set, validation set and test set are 80%, 60% and 60%. Finally, we confirmed that this three-stage model can accurately predict the strongest oscillator strength excitation state absorption wavelength of TMC and the quantum yield of singlet oxygen at that wavelength. This enables high-throughput screening of the TMC virtual space, facilitating the experimental development of new TMC photosensitizers. In future research, the work will develop molecular generation models based on reinforcement learning and diffusion models to construct the TMC virtual space. These models will be combined with the prediction model proposed in this paper for the discovery and experimental verification of new TMC photosensitizers. [1] MCKENZIE L, BRYANT H, WEINSTEIN J. Transition metal complexes as photosensitizers in one- and two-photon photodynamic therapy [J/OL]. Coordination

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KEYWORDS

photodynamic therapy; transition metal complex photosensitizers; quantitative structure-property relationship; deep learning

OS-D3-05

STUDENT ORAL

15:30~15:45 · Session D3 · D402

Multi-Objective Optimization of Reactive Distillation Column for Silane Production: Impact of Alternative Controllability Criteria and Bidirectional Perturbations

Josué J. Herrera Velázquez[1,3], J. Rafael Alcántara Avila[2], Salvador Hernández[1], and Julián Cabrera Ruiz[1,*]

[1] *Universidad de Guanajuato, Mexico*
[2] *Pontificia Universidad Católica del Perú, Peru*
[3] *Instituto Tecnológico Superior de Guanajuato, Mexico*

ABSTRACT

Photovoltaic solar energy based on polycrystalline silicon (from silane, SiH4) is a viable alternative to fossil fuels; however, reducing production costs remains a key challenge for large-scale deployment. This study proposes an Aspen Plus®–Python interface for the multi-objective optimization of a reactive distillation column for silane production, incorporating multiple reactive zones and using the NSGA-II algorithm. Total Annual Cost (TAC), reboiler duty (QH), and the open-loop controllability criterion (Aγ+γsm) were optimized simultaneously, considering several variations of the latter. These variations include positive and negative perturbations, as well as the use of the minimum singular value, since the current formulation considers only the condition number. Dynamic boundaries enabled the evaluation of configurations with one to three reactive zones. Results show that formulation based on positive disturbances perform best with approximate functions, however, the proposed variants adequately reproduce the expected behavior when compared with rigorous controllability analyses. Designs with two reactive zones minimize QH and Aγ+γsm, whereas three-zone configurations minimize TAC, yielding the optimal multi-objective solution. Compared with literature designs, the proposed approach improves TAC by 2.94%, QH by 27.30%, and Aγ+γsm by 21.62%. First-order approximations show strong agreement with rigorous transfer function behavior.

KEYWORDS

Silane, Reactive Distillation, Multi-Objective Optimization, Open-Loop Controllability, Aspen Plus – Python

OS-D3-06

STUDENT ORAL

15:45~16:00 · Session D3 · D402

Multiphase computational fluid dynamics of methane pyrolysis in a molten-metal bubble column reactor with carbon coverage

Jun-Ho Yang, Son Ich Ngo, Young-Il Lim*

Department of Chemical Engineering, Hankyong National University, Korea

ABSTRACT

The molten-metal bubble column reactor (MMBCR) for methane pyrolysis has attracted considerable attention as a promising route for CO2-free hydrogen production. However, when the reaction occurs at the gas bubble–liquid metal interface, it remains unclear to what extent the solid carbon formed accumulates on the bubble surface and results in carbon coverage that reduces the catalytic interfacial reaction due to steric hindrance. In this study, a computational fluid dynamic (CFD) was performed to investigate the effect of bubble surface carbon deposition on reaction rates in a Ni27Bi73 molten-metal bubble column reactor. A level-set volume-of-fluid (LS-VOF) CFD model was employed to capture the bubble interface and to visualized carbon accumulation at the bubble interface. This study provides fundamental insight into the mechanism of performance degradation caused by carbon accumulation in MMBCRs

KEYWORDS

Computational fluid dynamics, methane pyrolysis, Hydrogen production, Molten-metal bubble column reactor, Carbon coverage

ACKNOWLEDGEMENTS

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OS-D3-07

STUDENT ORAL

16:00~16:15 · Session D3 · D402

Dynamic operational planning of modular methanol synthesis via forecast-driven rolling-horizon optimization

Youngkeun Kim[1], Sungmin Lee[1], Jeongdong Kim[2,*], and Junghwan Kim[1,*]

[1]*Department of Chemical and Biomoleular Engineering, Yonsei University, Korea*
[2]*Department of Chemical Engineering, Massachusetts Institute of Technology, USA*

ABSTRACT

As global decarbonization accelerates, managing renewable intermittency and the operational rigidity of large-scale chemical plants remains a critical challenge for sustainable fuel production. To overcome these inherent limitations, this study proposes a dynamic optimization framework for a modular Power-to-Methanol (PtM) system. Integrating multi-step time-series forecasting with a rolling-horizon mixed-integer linear programming (MILP) strategy, the framework couples system-level planning with process-level transient dynamics, strictly enforcing realistic 3-hour startup and shutdown constraints to ensure practical feasibility. Evaluations of the proposed forecasting-based framework demonstrate remarkable operational fidelity. Compared to the global optimum, the proposed framework showed only a 12.33% profit gap and a 4.83% deviation in grid interaction, providing its superior adaptability over conventional stochastic MILP. Furthermore, comparative analysis reveals that the modular architecture economically outperforms an equivalent large-scale configuration in 85.1% of stochastic scenarios, securing robust profitability while sustaining PtM conversion objectives. These findings provide actionable guidance for modular PtM systems and highlight their potential as a flexible and economically resilient pathway for renewable methanol production under real-world uncertainty.

KEYWORDS

Modular power-to-methanol, Mixed-integer linear programming, Rolling-horizon optimization, Renewable intermittency, Operational flexibility

ACKNOWLEDGEMENTS

This work was supported by the Korea Institute for Advancement of Technology (KIAT) grant funded by the Korea Government (MOTIE) (RS-2024-00416131, HRS Program for Industrial Innovation).

OS-D3-08

STUDENT ORAL

16:15~16:30 · Session D3 · D402

Simplified PID Control for H_2/CO Optimization in Wood Biomass Gasification

Yu Hui Kok, Yuka Sakai and Yasuki Kansha*

The University of Tokyo, Japan

ABSTRACT

Gasification is a critical thermochemical process for converting biomass, such as Japanese Cypress, into versatile syngas. However, a significant gap exists between rigorous high-order kinetic models and the standard Proportional-Integral-Derivative (PID) control infrastructure used in industrial facilities. This research bridges that gap by numerically linearizing non-linear kinetic rate laws into a low-order architecture compatible with industrial loops. Focusing specifically on the pyrolysis stage of gasification, this study utilizes Thermogravimetric and Differential Analysis (TG-DTA) to establish intrinsic reaction rate laws for Japanese Cypress. These equations were linearized around optimal operating points to develop a representative First Order Plus Dead Time (FOPDT) plant transfer function in the Laplace domain, accounting for thermal lag and mass-transfer limitations. A PID control scheme, tuned via Internal Model Control (IMC) principles, was designed to modulate the pyrolysis temperature and maintain a target H2/CO ratio. Results demonstrate that precise regulation of the thermal gradient effectively stabilizes syngas composition despite the non-linearities of volatile cracking. By treating the pyrolysis stage as a precision control element, it ensures the precursor gas quality is optimized before any subsequent processing steps. This approach offers a robust solution for maintaining gas quality in decentralized biorefineries where feedstock variability necessitates high-performance automated regulation.

KEYWORDS

Biomass, Pyrolysis, Gasification, System Identification, PID

OS-D3-09

STUDENT ORAL
16:30~16:45 · Session D3 · D402

A non-cooperative game approach to coordinating multiple stakeholders' benefits and carbon emission reduction strategies in coal-based chemical industrial parks

Kai Li[1], Jing Wang[1,2] and Yongzhong Liu[1,2,*]

[1] *Department of Chemical Engineering, Xi'an Jiarenotong University, China*
[2] *University of Shaanxi Province, China*

ABSTRACT

The integration of coal mining, coal-fired power plant, renewable energy and chemicals production into coal-based chemical industrial parks is of great significance for the low-carbon transition of coal chemical industry. The use of renewable hydrogen coupled with carbon capture, utilization and storage (CCUS) to produce green chemicals has emerged as a viable pathway to improve energy efficiency and achieve net-zero emissions. However, the existing optimization models for the integration of resource and energy often overlook the coordination of conflicting interests among multiple stakeholders in the parks. In this work, a multi-stakeholder non-cooperative game model, including coal mine, coal-fired power plant, renewable energy enterprise, CCUS operator, chemical production lines based on coal and renewable energy, was proposed by analyzing the coupling relationships between material and energy flows and the interactive characteristics of stakeholders' benefits. An iterative algorithm was employed to obtain the Nash equilibrium point and determine the optimal pricing and demand schemes. Four scenarios were established for comparative analysis based on different decision-making modes and CO2 reduction schemes. The results indicate that, compared with the integrated optimization model, the proposed non-cooperative game approach effectively balances benefits of all stakeholders while providing theoretical guidance and decision support for achieving net-zero carbon emissions in t coal-based chemical industrial parks.

KEYWORDS

Coal-based chemical industrial park, Multiple stakeholders, Non-cooperative game approach, CCUS, Pricing and demand schemes

ACKNOWLEDGEMENTS

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OS-D3-10

STUDENT ORAL

16:45~17:00 · Session D3 · D402

Process Simulation and Technical Feasibility Assessment of CO_2-Based Fischer–Tropsch E-Fuel Production

Kangyeob Kim, Jin-Kuk Kim*

Department of Chemical Engineering, Hanyang University, Korea

ABSTRACT

The aviation sector is widely recognized as one of the most challenging industries to decarbonize due to its long-haul transportation characteristics and limited electrification potential. Consequently, the deployment of Sustainable Aviation Fuel (SAF) has emerged as an essential pathway for achieving mid- to long-term greenhouse gas emission reductions. In particular, electro-based SAF (E-SAF), produced from renewable hydrogen and captured carbon dioxide, has gained increasing attention as a promising alternative that enables significant emission mitigation while maintaining compatibility with existing aviation fuel infrastructure. In this study, aprocess simulation of a CO2-based E-SAF production pathway was conducted, with a focus on Fischer–Tropsch (FT) synthesis as a representative conversion route. The overall process was modeled to evaluate key performance indicators, including energy efficiency, carbon conversion efficiency, and system-level energy consumption. Furthermore, sensitivity analyses were performed on critical variables, such as reactor operating conditions and recycle configurations to identify dominant design parameters governing process performance. The impacts of variations in key process parameters and system configurations on overall fuel productivity and system-level energy demand were systematically analyzed. Based on the simulation results, optimal operating conditions and process configurations were proposed to enhance the technical and economic feasibility of CO2-based E-SAF production systems.

KEYWORDS

SAF, CCU, Fisher-Tropsch, Techno-economic analysis, E-fuel

ACKNOWLEDGEMENTS

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OS-D4-01

STUDENT ORAL

14:30~14:45 · Session D4 · D408

Separation Network Design for Light Olefin Recovery in Plastic Pyrolysis Refineries

Wen-Yang Lee and Jeffrey. D. Ward*

National Taiwan University, Taiwan

ABSTRACT

Process Systems Engineering tools are applied to the design and optimization of light olefin recovery from plastic pyrolysis. A conceptual plastic pyrolysis refinery is developed to evaluate separation performance and economic feasibility for different plastic feed cases[1]. . The first HDPE pyrolysis, where multiple cracked-gas compositions are generated to represent different pyrolysis operating conditions. These compositions are introduced into a unified separation flowsheet to examine impact on light olefin recovery and process cost. The second mixed plastic feed containing LDPE and PET. oxygen-containing . The separation section[2] for light olefin recovery is optimized with total annual cost (TAC) as the objective function. Simulated annealing (SA) is employed to , with the number of theoretical stages and feed stage locations treated as variables. The results the trade-offs between separation performance, process complexity, and economic performance across different plastic feed cases.

KEYWORDS

Light olefin recovery;

OS-D4-02

STUDENT ORAL

14:45~15:00 · Session D4 · D408

High-Value-Added Byproduct Resource Recycling Feedback Driving Synergistic Optimization of Chemical Process Systems Toward Resource Utilization Efficiency Improvement

Wenjing Li, Qiao Zhang*

School of Chemical Engineering & Technology, Xi'an Jiaotong University, China

ABSTRACT

This study proposes a methodology for High-Value-Added Byproduct Resource Recycling Feedback Network (HBRRFN) to enhance inter-system synergy in chemical processes. The HBRRFN employs feedback units to coordinate the allocation of multiple mass and energy resources for their efficient utilization. A mixed-integer nonlinear programming (MINLP) model is developed to obtain the optimal system portfolio through feedback paths selection and system scale adjustment. An industrial case involving propane dehydrogenation, ethane cracking, coal-to-methanol, and gas-to-urea is used to demonstrate the effects of recycling feedback of hydrogen, light hydrocarbons, fuel gas, and multi-grade waste heat. The best economic and environmental portfolios are determined, and the urea system is specifically identified as a crucial system in reinforcing synergy for overall efficiency improvement. Multi-objective optimization guides the Pareto-optimal solution, achieving a 6.62% environmental gain at 0.01% economic loss, with 20.0% byproduct recovery and 25.4% waste heat utilization. Overall, the HBRRFN provides a generalizable superstructure that supports system-level restructuring and primary-resource substitution beyond conventional secondary-resource allocation.

KEYWORDS

HBRRFN; Feedback Units; Synergistic Optimization; Resource Utilization Efficiency; Crucial System

ACKNOWLEDGEMENTS

The financial support from the National Natural Science Foundation of China under grant 21736008 is gratefully acknowledged.

OS-D4-03

STUDENT ORAL

15:00~15:15 · Session D4 · D408

AI-Driven Sustainable ALD Recipe Design Via Multi-Objective Optimization and Process-Level Life Cycle Assessment

Wonho Lee, Jeehoon Han*

POSTECH, Korea

ABSTRACT

As energy and material consumption in semiconductor manufacturing continue to increase, integrating environmental considerations into process design has become essential. Atomic Layer Deposition (ALD) recipe development has traditionally been driven by target Thin-Film Transistor (TFT) performance with limited attention to environmental impacts at the process level. This research advances ALD recipe optimization by systematically incorporating Life Cycle Assessment (LCA) into the evaluation stage. A Tandem Neural Network (TNN) surrogate model is developed to capture the nonlinear relationships between ALD process variables and TFT performance metrics, enabling the efficient identification of multiple candidate recipes that satisfy predefined electrical specifications. Both multi-objective optimization and hierarchical optimization are implemented and comparatively assessed, with hierarchical optimization demonstrating greater reliability in meeting high-priority TFT performance criteria. For the performance qualified recipes, process-level LCA is subsequently conducted to quantify environmental impacts. By comparing their environmental profiles, an ALD recipe is selected that maintains the required TFT performance while exhibiting improved environmental performance. The results demonstrate that applying LCA to technically feasible semiconductor process recipes provides a systematic pathway toward environmentally preferable ALD process design without compromising device performance.

KEYWORDS

Atomic Layer Deposition (ALD), Life Cycle Assessment (LCA), Tandem Neural Network (TNN), Hierarchical optimization

ACKNOWLEDGEMENTS

This research was supported in part by the Nano & Material Technology Development Program through the National Research Foundation of Korea funded by the Ministry of Science and ICT (RS-2025-25442614) and in part by the National Research Foundation of Korea(NRF) grant funded by the Korea government(MSIT)(RS-2026-25480561)

OS-D4-04

STUDENT ORAL

15:15~15:30 · Session D4 · D408

Selection of entrainers for different separation sequences in extractive distillation of methanol/methyl propionate

Li Xinying, Jiang Yangyang, Shang Zewen, Cao Jingxi, Liu Xuhan, Li Xiaohan, Cheng Huanong*

College of Chemical Engineering, Qingdao University of Science and Technology, China

ABSTRACT

This study proposes an entrainer screening and mechanistic analysis method combining intermolecular interaction energy and process economics for the methanol-methyl propionate azeotropic system. Separation sequences were classified based on the interaction energy magnitude, and entrainers were ranked by interaction energy differences within the same sequence. Combined with total annual cost (TAC) calculation, ternary vapor-liquid equilibrium experiments, and NRTL model fitting, [MMIM][DMP] was identified as the best entrainer with a TAC of 7.376×105 $·Y-1. Quantum chemical analyses (AIM, IRI, etc.) revealed that entrainers containing N/O lone-pair electrons break the azeotrope via strong hydrogen bonds. The MP-prior separation is dominated by electrostatic and dispersion interactions, while the MeOH-prior separation relies mainly on dispersion interactions. Method comparison validated the accuracy of the interaction energy difference approach.

KEYWORDS

extractive distillation; separation sequence; quantum chemistry; mechanism analysis; TAC

ACKNOWLEDGEMENTS

The work was supported by the National Natural Science Foundation of China (Grant No. 22274085).

OS-D4-05

STUDENT ORAL

15:30~15:45 · Session D4 · D408

Thermodynamic-Guided Computer Aided Molecular Design Framework of Stable Synthetic Ester Lubricants

Xiao Syuen Lim, Lik Yin Ng, and Nishanth Chemmangattuvalappil *

School of Engineering, Sunway University, Malaysia

ABSTRACT

Current lubricant development strategies rely heavily on additive-based stabilization and empirical formulation, offering limited control over degradation pathways that are fundamentally governed by molecular structure. In this work, we systematically embed thermodynamic stability into the molecular design process by developing a thermodynamics-guided Computer-Aided Molecular Design (CAMD) framework. The framework can generate chemically stable synthetic ester base oils candidates for ISO Viscosity Grade 46. The CAMD algorithm is developed by integrating property prediction models with the thermodynamic feasibility of chemical reactions leading to ester decomposition. The stability conditions have been modeled based on the potential decomposition mechanisms. By calculating the enthalpy and entropy of potential molecular structures, the algorithm screens candidates based on thermodynamic barriers rather than post-formulation constraints. The results show that each generated compound exhibits positive Gibbs free energy for both hydrolysis and thermal decomposition, confirming non-spontaneity under operational conditions. These molecules achieve enhanced stability through strategic branching and unsaturation, thereby increasing thermodynamic barriers compared to linear structures. As base oil constitutes approximately 90% of a lubricant formulation, rationalizing the molecular selection process shifts lubricant design toward a predictive, molecular-level optimization strategy that ensures both rheological performance and thermal stability.

KEYWORDS

Synthetic Ester Lubricants; Viscosity; Gibbs Free Energy; Computer-Aided Molecular Design; Thermodynamic Stability.

OS-D4-06

STUDENT ORAL

14:45~15:00 · Session D4 · D408

Process Design and 4E Analysis of an Integrated Methane Pyrolysis-Dual Chemical Looping System for Ammonia Production

Inhye Kim[1], Minseok Im[1], Sunghyun Cho[1,2,*]

[1]*School of Chemical Engineering, Jeonbuk National University, Korea*
[2]*Clean Energy Research Center, Jeonbuk National University, Korea*

ABSTRACT

Ammonia is increasingly recognized as a carbon-neutral fuel and hydrogen carrier. Nevertheless, conventional production based on the Haber-Bosch process remains highly energy-intensive and carbon-emitting. This study proposes an alternative ammonia synthesis pathway integrating methane pyrolysis with a dual chemical looping system employing $Fe2O3$ and $Al2O3$ as oxygen carriers. The process was conceptually designed and systematically evaluated using energy, exergy, environmental, and economic (4E) analyses. Its performance was benchmarked against conventional and single-loop configurations to quantify improvements in efficiency, emissions, and cost. The integrated configuration enhances the utilization of thermal and material streams through internal heat recovery and effective management of solid carbon and looping intermediates. Compared with the conventional route, energy and exergy efficiencies increased by 8.4% and 19.0% respectively. The global warming potential decreased by 15.85 kg CO2-eq per kg NH3, and the levelized cost of ammonia decreased to 336.97 USD per ton, corresponding to a 60.9% reduction. Sensitivity analyses were conducted to assess the influence of fluctuations in key economic parameters, demonstrating the stability of the proposed system. Overall, the results indicate that the dual chemical looping-integrated pathway provides a technically viable and economically competitive option for low-emission ammonia production.

KEYWORDS

Ammonia; Chemical looping; Methane pyrolysis; Techno-economic analysis; Life cycle assessment; Exergy analysis

OS-D4-07

STUDENT ORAL

15:00~15:15 · Session D4 · D408

Clean hydrogen production via waste plastic-biomass co-gasification with carbon capture and sequestration: Techno-economic and environmental assessment under policy frameworks

Minju Jang and Joonjae Ryu*

Department of Chemical Engineering, University of Seoul, Korea

ABSTRACT

Co-gasification of biomass and waste plastics with carbon capture and sequestration (CCS) offers a promising pathway for clean hydrogen production, as it combines the negative emission potential of biomass with the enhanced hydrogen yield and waste management benefits of waste plastics. However, its techno-economic viability under emerging clean hydrogen policy frameworks remains unclear. In this study, a detailed process model was developed for the co-gasification of rice husk and waste polypropylene, incorporating upstream pretreatment, downstream syngas cleaning and upgrading, and heat integration strategies. Techno-economic analysis (TEA) and life cycle assessment (LCA) were conducted for various blending ratios, with and without CCS. The integrated TEA-LCA-policy assessment revealed that the lowest levelized cost of hydrogen (LCoH) of \$1.11/kg-H2 could be achieved at a 40% plastic mix ratio with CCS, meeting Tier-1 clean hydrogen criteria under IRA Section 45V. Biomass-rich systems benefited more under IRA 45V, while plastic-rich systems favored IRA 45Q from an economic perspective. Overall, these results highlight that co-gasification with CCS can deliver cost-competitive clean hydrogen when aligned with policy incentives, emphasizing the importance of coupling TEA, LCA, and policy analyses for a holistic evaluation of emerging hydrogen technologies.

KEYWORDS

Co-gasification, Hydrogen production, Plastic recycling, Clean hydrogen policy, Techno-economic analysis, Life cycle assessment

ACKNOWLEDGEMENTS

This work was supported by the ministry of climate, energy, and environment (MCEE) (RS-2026-25502834).

OS-D4-08

STUDENT ORAL

16:15~16:30 · Session D4 · D408

Energy-saving strategies for waste heat recovery in extractive pressure-swing distillation process of chloroform/ethanol/water ternary azeotropic mixture

Xiaoyan Zhang, Lulin Sun, Hongbo Xu, Qiyan Yang, Xin Li*, Yinglong Wang, Peizhe Cui

College of Chemical Engineering, Qingdao University of Science and Technology, China

ABSTRACT

Conventional distillation struggles to effectively separate complex mixtures, often requiring special processes that suffer from high energy consumption. Three schemes—pressure-swing distillation (PSD), extractive distillation (ED), and extractive pressure-swing distillation (EPSD)—were evaluated for separating the chloroform–ethanol–water ternary azeotropic system. Multi-objective optimization identified EPSD as the optimal base process. Traditional heat integration showed limited energy-saving potential, while vapor recompression increased electricity demand and equipment costs. Observing that the top of the high-temperature column operates at a lower temperature than the bottom of the low-temperature column, an intermediate heat exchange-assisted heat integration process (IHE-HI1-EPSD) was proposed. Further analysis of sensible heat recovery enabled additional heat exchange between the bottom streams of both columns, leading to the improved IHE-HI2-EPSD configuration. A comprehensive evaluation framework assessing economic performance, energy consumption, and environmental impact demonstrated that IHE-HI2-EPSD reduces total annual cost by 22.44% and cuts energy use and gas emissions by 48.49%. The proposed process offers significant energy-saving advantages and provides a sustainable solution for azeotropic separation.

KEYWORDS

Phase diagram analysis; Intensification strategy; Process optimization; Performance analysis; Multi-objective optimization

OS-D4-09

STUDENT ORAL

16:30~16:45 · Session D4 · D408

Theoretical Analysis of Conditions for Negative Transfer in Frustratingly Easy Domain Adaptation with Linear Regression

Yuki Kobayashi[1], Sanghong Kim[2], and Manabu Kano[1,*]

[1] *Department of Informatics, Kyoto University, Japan*

[2] *Department of Applied Physics and Chemical Engineering, Tokyo University of Agriculture and Technology, Japan*

ABSTRACT

Transfer learning (TL) intends to improve model performance in a target domain (TD) with small data by leveraging data from a similar source domain (SD). If the data of SD and TD differ significantly, TL can degrade model performance relative to a model trained without TL, which is called negative transfer (NT). However, it is unclear under what conditions NT occurs. Frustratingly easy domain adaptation (FEDA) is a TL method, and several studies have successfully applied it in the process industry. This study derived a mathematical condition for NT when FEDA and ordinary least squares (OLS) regression are used. The derivation assumes linear input-output relationships in SD and TD, with coefficient shifts in a subset of variables. We also conducted numerical simulations by varying the SD and TD sample sizes (Ns, Nt), the number of shifted coefficients (pshift), and the coefficient shift magnitude (Δβ) to examine their impacts on NT. As a result, Ns had little effect on NT, while NT became more prone to occur as Nt, pshift, and Δβ increased. This study advances the theoretical understanding of the mechanism behind NT in the combination of FEDA and OLS.

KEYWORDS

Transfer learning, Negative transfer, Frustratingly easy domain adaptation, Ordinary least squares, Mathematical analysis

ACKNOWLEDGEMENTS

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OS-D4-10

STUDENT ORAL

16:45~17:00 · Session D4 · D408

Predictive Modeling of a renewable methanol synthesis reactor under periodic operations by Kolmogorov-Arnold Networks

Minghui Yu[1], Jing Wang[1,2] and Yongzhong Liu[1,2,*]

[1]Department of Chemical Engineering, Xi’an Jiaotong University, China
[2]University of Shaanxi Province, China

ABSTRACT

Under periodic operating conditions, the internal temperature, component concentrations, and conversion rate of a renewable methanol synthesis reactor exhibit significant nonlinear dynamic behaviors over time. Mechanistic models are often computationally intensive and costly, making them unsuitable for rapid prediction and online optimization. This work employs Kolmogorov-Arnold Networks (KAN) to develop a surrogate model for predicting dynamic performances of a methanol synthesis reactor under periodic operation. The model takes operational variables, including inlet flow rates, temperature, and pressure, and periodic operation features, such as period, amplitude, and phase shift, as inputs to predict key performance indicators, including outlet methanol mole fraction, reactor temperature distribution, and conversion. Training data are obtained by simulations on the COMSOL software package, which are divided into training, validation, and test sets for the model development and evaluation. The effects of different learnable basis functions, such as B-spline, polynomial, Fourier series, etc., and their combinations, on the accuracy of periodic dynamic performances are investigated. Results show that the developed KAN surrogate model achieves fast and accurate predictions under conditions of strong nonlinearity, periodic disturbances, and multivariable coupling, while maintaining interpretability. This work provides an efficient data-driven approach for rapid prediction, real-time control, and online optimization of reactors under periodic operation.

KEYWORDS

Methanol synthesis reactor, Periodic operation, Dynamic characteristics, Surrogate model, Kolmogorov-Arnold Networks

ACKNOWLEDGEMENTS

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P-01

POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Comparative Techno-Economic and Environmental Analysis of Tar Removal and Syngas Upgrading Pathways in SNG Production from Plastic Waste

Doyeong Ahn, and Inkyu Lee*

School of Chemical Engineering, Pusan National University, Korea

ABSTRACT

Chemical recycling of plastic waste (PW) offers the advantage of recovering energy in the form of usable fuels. Producing synthetic natural gas (SNG) is one of the attractive PW recycling pathways. It converts PW into a widely used energy carrier without changing the existing natural gas infrastructure. However, the PW-to-SNG process has two limitations: (i) significant tar formation, which causes operational issues in downstream units, and (ii) production of syngas with an insufficient hydrogen-to-carbon (H/C) ratio for natural gas synthesis. This study proposes four cases by combining two tar removal technologies and two H/C ratio increasing strategies and compares their environmental and economic performance. Tar was removed using oil-based scrubbing (OS) and steam reforming (SR), while the H/C ratio was increased via CO2 removal with acid gas removal unit (CR) and external H2 addition (HA). The OS-HA case shows the lowest greenhouse gas emissions but the highest levelized cost of SNG (LCO-SNG), whereas the SR-CR case shows the opposite trend. Sensitivity analysis indicates that only HA-based cases achieve LCO-SNG below the cost of conventional natural gas. This study demonstrates that the PW-to-SNG process could offer a promising route to carbon neutrality by replacing fossil natural gas and valorizing plastic waste.

KEYWORDS

Plastic waste, Synthetic natural gas, Techno-economic analysis, Environmental analysis, Process design

ACKNOWLEDGEMENTS

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korean government (MSIT) (RS-2024-00341380).

P-02

POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Prediction Rationale Based on Occupied Space Information of Three-Dimensional Structures and Molecular Descriptors in Biodegradability Prediction

Atsushi Yoshida*, Kazuhiro Takeda

Shizuoka University, Japan

ABSTRACT

Tests based on the Chemical Substances Control Law to determine biodegradability are costly and time-consuming. To improve prediction efficiency, a machine learning model using 3D structural information with electronic and energy -based properties was developed. Among these, ionization energy gave the best accuracy. To explore structure- dependent trends, transfer learning was applied by fine-tuning a pre -trained model on structural groups such as linear, monocyclic, polycyclic, and heterocyclic compounds, leading to improved classification performance. Furthermore, to verify the interpretability of predictions based on molecular descriptors and 3D voxel representations in this model, interpretability techniques such as SHAP, Grad -CAM, and Integrated Gradients were introduced. These analyses enabled the visualization and quantification of molecular descriptors contributing to biodegradability predictions, as well as spatial regions and atomic positions within molecules. Moving forward, molecular descriptors and three - dimensional structural features emphasized by the model in biodegradability prediction will be systematically analyzed using this methodology, thereby advancing the elucidation of structural factors involved in degradation behavior. Furthermore, based on the insights gained, we aim to optimize model design and enhance the transparency of prediction rationale, thereby improving the reliability and practicality of machine learning models.

KEYWORDS

biodegradability; machine learning; 3D structures; molecular descriptors;

P-03

POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Dynamic Modeling of a Hydrogen-Based Fluidized-Bed Reactor for Iron Ore Reduction

Min Cheol Bae[1], Sang Hwan Son[1,2,*]

[1]School of Chemical Engineering, Pusan National University, Korea
[2]Institute for Environment and Energy, Korea

ABSTRACT

Conventional ironmaking is a significant source of global CO2 emissions due to the use of coke as the reductant. Hydrogen-based iron ore reduction has emerged as a promising low-carbon alternative. Fluidized-bed reactors provide efficient gas–solid contact and enable the direct use of untreated ore, which can reduce preprocessing costs. Nevertheless, the absence of commercially deployed hydrogen-based fluidized-bed reactors necessitates a mechanistic understanding of coupled reaction and flow behavior for reactor design and operation. This study presents a dynamic model for a hydrogen-based fluidized-bed reactor. Mass and energy balance equations are established for the bubble and emulsion phases, and kinetic expressions for stepwise iron ore reduction and dolomite calcination are incorporated. The model predicts transient changes in gas concentration, reduction degree, and temperature under a range of operating conditions, thereby enabling a quantitative evaluation of reactor performance.

KEYWORDS

Iron Ore Reduction, H2-Based Reduction, Dynamic Modeling, Fluidized Bed Reactor

ACKNOWLEDGEMENTS

POSCO, Ministry of Trade, Industry and Energy (South Korea)

P-04

POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Sustainable Integrated Process for Methyl Formate via CO_2 Hydrogenation over Ru-Based Heterogeneous Catalysts

Baejeong Kim, Taeksang Yoon, Minji Kang, Hongjin Park, Sungho Yoon* and Chul-Jin Lee*

Department of Intelligent Energy and Industry, Chung-Ang University, Korea

ABSTRACT

Carbon capture and utilization (CCU) through CO2 hydrogenation offers a promising pathway for producing value-added C1 chemicals such as methyl formate (MF). However, practical implementation remains challenging due to the need for efficient reaction–separation integration during scale-up. In this study, a recyclable heterogeneous catalyst, Ru-MACHO-POMP, was applied for CO2 hydrogenation in methanol using tripropylamine (TPA) as a base. Product formation was quantified by quantitative NMR analysis to evaluate catalytic performance and stability. To address downstream separation challenges, reactive distillation was introduced to selectively recover an MF-rich distillate while retaining the TPA-containing bottom phase for reuse. Aspen Plus modeling was employed to assess the feasibility of the integrated process configuration and to support process design. The catalyst exhibited stable activity over multiple recycling cycles, and the reaction–separation integration demonstrated technical feasibility. This work presents an integrated CO2-to-MF pathway combining recyclable heterogeneous catalysis, separation design, and preliminary TEA/LCA evaluation toward sustainable MF production.

KEYWORDS

CCU, heterogeneous catalyst, TEA, LCA, separation

ACKNOWLEDGEMENTS

This work(research) was supported by ITECH R&D program of MOTIE/KEIT [project No. RS-2023-00266831, Development of Novel Plasma Process for Hydrocarbon Cracking].

P-05

POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Effect of operating conditions on hydrogen production via non-oxidative polyethylene pyrolysis in a multi-stage molten-tin-based reactor

Bang Thanh Le[1], Son Ich Ngo[1,2], Young-Il Lim[1,*], Young Jae Lee[3], and Uen-Do Lee[3]

[1]Department of Chemical Engineering, Hankyong National University, Korea
[2]Faculty of Heat and Refrigeration Engineering, Industrial University of Ho Chi Minh City, Vietnam
[3]Korea Institute of Industrial Technology (KITECH), Korea

ABSTRACT

Plastic waste presents a significant environmental challenge, necessitating sustainable valorization strategies. In this study, a one-dimensional (1D) model of a multi-stage molten-tin-based reactor was developed to enhance clean hydrogen production via non-oxidative polyethylene (PE) pyrolysis. In the first stage, PE underwent thermal decomposition to form H2, light hydrocarbons, and solid carbon. In the second-stage packed-bed reactor, coke was removed and non-condensable gases underwent further non-catalytic reactions. The remaining hydrocarbons were subsequently converted to H2 and solid carbon in a molten-metal-filled third stage through catalytic and non-catalytic reactions. The 1D model integrated mass and momentum balances, reaction kinetics, and hydrodynamic correlations. Using the validated 1D framework, the effects of operating pressure, temperature, gas holdup, and reactor dimensions on hydrogen yield were systematically evaluated. This model provides a quantitative basis for reactor optimization and scale-up of hydrogen production from plastic waste.

KEYWORDS

Hydrogen production, Polyethylene pyrolysis, Molten metal bubble column reactor, Multi-stage reactor design, Hydrodynamics.

ACKNOWLEDGEMENTS

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korean Government (MEST) (grant number: RS-2026-25472336 and 2022M3J5A1051728).

P-06

POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Upcycling Polymeric Fibrous Waste into Methanol through Carbon Dioxide–Assisted Pyrolysis: A Techno-Economic and Environmental Assessment

Changbeom Shin[1], Taean Go[1], Hyungtae Cho[2], Jaewon Lee[1,*]

[1] *Hanyang University ERICA, Korea*
[2] *Kyung Hee University, Korea*

ABSTRACT

Methanol is gaining attention as an alternative fuel, and green methanol produced from renewable resources, such as waste and captured carbon, may reduce life-cycle carbon dioxide (CO2) emissions. This study proposes an integrated pathway for green methanol production that combines syngas from carbon dioxide (CO2)–assisted pyrolysis of polymeric fibrous waste with hydrogen-rich gas produced via biogas steam reforming (BSR). The hybrid configuration is designed to supplement hydrogen availability and more effectively meet the stoichiometric hydrogen requirement for methanol synthesis. Carbon dioxide (CO2) generated during the pyrolysis and reforming steps is also captured, compressed, and cooled for storage. To assess practical viability, we conducted a techno-economic analysis (TEA) and a life cycle assessment (LCA). Compared with a conventional incineration baseline, the proposed route may support circular resource use by converting polymeric fibrous waste into a value-added fuel. Under favorable assumptions regarding feedstock properties, energy supply, and carbon management, the system could potentially approach net-negative greenhouse gas emissions. Overall, the results indicate a plausible pathway for waste upcycling and lower-carbon methanol production.

KEYWORDS

Process Design, Green Methanol, Pyrolysis, Waste-to-Energy, TEA, LCA

P-07

POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Novel Energy-Saving Strategies of a Transesterification Reactive Distillation Process with Side-Stream configurations

Yu-Sheng Chen[1] , Irvy Ai Xia Teh[2], Hao-Yeh Lee[1,*], and Zong Yang Kong[3]

[1]*Department of Chemical Engineering, National Taiwan University of Science and Technology, Taiwan*
[2]*Faculty of Engineering, Swinburne University of Technology, Malaysia*
[3]*School of Engineering, Sunway University, Malaysia*

ABSTRACT

Distillation columns are major energy consumers in chemical processes, particularly in reactive distillation (RD) systems. Conventional heat-integrated RD commonly relies on vapor side streams, which increase operational complexity and reduce controllability. In contrast, side-stream reactive distillation using liquid side streams offers greater operational flexibility and improved controllability, making it a promising alternative for energy-efficient design. This study investigates a non-ideal transesterification reactive distillation process for n-butyl acetate production, consisting of a reactive distillation column (RDC) and a separation column with azeotropic behavior. Two optimization strategies, minimizing RDC reboiler duty and minimizing total reboiler duty, are compared under product specifications using a two-stage sequential optimization approach. Energy consumption and total annual cost (TAC) are evaluated before and after heat integration. Results show that minimizing total reboiler duty provides only limited energy savings prior to heat integration. In contrast, minimizing the RDC reboiler duty initially leads to a slight increase in overall energy consumption. After heat integration, this strategy achieves up to 31.5% reduction in total energy consumption and approximately 24% reduction in TAC.

KEYWORDS

Reactive distillation; Side-stream design; Process simulation; Aspen Plus

ACKNOWLEDGEMENTS

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P-08

POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Criticality Analysis for Redundancy Planning and Preventive Maintenance in Industrial Symbiosis

Yick Eu Chew[1], Bing Shen How[1], Jean Pimentel[2], Petar Sabev Varbanov[2,3], Ferenc Friedler[2], Viknesh Andiappan[1,*]

[1]Faculty of Engineering, Swinburne University of Technology Sarawak, Malaysia
[2]Department of Systems Sciences, Széchenyi István University, Hungary
[3]Faculty of Mechanical Engineering, Brno University of Technology - VUT Brno, Czech Republic

ABSTRACT

Hard-to-abate sectors contribute significantly to global CO2 emissions, but their decarbonisation is costly and technically challenging. Smart energy systems offer a cost-effective decarbonisation solution for hard-to-abate sectors when implemented in an industrial symbiosis. In an industrial symbiosis, smart energy systems can act as anchor tenants with shared carbon capture, transport, and storage infrastructure. This collaborative approach allows multiple hard-to-abate plants to reduce emissions while benefiting from economies of scale. However, such tightly integrated systems are vulnerable to operational disruptions. Maintenance of a single equipment can propagate across the network, reducing energy generation and deviating from normal operation. However, implementing redundancy for every unit is economically and practically infeasible. Therefore, identifying the most critical equipment within the energy system is essential for prioritising maintenance efforts and allocating limited financial resources effectively. This study develops a criticality analysis framework that combines the Shapley–Shubik power index with P-graph methodology to identify key equipment within a smart energy system. Based on the identified critical units, a mixed-integer linear programming model is formulated to design a preventive maintenance plan that minimises operational disruptions. The model is implemented and solved using Pyomo in Python. This proposed maintenance framework is demonstrated through a case study of a combined heat and power unit in a smart energy system of industrial symbiosis.

KEYWORDS

System Resilience; Operational Scheduling; Reserve; Flexibility

P-09 **POSTER**

13:30~14:30 · Poster Session P1 · Engineering Building D

Comparative Techno-Economic and Life Cycle Assessment of Thermochemical Pathways for Waste Plastic Valorization: Fuel, Hydrogen, and Circular Polyethylene Production

Chanmok Kim, Donghyeon Kim, Heehyun Choi, Hyeonseo Im, and Jiyong Kim*

School of Chemical Engineering, Sungkyunkwan University, Korea

ABSTRACT

The accumulation of end-of-life plastics necessitates the development of scalable thermochemical conversion strategies that go beyond conventional mechanical recycling. This study presents a comparative techno-economic analysis and life cycle assessment (LCA) of three waste plastic valorization pathways rigorously modeled in Aspen Plus: (1) pyrolysis followed by hydrotreatment and separation to produce gasoline-range fuels (plastic-to-fuel, P2F), (2) steam gasification with water-gas shift and pressure swing adsorption for hydrogen production (plastic-to-hydrogen, P2H2), and (3) pyrolysis followed by hydrotreatment of pyrolysis oil, and olefin purification to produce polymer-grade light olefins (e.g., ethylene and propylene) for polyolefin resynthesis via catalytic polymerization (plastic-to-plastic, P2P). A uniform waste polyolefin feedstock is adopted across all scenarios to ensure a fair comparison. Economic performance is assessed in terms of minimum selling price and net present value, while environmental impacts are quantified within a cradle-to-gate LCA framework, employing global warming potential as the primary impact indicator. Sensitivity analyses are conducted on feedstock composition, plant capacity, and energy source to identify the dominant cost and emission drivers. This work aims to provide a systematic framework for evaluating the economic feasibility and environmental sustainability of competing thermochemical plastic upcycling and closed-loop recycling pathways.

KEYWORDS

Waste plastic valorization, Techno-economic analysis, Life cycle assessment, Thermochemical recycling,

P-10

POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

A Dynamic Simulation and Economic Evaluation Framework for Cyclic Distillation of Close-Boiling Mixtures

Cheng-Yen Lai and Jeffrey D. Ward*

Department of Chemical Engineering, National Taiwan University, Taiwan

ABSTRACT

The separation of close-boiling mixtures remains a major challenge in distillation due to high energy consumption and stringent product purity requirements [1]. While conventional distillation is widely applied, its economic and energetic limitations motivate the exploration of alternative process intensification strategies.

In this work, a unified dynamic simulation and economic evaluation framework is developed to investigate cyclic distillation for close-boiling separations. Cyclic distillation operates under periodic non-steady-state conditions with alternating vapor and liquid flow [2,3], enabling the systematic study of transient column behavior and its impact on separation performance. Propane–propylene separation [4] is employed as a representative case study to demonstrate the modeling approach and to analyze the sensitivity of separation performance and total annualized cost (TAC) to key design and operating variables, including the number of stages, feed location, vapor flow rate, and cycle duration.

The proposed framework is also applied to close-boiling mixtures and cyclic distillation is compared with other process intensification strategies, including heat-pump-assisted distillation and multiple-effect distillation. The results of this work aim to provide insight into the economic and operational trade-offs associated with cyclic distillation and its performance with alternative distillation intensification strategies [5].

KEYWORDS

Cyclic distillation; Close-boiling separations; Process intensification; Dynamic simulation; Total annualized cost

ACKNOWLEDGEMENTS

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P-11 **POSTER**
13:30~14:30 · Poster Session P1 · Engineering Building D

Process design of ammonia decomposition system for hydrogen and power co-generation with low nitrogen oxide emissions

Seoyeon Cho, and Inkyu Lee*

School of Chemical Engineering, Pusan National University, Korea

ABSTRACT

Ammonia is regarded as a promising hydrogen carrier due to its high energy content and mild liquefaction condition. Generally, in a conventional ammonia decomposition process, ammonia is converted into hydrogen in the catalyst-packed reactor, and the reactor effluent gas is purified through a pressure swing adsorption (PSA). PSA tail gas is combusted in the furnace to supply the decomposition reaction heat. There are two major features of the conventional process. (1) First, external heating to supply the reaction heat requires combustion fuel such as PSA tail gases. (2) Furthermore, the combustion of PSA tail gases leads to significant emissions of nitrogen oxides (NOx). These factors adversely affect economic and environmental performance of the process, respectively. Therefore, this study proposes a novel concept of the ammonia decomposition process. The proposed process (1) supplies reaction heat via an ammonia autothermal reaction, (2) utilizes PSA tail gas for power generation in a solid oxide fuel cell (SOFC), and (3) combusts SOFC-off gases. We conducted the process simulation and techno-economic analyses. The results show that the proposed process generated 23.4 MW of additional power, a 12.6% lower levelized cost of hydrogen, and a 77.1% reduction in NOx emissions compared to the conventional process.

KEYWORDS

process design, hydrogen production, power generation, ammonia autothermal reforming, solid oxide fuel cell, nitrogen oxides

ACKNOWLEDGEMENTS

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P-12

POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Multi-Dataset Sustainable Process Simulation of Food Waste to Biogas system

Mingyo Choi[1], Jaewon Byun[2], Jeehoon Han[1,*]

[1]*Department of Chemical Engineering, Pohang University of Science and Technology (POSTECH), Korea*
[2]*Chonnam National University, Korea*

ABSTRACT

Population growth and economic growth in global leads to significant environmental problems such as greenhouse gas emissions and air pollutant releases. Among these exponential increases of food waste (FW) has emerged as an urgent and critical issue in society at large. This study focuses on the sustainable strategies of FW as a source of energy to address a problem deeply embedded throughout society. However, difficulties exist in reflecting regional and seasonal variations in FW characteristics. Furthermore, it is difficult to consider inhibitor factors that impact bio-process efficiency, presenting challenges in developing and operating processes for optimal production. Therefore, this study aimed to develop an integrated model combining the conversion process using a kinetic model based on MATLAB and the separation process using Aspen Plus V14, to conduct research targeting optimal process design considering regional characteristics. Furthermore, to more adequately reflect actual plant operating conditions, dynamic simulations were performed considering conditions where the inflow rate fluctuates over time. Implementing the AD kinetics via MATLAB, was possible to analyze changes in the biogas production process based on regional and seasonal variations of FW. Predicting FW composition and developing corresponding biogas production strategies, this study highlights the establishment of multi-dataset process simulation system.

KEYWORDS

Biogas, Anaerobic digestion, Food waste, Process simulation

ACKNOWLEDGEMENTS

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P-13

POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Learning Temperature-Aware Molecular Representations for Organic Solubility Prediction

Chonghyo Joo and Lauren Ye Seol Lee*

Department of Chemical Engineering, University College London, UK

ABSTRACT

Accurate prediction of organic solubility across temperature is essential for solvent selection and process design. Although many machine learning models have been developed for solubility prediction, most focus on fixed-temperature setting or treated temperature as a simple scalar input, limiting their ability to capture nonlinear temperature-dependent effects in solute-solvent behavior. To address these challenges, we introduce a temperature conditioning approach that embeds temperature directly into latent features through feature-wise linear modulation (FiLM) following radial basis function kernel expansion. The proposed method is evaluated using two representative architectures: Chemprop, which learns graph-based molecular representations, and Fastprop, which uses fixed molecular descriptors. Models are trained on BigSolDB dataset and evaluated under both interpolation conditions and extrapolation to unseen solutes using different datasets. The results show that the temperature conditioning layer improves predictive performance and temperature sensitivity, with particularly strong gains observed for the graph-based Chemprop model. These findings suggest that representation-level temperature conditioning is an effective strategy for capturing temperature-dependent molecular interactions in solubility prediction.

KEYWORDS

Molecular representation, Solubility, Organic solvents, Machine learning

ACKNOWLEDGEMENTS

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P-14

POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

A Comparative Study of International Renewable Energy Supply Chains Utilizing Green Ammonia as Energy Carrier

Chun-Cheng Li[1], Chong Wei Ong[1,2], Cheng-Liang Chen[1,2,*]

[1] *Department of Chemical Engineering, National Taiwan University, Taiwan*
[2] *Department of Chemical and Environmental Engineering, University of Nottingham Malaysia, Malaysia*

ABSTRACT

Addressing the global challenge of climate change requires innovative solutions for transitioning to renewable energy systems. This study analyses international renewable energy supply chains using green ammonia as a carrier to support net-zero emissions by 2050, connecting energy-rich exporters (Australia, Qatar, Chile) with energy-deficient importers (Japan, South Korea, Taiwan). In exporting regions, renewable electricity powers solid oxide electrolysers (SOECs) for hydrogen production and air separation units (ASU) for nitrogen. These are combined via the Haber-Bosch process to produce green ammonia for transport. In importing regions, two pathways are evaluated: direct combustion in a gas turbine combined cycle (GTCC) with Selective Catalytic Reduction (SCR) for NOx control, and ammonia cracking to supply hydrogen for solid oxide fuel cells (SOFCs). This research provides detailed process simulations, economic evaluations, and life cycle assessments (LCAs) for both pathways. By calculating the levelized costs of hydrogen and electricity alongside global warming potential (GWP), this study determines the overall feasibility and environmental impact of these green ammonia-based energy transport systems.

KEYWORDS

Renewable electricity, International supply chain; Ammonia, Gas turbine combined cycle, Cracking, Solid oxide fuel cells

ACKNOWLEDGEMENTS

The author would like to thank Professor Cheng-Liang Chen and colleagues in the Department of Chemical Engineering for their support and helpful suggestions in completing this study.

P-15 **POSTER**

13:30~14:30 · Poster Session P1 · Engineering Building D

Dynamic Multi-Objective Operational Optimization of the Green Hydrogen Ammonia Synthesis Process under Uncertainty Disturbance

Zijun Wang[1], Shida Gao[2], Kangkang Feng[3], Xiangjian Shi[3], **Cuimei Bo**[1,*]

[1]*College of Electrical Engineering and Control Science, Nanjing Tech University, China*
[2]*Shanghai Jiao Tong University, China*
[3]*Nanjing Nanrui Jibao Engineering Technology Co., China*

ABSTRACT

Green hydrogen-coupled ammonia synthesis is a promising pathway for the low-carbon transition of the fertilizer industry. However, the fluctuation of renewable energy output conflicts with the strict requirements of ammonia synthesis for safe and stable operation, posing major challenges to online optimization. To address this issue, this paper proposes a dynamic multi-objective operational optimization method for ammonia synthesis under fluctuating green hydrogen loads. A flexible power-hydrogen-ammonia process and a mechanistic model are first developed. Then, a dynamic multi-objective optimization model is established to maximize hydrogen conversion and minimize total energy consumption under constraints on product purity and critical operating variables. Furthermore, a DAPB-NSGAII algorithm is proposed by integrating an online Gaussian process surrogate, environmental change detection, Pareto-based dual-metric infill sampling, and centroid-prediction-based population reconstruction, enabling efficient tracking of the Pareto front in time-varying environments. Results show that the proposed method outperforms comparative algorithms in HV and IGD on dynamic benchmark problems, and achieves faster load-transition response and better operational decisions in a 150 h online optimization case.

KEYWORDS

green ammonia synthesis, load fluctuation, dynamic multi-objective optimization, Gaussian process surrogate model

ACKNOWLEDGEMENTS

This work was supported by the National Natural Science Foundation of China (62333010).

P-16 **POSTER**

13:30~14:30 · Poster Session P1 · Engineering Building D

Process Design and Optimization Based on Techno-Economic Evaluation of Green Hydrogen Considering Variations in Cell Number and Operating Conditions of Alkaline Water Electrolysis Stacks

Dong-ha Kim, Joonjae Ryu*

Department of Chemical Engineering, Center for Innovative Chemical Processes, Institute of Engineering, University of Seoul,163 Seoulsiripdaero, Dongdaemun-gu, 02504, Seoul, South Korea

ABSTRACT

The hydrogen economy is a pivotal component of global efforts to achieve carbon neutrality, with green hydrogen production via water electrolysis emerging as a core technology. Among various methods, Alkaline Water Electrolysis (AWE) offers high potential for commercialization; however, maximizing its economic feasibility requires a sophisticated understanding of the trade-offs between system scale and efficiency. This study focuses on the Techno-Economic Analysis (TEA) and process optimization of AWE systems, specifically considering variations in cell integration (cell number) and diverse operating conditions. A rigorous process model was developed using Aspen Custom Modeler (ACM) to simulate the electrochemical behavior of AWE cells and stacks. Unlike conventional models that treat cell numbers as fixed constants, this research incorporates scale-dependent loss mechanisms—such as shunt current and pressure drops—to evaluate their impact on overall system performance. Unit operations are modeled based on theoretical electrochemical principles and experimental correlations, aiming for a high accuracy predictive model. Based on this precisely engineered model, the study performs an integrated optimization of cell numbers and operating variables (temperature, pressure, and flow rate) to derive the optimal green hydrogen production scenario.

KEYWORDS

Alkaline Water Electrolysis, Green Hydrogen, Techno-Economic Analysis, Aspen Custom Modeler

ACKNOWLEDGEMENTS

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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POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Production of Methanol from Waste Expanded Polystyrene through Pyrolysis-integrated Process: Techno-economic analysis

Dongho Choi, Hyungtae Cho*

Department of Chemical Engineering, College of Engineering, Kyung Hee University, Yongin, Republic of Korea

ABSTRACT

Waste expanded polystyrene (WEPS) has become a significant environmental concern, particularly marine ecosystems, necessitating effective disposal strategy. As a measure of it, this study proposes a process that use of WEPS as feedstock for low-carbon fuel. Notably, methanol is recognized as a next-generation low-carbon fuel in maritime industry. In previous work, the presence of CO2 enhances syngas production during catalytic pyrolysis of waste EPS compared to conventional catalytic pyrolysis under inert condition. Based on these experimental findings, two WEPS-to-methanol processes were developed: one integrating CO2-assisted catalytic pyrolysis and the other involving conventional one. The process integrating CO2-assisted catalytic pyrolysis demonstrated a substantial increase in the methanol productivity compared to that including conventional one, highlighting the merits of introducing CO2 in catalytic pyrolysis of WEPS. Additionally, the cost of methanol production was significantly lower in the process incorporating CO2-assisted catalytic pyrolysis, emphasizing its economic viability. This approach highlights the potential for transforming WEPS into valuable resources while addressing environmental challenges, paving the way for sustainable waste management practices and contributing to a circular economy that prioritizes the reduction of plastic waste.

KEYWORDS

Methanol, Plastic waste, Expanded polystyrene, Thermochemical process, Catalytic pyrolysis, Circular economy

ACKNOWLEDGEMENTS

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POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

System Optimization and Techno-Economic Analysis for Renwable Energy-based Green Ammonia Production

Donghyeon Jeon, Jin-Kuk Kim*

Department of Chemical Engineering, Hanyang University, Korea

ABSTRACT

Low-carbon ammonia (NH3) has emerged as a strategic energy carrier within the Power-to-X framework. Compared with hydrogen, NH3 provides higher volumetric energy density and can be liquefied under relatively moderate conditions, making it more suitable for bulk storage and long-distance transport. However, the economic feasibility of green NH3 remains challenged due to the high electricity consumption for water electrolysis and high capital expenditures associated with electrolyzer systems and renewable energy infrastructure. In this study, gray, blue, and green NH3 production processes are set up. Renewable energy systems integrating solar PV, wind turbines, and battery storage are considered for green NH3 production, while amine-based capture for the removal of CO2 from steam methane reformer flue gas is introduced for the blue NH3 process. The capacity of renewable energy systems is optimized via particle swarm optimization subject to region-specific hourly weather profiles and time-varying grid electricity pricing. Through an integrated process-energy system analysis, cost-effective renewable energy supply pathways are systematically identified for green NH3 production. Also, sensitivity and scenario analyses considering the level of dependency on grid electricity, carbon pricing, and technology maturity levels are conducted to quantitatively assess the impact of renewable energy supply and integration strategies on techno-economic competitiveness of green NH3 compared with gray and blue NH3.

KEYWORDS

Hydrogen, Ammonia, Renewable energy system, Carbon-neutrality

ACKNOWLEDGEMENTS

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POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Energy Management and Optimization of an Off-Grid Wind-Photovoltaic-Hydrogen Storage- Methanol System

Fei Wang, Qiao Zhang*

School of Chemical Engineering & Technology, Xi'an Jiaotong University, China

ABSTRACT

Driven by global energy transition and carbon neutrality targets, power-hydrogen-chemical systems integrating wind and solar energy with hydrogen production and methanol synthesis have emerged as a promising pathway for deep decarbonization. However, due to the intermittency of renewable energy, existing energy management strategies struggle to simultaneously ensure process stability and economic performance, often relying on excessive capacity redundancy. This study proposes a multi-timescale energy management framework for an off-grid wind-photovoltaic-hydrogen storage-methanol system. A dynamic priority control based on battery state of charge enables real-time power allocation and stabilizes system operation, while a multi-objective optimization model is employed to determine the cost-optimal configuration. The results indicate that the optimal configuration is achieved when the capacities of the electrolyzer, battery, and hydrogen storage are 0.72, 0.72, and 0.80 times their nominal values, respectively, yielding a minimum levelized methanol cost of 4535.90 CNY/t and a renewable curtailment rate of 13.80 %. The proposed strategy effectively reduces system redundancy while maintaining stable chemical operation, providing a practical pathway for the large-scale deployment of green methanol.

KEYWORDS

Off-grid energy system; Power-to-methanol (PtM); Energy management system (EMS); Multi-timescale control; Dynamic priority strategy

P-20 POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Sustainable Strategy for Polybutylene Adipate Terephthalate Production Utilizing Biomass-derived Monomers and Lignin Blending

Gihyun Kwon (Underline Presenting Author), and Jeehoon Han*

Department of Chemical Engineering, Pohang University of Science and Technology, Korea

ABSTRACT

Poly(butylene adipate-co-terephthalate) (PBAT) has attracted significant attention as a promising biodegradable plastic for agricultural mulch films and packaging applications. However, the high carbon footprints of its constituent monomers remain a key barrier to its large-scale commercialization. Previous studies have attempted to improve its environmental performance by incorporating sustainable fillers such as lignin, but its relatively high carbon footprint still limits its competitiveness compared with other biodegradable polymers. This study evaluated the potential to reduce the environmental impacts of PBAT by producing the fossil-derived monomers from lignocellulosic biomass and blending PBAT with lignin. The results indicate that synthesizing 1 kg of PBAT requires 0.41 kg of 1,4-butanediol, 0.37 kg of adipic acid, and 0.33 kg of terephthalic acid, which in turn require 16.5 kg of corn stover. Compared with fossil-based PBAT, the global warming potential of bio-based PBAT can be reduced by 71.0%. Furthermore, blending approximately 5 wt% lignin into PBAT composites can reduce carbon emissions to 2.63 kgCO2 eq., demonstrating the effectiveness of biomass-derived monomer production and lignin incorporation in improving the sustainability of PBAT. These findings suggest the potential to enhance the compatibility between biomass-derived PBAT and lignin, thereby further improving the environmental impacts of PBAT composites. (191 words)

KEYWORDS

Polybutylene adipate terephthalate, Biomass, Biodegradable polymer, Lignin, Global warming potential

ACKNOWLEDGEMENTS

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POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Structured Surrogate Modeling and Reinforcement Learning for Grade Transition Control in Polypropylene Reactors

Guyang Liu, Jingyi Lu*, Wenli Du*

East China University of Science and Technology, China

ABSTRACT

Grade transition in polypropylene reactors is a critical yet challenging operation because it must balance product quality, transition time, temperature safety, and post-switch stability. This work addresses the control of melt flow index (MFI) transitions in propylene polymerization reactors and formulates grade switching as a constrained dynamic optimization and closed-loop control problem. The reactor is described by a 14-dimensional state vector and three manipulated variables: propylene feed rate, hydrogen feed rate, and cooling-water flow rate. To avoid the high computational cost of repeatedly integrating a stiff mechanistic model during policy training, a structured data-driven surrogate is developed to approximate one-step state transitions. Rather than using a fully black-box mapping, the surrogate sends the same state input to three parallel encoding branches to learn concentration, microscopic chain-moment, and thermodynamic features, whose structured encoding and fusion better capture the heterogeneity of polymerization dynamics. Based on this fast surrogate environment, PPO is used to learn closed-loop switching policies for both low-to-high and high-to-low grade transitions. Results show that the proposed method achieves excellent set-point tracking without a mechanistic model, while offering faster computation and rapid response. It provides an effective modeling and control framework for high-dimensional nonlinear industrial systems with sufficient historical data.

KEYWORDS

Polypropylene reactor; Grade transition; Melt flow index;Reinforcement learning

P-22

POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Physics Informed Neural Network for Viscoelastic Flows: Application to EPDM Die Swell Prediction

Gwanghyeon Kwon[1], Hyeong Ro Yoon[1], Seokyoung Hong[1,2], and Jong Min Lee[1,*]

[1]*Department of Chemical and Biological Engineering, Seoul National University, Korea*
[2]*School of Energy and Chemical Engineering, Ulsan National Institute of Science and Technology, Korea*

ABSTRACT

During the polymeric extrusion process, the die swell phenomenon is inherently inevitable, posing significant challenges in achieving precise dimensional accuracy for the final product. Empirical die-tuning necessitates costly and time-consuming iterative cycles, which creates a critical need for high-fidelity direct extrusion modeling to predict swelling behavior and facilitate efficient inverse die design. To address the challenges of data sparsity and complex viscoelastic rheology in industrial manufacturing, this study proposes a physics-informed neural network (PINN) for efficient extrusion modeling. High-fidelity training datasets were generated under diverse process conditions, by varying the injection velocities and temperatures, using the FEM-based open-source platform, FEniCS. The PINN, trained on a sparse dataset representing limited sensor orientations with the Oldroyd-B constitutive model and fundamental conservation laws (mass and momentum balances) embedded into the loss function, enabled the prediction of multi-physics profiles and the swelling ratio of sponge ethylene-propylene rubber (EPDM) compounds. As a result, PINN significantly outperformed standard deep neural networks (DNN) in predicting multiphysics profiles and swelling ratios. Achieving lower root mean square errors (RMSE) for all variables, the PINN demonstrated superior physical consistency and data efficiency in capturing non-linear rheological behavior of EPDM.

KEYWORDS

Polymeric extrusion, Die swelling, PINN, EPDM

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POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Sustainable Design and Economic Analysis of LOHC Dehydrogenation Process using Bayesian Optimization

Hyungjun Joo, Yeonsoo Kim*

Department of Chemical Engineering, Kwangwoon University, Korea

ABSTRACT

Liquid Organic Hydrogen Carriers (LOHC), specifically methylcyclohexane, presents a viable hydrogen storage solution. However, the highly endothermic dehydrogenation process requires substantial thermal energy, often compromising system sustainability through fossil fuel combustion. This study proposes an integrated dehydrogenation process coupled with a hydrogen blended natural gas co-firing turbine to supply reactor heat and power. To systematically resolve the conflicting objectives of economic feasibility and environmental sustainability, we developed a rigorous process model using Aspen HYSYS, simulating an industrial scale packed bed reactor. Addressing the high computational cost of rigorous simulations, a multi objective Bayesian optimization framework was implemented via a Python-Aspen interface. By utilizing Gaussian process surrogate model, the algorithm efficiently navigated the complex design space. The optimization adjusted decision variables, including reactor conditions and co-firing ratio, with high data efficiency. The resulting Pareto optimal frontiers quantify the trade-offs between minimizing costs and reducing emissions, providing robust guidelines for selecting optimal operational strategies under varying economic and environmental constraints.

KEYWORDS

Optimization, Hydrogen, LOHC, Machine Learning

ACKNOWLEDGEMENTS

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POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Mathematical Modeling and Simulation of an Energiron ZR Shaft Furnace for Hydrogen-Based Direct Reduction

Halyn Chung[1], and Sang Hwan Son[1,2,*]

[1]*School of Chemical Engineering, Pusan National University, Korea*
[2]*Institute for Environment and Energy, Korea*

ABSTRACT

The steel industry, one of the major contributors to global CO2 emissions, is transitioning from conventional coke-based ironmaking to natural-gas- and hydrogen-based direct reduction. Shaft furnaces are a commercially established option for this transition, and Energiron ZR is characterized by in-situ CH4 reforming, which provides flexibility in reducing-gas composition and supports low-CO2 operation. However, compared with Midrex-based systems, relatively few modeling and simulation studies have been reported for Energiron ZR shaft furnaces. This work presents a two-dimensional axisymmetric mathematical model of an Energiron ZR shaft furnace with radial gas injection, implemented in MATLAB. The model describes countercurrent gas–solid flow by solving momentum, mass, and energy conservation for the gas phase together with mass and energy balances for the solid phase. The reduction of iron ore pellets is formulated using a three-interface unreacted shrinking core model to capture the stepwise progression of reduction within individual pellets. The governing equations are solved iteratively to obtain converged distributions of gas composition, temperature, velocity, and solid conversion. The model offers spatially resolved insight into reactor behavior and provides an efficient framework for process analysis and optimization.

KEYWORDS

Hydrogen-based direct reduction, Shaft furnace, Energiron ZR, Mathematical modeling

ACKNOWLEDGEMENTS

Hyundai Steel

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POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Multi-stage stochastic programming for sustainable syngas injection into blast furnaces via waste plastics valorization

Heedo Ryou[1], Jinsu Kim[2], and Jeehoon Han[1,*]

[1]*Department of Chemical Engineering, Pohang University of Science and Technology, Korea*
[2]*Department of Petrochemical Materials, Chonnam National University, Korea*

ABSTRACT

The increasing production of plastics and the growing volume of waste plastics increasingly necessitate the development of effective recycling technologies. A strategy for the valorization of waste plastics, including conversion into syngas via gasification and syngas injection into blast furnaces to replace fossil-derived reducing agents is developed. A process modeling framework for the integrated process covers waste plastics feedstock preparation, syngas production, and blast furnace injection. The framework is used to conduct both a techno-economic and life cycle assessment. Multi-stage stochastic programming is also used to optimize operating and integration decisions under uncertainty in feedstock composition and process performance with CO2 reduction potential and syngas production cost as key indicators. The results identify operating and integration conditions under which waste plastic-derived syngas can deliver scalable decarbonization benefits in steel industry, providing a practical valorization pathway for waste plastics.

KEYWORDS

Waste plastics, Syngas injection, Blast furnace, Life-cycle assessment, Techno-economic analysis

ACKNOWLEDGEMENTS

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P-26 **POSTER**
13:30~14:30 · Poster Session P1 · Engineering Building D

ML-driven framework for system-level assessment of biomass and waste plastic co-gasification

Hyeonseo Im, Heehyun Choi, Chanmok Kim, Donghyeon Kim, Jiyong Kim*

School of Chemical Engineering, Sungkyunkwan University, Suwon, Republic of Korea

ABSTRACT

Biomass and waste plastic co-gasification is increasingly recognized as a promising pathway for converting renewable and waste-derived carbon into valuable products. However, its practical potential remains insufficiently understood because most existing studies focus only on reactor-scale syngas behavior without connecting it to downstream process performance. This study proposes an integrated ML-based framework to evaluate co-gasification as a feed-flexible waste-to-X platform. Using a literature-derived dataset, physics-informed ML models were developed to predict syngas composition from feedstock properties, blending ratio, and operating conditions. The predicted syngas was then used in process simulations for hydrogen production via steam gasification and electricity generation via air gasification, followed by TEA, LCA, and optimization under feed availability constraints. The ML model reproduced non-equilibrium experimental behavior more accurately than equilibrium-based approaches while maintaining high predictive performance. The results showed that waste plastic characteristics, feed cost, and upstream carbon intensity are key drivers of overall system outcomes. Optimization further demonstrated that the most favorable feed combinations and operating conditions vary with regional resource availability and the selected objective. Overall, the results suggest that co-gasification should be developed as a feed-adaptive system that integrates reactor behavior with process design, economics, environmental performance, and supply constraints.

KEYWORDS

Biomass–waste plastic co-gasification, Machine learning, Syngas prediction, Techno-economic assessment, Life-cycle assessment

ACKNOWLEDGEMENTS

None

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POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Environmental and Economic Feasibility Analysis of Sustainable Aviation Fuel Production via Methanol-to-Jet Pathways Using Bio-methanol

Heejeong Kim, Jiyun Yoo, Jeehoon Han*

Department of Chemical Engineering, Pohang University of Science and Technology, Korea

ABSTRACT

Global environmental policies have been reinforced in recent years, which is promoting the transition from fossil-based aviation fuels to sustainable aviation fuel (SAF) to reduce carbon emissions in the aviation industry. In this work, a SAF production pathway based on bio-methanol and the methanol-to-jet fuel (MtJ) process is evaluated. Biomethanol is converted into 100,000 t yr-1 of SAF through a sequence of methanol-to-olefins (MtO), oligomerization, and hydrogenation processes. The overall process is modeled using Aspen Plus and MATLAB, with the MtO and oligomerization units developed using kinetic-based rigorous models. Economic and environmental performance of the proposed process are evaluated through techno-economic analysis (TEA) and life cycle assessment (LCA). Based on these results, the main factors affecting the levelized cost and greenhouse gas (GHG) emissions are analyzed. Furthermore, a sensitivity analysis is performed with respect to different sources of renewable electricity and renewable hydrogen to identify potential pathways for improving the sustainability and economic feasibility of biomethanol-based SAF production.

KEYWORDS

Sustainable Aviation Fuel, Methanol to jet fuel, Biomethanol, Process simulation, Life Cycle Assessment, Techno-Economic Analysis

ACKNOWLEDGEMENTS

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POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

LSTM–Transformer Autoencoder for Anomaly Detection: Application to a Real-World Multimode Industrial Chemical Proces

Hyeokin Gwon[1], Hyukwon Kwon[2,3], Meng Qi[4], Hyungtae Cho[5,*], Jaewon Lee[2,*]

[1]Department of Materials Science and Chemical Engineering, Hanyang University, Korea
[2]Department of Chemical and Biomolecular Engineering, Yonsei University, Korea
[3]Korea Institute of Industrial Technology, Korea
[4]Department of Chemistry and Bioscience, Aalborg University, Denmark
[5]Department of Chemical Engineering, Kyung Hee University, Korea

ABSTRACT

Modern industrial processes consist of multiple interdependent unit operations where even small disturbances can cause production losses, quality issues, and environmental harm. Conventional fault-detection approaches typically assume static or linearly dynamic conditions, making them ill-suited for the nonlinear, high-dimensional nature of real industrial systems. This work introduces the LSTM–Transformer Autoencoder (LTAE), an anomaly-detection framework that combines an LSTM encoder for capturing sequential temporal patterns with a transformer-based decoder leveraging multi-head attention to model long-range dependencies and enable accurate signal reconstruction. On the Tennessee Eastman (TE) benchmark under single-mode operation, LTAE preserved a near-zero false alarm rate (FAR = 0.00) while improving fault detection rate (FDR) from 0.83 to 0.86. In a multimode industrial polyethylene (PE) process, it dramatically reduced FAR from 0.85 to 0.05 while maintaining FDR at 1.00. These findings confirm that LTAE provides reliable and generalizable anomaly detection across both operating environments, offering a viable path toward minimizing material waste, reducing energy inefficiencies, and lowering environmental impact in complex chemical manufacturing.

KEYWORDS

Machine learning, Process monitoring, Anomaly detection, Chemical process

ACKNOWLEDGEMENTS

This work was supported by the Industrial Technology Innovation Program (RS-2024-00507471, “Development and Demonstration of an Operations Optimization Platform for AI-Driven Autonomous Manufacturing in Refinery and Petrochemical Processes”) funded by the Ministry of Trade, Industry & Energy (MOTIE), Korea.

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POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Artificial Photosynthesis-Based Photocatalytic Hydrogen Production: A Techno-Economic and Land-Use Comparison with PV-Electrolysis

HyunJun Choi, Juyung Byun, Jin Ko and Junghwan Kim*

Department of Chemical and Biomolecular Engineering, Yonsei University, Korea

ABSTRACT

Hydrogen produced from renewable solar energy is a promising solution for carbon neutrality. Among solar-to-hydrogen technologies, photovoltaic-electrolysis (PV-EC) and photocatalytic (PC) water splitting are two representative pathways. PC systems inspired by artificial photosynthesis directly convert sunlight into hydrogen via a single-step water-splitting reaction, offering a structurally simpler route than PV-EC. However, PC systems remain underexplored at a systems level, and large-scale quantitative assessment is still lacking. This study performs a techno-economic and land-use assessment comparing a PC reactor model integrating Fresnel lens concentration against a proton exchange membrane (PEM) electrolyzer-based PV-EC system across seven countries using real meteorological data, both normalized to equivalent hydrogen output. Results show that PC achieves a lower LCOH of 7.03 $/kg compared to 7.12 $/kg for PV-EC in the United States (US), while PV-EC is more competitive in Australia and Saudi Arabia. PC systems achieve higher land productivity across all countries, with the US achieving 4.66 kg H2/m2/yr for PC compared to 1.57 kg H2/m2/yr for PV-EC, approximately three times higher. These findings provide country-specific insights into the potential for deploying artificial photosynthesis-based photocatalytic hydrogen production.

KEYWORDS

photocatalytic water splitting, artificial photosynthesis, techno-economic analysis, land-use assessment, PV-electrolysis

ACKNOWLEDGEMENTS

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POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Optimization of a Waste Resource Supply Chain Based on Process Modeling of Co-Gasification of Waste Plastics and Biomass

Juhan Hwang and Joonjae Ryu*

Department of Chemical Engineering, University of Seoul, Korea

ABSTRACT

As the global imperative for carbon neutrality continues to intensify, there is a growing demand for integrated approaches that encompass the design of supply chains capable of efficiently transporting and utilizing waste resources, alongside the incorporation of clean energy production technologies. In this study, a waste resource supply chain was designed by leveraging data derived from process simulation of co-gasification involving waste plastics and biomass. In particular, the domestic generation volumes and regional distributions of waste resources were analyzed to formulate eight distinct scenarios (Cases), from which optimal strategies for minimizing transportation costs and logistics-associated carbon emissions were derived through mathematical modeling and optimization. Furthermore, by incorporating the transportation costs, waste resource procurement costs, and greenhouse gas emissions from logistics—as quantified through the optimization results—both Life Cycle Assessment (LCA) and Techno-Economic Analysis (TEA) were conducted to provide a comprehensive evaluation of environmental and economic feasibility.

KEYWORDS

Waste Resources, Co-Gasification, Supply Chain, Optimization, LCA, TEA

ACKNOWLEDGEMENTS

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POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Single-Amine Strategy for CO_2 Hydrogenation to Formic Acid: Process Simplification Using NBIM Coupled with Heterogeneous Ru-MACHO-POMP Catalysis

Jaehyeong Choi[1,2], Jiseong Baek[3], Hongjin Park[3], Minsol Kim[1,2], Kibong Lee[2], Ung Lee[1,4,2,*] and Sungho Yoon[3,*]

[1]*Clean Energy Research Center, Korea Institute of Science and Technology (KIST), Korea*
[2]*Department of Chemical and Biological Engineering, Korea University, Korea*
[3]*Department of Chemistry, Chung-Ang University, Korea*
[4]*Division of Energy and Environmental Technology, KIST School, Korea*

ABSTRACT

The catalytic hydrogenation of CO2 to formic acid (FA) is a promising route for sustainable C1 chemical production and hydrogen storage. However, practical implementation is limited by complex separation processes in conventional dual-amine systems, where an amine-exchange step imposes additional energy and capital penalties. In this work, we propose a single-amine strategy employing N-butylimidazole (NBIM) simultaneously as both the reaction and separation amine, eliminating the amine-exchange step. To compensate for the lower basicity of NBIM, heterogeneous catalysts were systematically screened, and Ru-MACHO-POMP exhibited the highest activity, achieving 53 kgFA/kgcat./d at 80 °C and 80 bar. Temperature-dependent studies identified 80 °C as the optimal condition, balancing productivity with a high acid-to-amine ratio (AAR ≈ 0.9) that minimizes downstream separation energy. Process simulation and techno-economic analysis (TEA) using Aspen Plus yielded a levelized cost of \$0.583 kg-1 for 85 wt% FA, competitive with fossil-based routes. Life-cycle assessment (LCA) identified steam consumption as the dominant environmental contributor; implementing mechanical vapor recompression (MVR) reduced the global warming potential from 4.87 to 0.63 kg CO2-eq/kg FA. Multi-objective optimization and SHAP analysis provided a quantitative roadmap linking catalyst performance and separation design to economic and environmental targets.

KEYWORDS

CO2 hydrogenation, Formic acid, Heterogeneous catalysis, Techno-economic analysis, Life cycle assessment, Process Optimization

P-33

POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Deep Reinforcement Learning-Based Thermal Management of Battery Fullpack in Electric Vehicle

Dabin Jeong and Yeonsoo Kim*

Department of Chemicl Engineering, Kwangwoon University, Korea

ABSTRACT

Ensuring battery safety while minimizing energy consumption is a key challenge in electric vehicle (EV) thermal management. In this study, a deep reinforcement learning (DRL)-based control strategy is proposed to enhance the performance of the battery thermal management system (BTMS) using the Deep Deterministic Policy Gradient (DDPG) algorithm. The proposed controller regulates the coolant flow rate, coolant inlet temperature, and a three-way valve signal. To capture the inherent thermal dynamics and temporal dependencies of battery systems, a gated recurrent unit (GRU) is integrated into the DDPG framework. In addition, a hybrid discrete–continuous action space is adopted to simultaneously handle mode selection and continuous control variables. Also, an actor loss regularization term is applied to promote smooth control actions, reflecting realistic actuator behavior. The performance of the proposed DRL-based controller is evaluated through a comparative study with a zone-based model predictive control (MPC) strategy and nonlinear programming method. Under charging rates of 3C and 2.5C, simulation results demonstrate that the proposed approach effectively maintains thermal stability while achieving lower energy consumption.

KEYWORDS

Electric vehicle, Battery thermal management, Reinforcement learning, Deep deterministic policy gradient

ACKNOWLEDGEMENTS

This work is supported by the Specialized Graduate School Program in the (field of support) funded by the Government of the Republic of Korea (Ministry of Climate, Energy and Environment) and administered by the Korea Environment Corporation.

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POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Integration of Water Electrolysis with Oxy-fuel SMR for Advanced Blue Hydrogen Production

Narin Jeong, Kang Cheongmin*, Young Woo Chon*

Department of Environmental Engineering, Inha University, Korea

ABSTRACT

As the global energy sector shifts toward a green hydrogen economy, blue hydrogen has emerged as a critical transitional bridge. However, the high CAPEX and OPEX associated with conventional Carbon Capture and Storage (CCS) remain significant barriers. This study introduces an innovative blue hydrogen production framework that integrates Steam Methane Reforming (SMR) with water electrolysis (SOEC and PEMEC) to mitigate these economic challenges. The core of this proposal lies in the synergistic use of resources: the oxygen byproduct from electrolysis is utilized for oxy-fuel combustion within the SMR unit. This approach enables streamlined CO2 separation through simple steam condensation. Additionally, thermal efficiency is optimized by recovering waste heat from the SMR flue gas to preheat the electrolyzer feed water. Through rigorous techno-economic, sensitivity, and greenhouse gas (GHG) assessments, the SMR+SOEC configuration was identified as the most superior model. This research offers a strategic direction for the evolution of high-efficiency blue hydrogen systems.

KEYWORDS

Blue hydrogen, Steam methane reforming (SMR), Oxy-fuel combustion, Electrolysis, Techno-economic anlaysis

ACKNOWLEDGEMENTS

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POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

A framework for knowledge-integrated process modeling from natural language using large language models

Jin Ko[1], Minji Kim[1], Juyeon Kim[2], Youngwon Lee[2], Youlim Chung[2], Jonggeol Na[2,*] and Junghwan Kim[1,**]

[1] *Department of Chemical and Biomoleular Engineering, Yonsei University, Korea*
[2] *Department of Chemical Engineering and Materials Science, Ewha Womans University, Korea*

ABSTRACT

Large language models are increasingly explored to enable natural language-driven process modeling, addressing the complexity of conventional simulators such as Aspen Plus. However, existing LLM-based studies often rely on unstructured outputs or remain limited in applicability, resulting in uncertain reliability due to insufficient integration of process knowledge and inadequate validation. To address these limitations, this study proposes a knowledge-integrated process modeling framework that enables automatic generation of Aspen Plus simulations from natural language inputs using an LLM agent. The proposed framework consists of three steps: (i) natural language interpretation, (ii) flowsheet generation, and (iii) simulation refinement. First, relevant information is extracted from natural language inputs and a literature database and transformed into a structured process schema, while ambiguities and missing information are identified to clarify key design choices. Subsequently, an Aspen flowsheet is constructed based on process modeling knowledge, with validation and completion ensuring model consistency and physical validity under LLM-assisted automation. Finally, simulation results and logs are used to analyze errors, and the model is iteratively improved through LLM-based refinement. This work enhances simulation reliability through a knowledge-integrated, LLM-based approach and enables reliable automation of process modeling, providing a foundation for scalable digital design environments.

KEYWORDS

Large language models, Process modeling, LLM agent, knowledge integration

ACKNOWLEDGEMENTS

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POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Parallel Computing Strategy of Isotherm Parameters Regression for p-Xylene Simulated Moving Bed Process via Internal Network Approach

Jing-Yang Tseng[1], I-Lung Chien[2], and Hao-Yeh Lee[1,*]

[1]*Department of Chemical Engineering, National Taiwan University of Science and Technology, Taiwan*
[2]*Department of Chemical Engineering, National Taiwan University, Taiwan*

ABSTRACT

P-Xylene (PX) separation using Simulated Moving Bed (SMB) technology plays a critical role in the petrochemical industry. This study develops a high-fidelity SMB model in Aspen Chromatography®, integrated with Python-based parameter regression. To ensure model generalizability across various scenarios, diverse data is necessary during regression. However, SMB systems involve highly dynamic transport phenomena characterized by numerous time-dependent partial differential equations (PDEs), leading to intensive computational demands. Furthermore, due to the COM architecture of Aspen software, Python cannot independently command separate simulation instances within a multi-file environment, constraining the feasibility of concurrent operations. To solve this problem, a parallel regression strategy based on an internal network architecture is proposed. Tasks are distributed from a physical host to multiple virtual machines, enabling simultaneous simulation under different operating conditions. The host coordinates parameter allocation and error aggregation, while each virtual machine independently executes a specific simulation instance. This method achieves a significant reduction of 50%–60% in the computation time compared to sequential approaches. Moreover, simultaneous incorporation of multiple operating conditions improves model generalizability and accuracy in capturing real plant dynamics. This scalable parallel architecture offers a cost-effective solution for high-computational dynamic systems and demonstrates strong potential for industrial-scale process modeling.

KEYWORDS

p-Xylene; Simulated Moving Bed; Aspen Chromatography; Parallel computing; Parex process

P-37

POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Industrial Plant Implementation and Assessment of Disturbance Observer-Based PID Control for Valve Hysteresis Compensation

Jinki Shoda*, Masaharu Daiguji

ENEOS Corporation, Japan

ABSTRACT

Valve hysteresis, such as valve stiction, poses a significant challenge for advanced control in process industries. It causes a discrepancy between the valve position setpoint and the actual position, resulting in degraded control performance, such as oscillations and poor setpoint tracking. Conventional solutions such as valve replacement or repairing needs high costs and plant shutdowns, making them difficult to implement in processes that demand continuous operation. Recently, Khamkaew et al. [2025] proposed a control scheme in which a disturbance observer (DOB) is incorporated into a conventional PID controller to compensate for valve stiction in process control systems, and demonstrated at the simulation level that the DOB-based approach significantly improves closed-loop performance under severe stiction conditions. In this study, the DOB-based PID control scheme was introduced to a flow control loop exhibiting hysteresis characteristics in an industrial process, and its potential for control performance improvement was investigated. To verify the effectiveness of the DOB-based PID control, the control performance with and without DOB-based compensation was compared in a flow control valve at a petrochemical plant. The results confirmed that DOB-based compensation suppressed oscillations and improved setpoint tracking, leading to better overall control stability. This study contributes new experimental evidence for the feasibility of DOB-based compensation in actual process plant environments. Khamkaew, J. and Jennawasin, T. Disturbance-observer Based PID Control Design for a Level Control System with Valve Stiction, In: Press: Proceedings of the 2025 SICE Festival with Annual Conference (SICE FES 2025). 2025.

KEYWORDS

Industrial Process, PID Control, Nonlinear Control, Process Control

P-38

POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Process Simulation and Economic Evaluation of Converting Mixed Plastic Waste into Methanol and Hydrogen

Jinwoo Gil[1], Dongho Choi[1], Jaewon Lee[2], Hyungtae Cho[1,*]

[1]*Department of Chemical Engineering, Kyung Hee University, Korea*
[2]*Department of materials Science and Chemical Engineering, Hanyang University, Korea*

ABSTRACT

Waste footwear has a complex compositional property, and thus its recycling is significant challenge. Thus, disposal of such waste has primarily achieved with incineration or landfill. However, such disposal methods have raised environmental concerns. To address these limitations, this study developed processes producing hydrogen or methanol from waste footwear, enabling both waste valorization and environmentally-benign disposal. In these processes, CO2-mediated catalytic pyrolysis was employed as a unit operation to convert waste footwear into syngas, which was subsequently routed to downstream units for hydrogen or methanol production. In the hydrogen production route, the productivity of hydrogen reached 2,100 tons, and its levelized cost of product (LCOP) was estimated to USD 5,300 ton-1. In the methanol production route, its productivity was 11,000 tons, with an LCOP of USD 1,300 ton-1. Although these production costs are higher than those of fossil-based hydrogen(USD 2,000 ton-1) and methanol(USD 600 ton-1), they remain lower than the costs typically reported for green hydrogen(USD 8,000 ton-1) and e-methanol(USD 2,500 ton-1) produced via renewable electricity-based pathways. This indicates that the proposed waste-to-chemical routes can offer a cost-competitive alternative among low-carbon production options.

KEYWORDS

Process Design, Hydrogen, Methanol, Waste-to-energy, Pyrolysis, Techno-economic analysis

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POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Integrated Process Evaluation for the Co-Production of Biodiesel and Bio-Lubricants from Biomass: Energy Analysis and Life Cycle Assessment

Jiyun Yoo[1], Yoonjae Lee[1], Seungjun Choi[1], Jaerak Ko[2], Soonho Hwangbo[2], and Jeehoon Han[1,*]

[1] *Department of Chemical Engineering, Pohang University of Science and Technology, Korea*
[2] *Department of Chemical Engineering, Gyeongsang National University, Korea*

ABSTRACT

Rising concerns over greenhouse gas emissions and the depletion of fossil resources have accelerated interest in renewable fuels and high-value biobased products. In this study, previously independent pathways were consolidated into a single process for the co-production of biodiesel and bio-lubricants from biomass, using oleic acid as a key intermediate. The integrated process was designed to enable energy integration and improved resource utilization. The present study evaluates the energy performance and flows of the integrated system and conducts a life cycle assessment (LCA) to determine whether process integration provides environmental benefits compared with the stand-alone production routes. Within the integrated framework, biomass is biologically converted into biodiesel and oleic acid, followed by chemical upgrading of hydroxymethylfurfural (HMF) and oleic acid to synthesize 2,5-tetrahydrofuran dimethanol-C18 diester, a lubricant-range product. Environmental impacts were evaluated using SimaPro with the Ecoinvent 3.0 database. Multiple allocation methods were applied to the co-production system to examine methodological sensitivity and to identify an appropriate approach for distributing environmental burdens. The abstract should be written in 200 words

KEYWORDS

Process integration, Biomass utilization, Energy analysis, Life cycle assessment, Co-production system

ACKNOWLEDGEMENTS

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P-40

POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Sustainable Integrated Steelmaking through Rotary Hearth Furnace-Based Steel Solid Waste Recycling: A Multi-Objective Optimization Approach

Jongil Bae[1], Myungsuk Son[2], Gayoung Lee[1], Jinsu Kim[3], and Jeehoon Han[1,*].

[1] *Department of Chemical Engineering, Pohang University of Science and Technology, Korea*
[2] *Korea Testing Laboratory, Korea*
[3] *Department of Petrochemical Materials, Chonnam National University, Korea*

ABSTRACT

Rotary Hearth Furnace (RHF) enables valorization of steel solid waste by converting solid waste into low-reduced iron and direct-reduced iron, which are subsequently utilized in Blast Furnace (BF) and Electric Arc Furnace (EAF), respectively. RHF facilitates material recirculation and supports a transition toward an electrified and less carbon-intensive EAF-based production route. In addition, reduced waste treatment requirements contribute to improved environmental and economic performance. This study develops a unified mathematical model representing the integrated RHF–BF–EAF steelmaking process, explicitly capturing material and energy balances across the interconnected units. The framework enables simulation of crude steel production under various operating conditions. A multi-objective optimization problem is formulated to simultaneously minimize unit production cost, carbon intensity, and mineral resource depletion. Pareto-optimal solutions are identified to quantify economic–environmental trade-offs within the integrated system. The integrated framework serves as a robust simulation and decision-support model for evaluating alternative steelmaking scenarios. The results demonstrate that coordinated operation across the RHF–BF–EAF integrated process enhances resource efficiency and reduces carbon intensity, providing practical guidance for sustainable integrated steel production.

KEYWORDS

Rotary Hearth Furnace, Solid Waste Recycling, Circular Steelmaking, Multi-Objective Optimization

ACKNOWLEDGEMENTS

This research was supported in part by the program of Development of Eco-friendly Chemicals as Alternative Raw Materials to Oil (No. 2022M3J5A1085257) through the National Research Foundation of Korea (NRF) funded by the Ministry of Science and ICT and in part by the National Research Foundation of Korea(NRF) grant funded by the Korea government(MSIT)(RS-2025-23323940).

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POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Surrogate Model-Based Optimization of Amine CO_2 Capture Process

Joonyoung Lee[1], Michael John Binns[2], Jin-Kuk Kim[1,*]

[1]Department of Chemical Engineering, Hanyang University, Korea
[2]Department of Chemical Engineering, Dongguk University, Korea

ABSTRACT

Monoethanolamine (MEA)-based wet CO2 capture is a technologically mature post-combustion capture process that can be readily available for industrial implementation. However, its economic feasibility is limited by the high regeneration energy required in the reboiler. Improving energy efficiency and reducing capture cost requires systematic process design and optimization, for the simultaneous consideration of multiple operating variables, including pressure, solvent loading, and temperature. Nevertheless, conventional physics-based process simulations suffer from high computational cost and convergence issues, which hinder their effective application in process optimization, subject to various design conditions. In this study, process modeling simulation study is first carried out for an MEA-based CO2 capture process, which incorporates a rate-based absorber model to account for mass transfer and reaction kinetics. High-fidelity simulation data were, then, generated through integrated workflows between MATLAB, Aspen HYSYS, and Python, with which data-driven surrogate models are constructed to represent CO2 capture behavior and system-wide performance. A wide range of machine learning surrogate models were proposed, and its predictive performance are evaluated and compared. Multi-objective optimization is performed to simultaneously minimize energy consumption and maximize CO2 capture efficiency, allowing the effective identification of optimal design and operating conditions. The ability of the proposed design framework to significantly enhance the energy efficiency of MEA-based CO2 capture processes is demonstrated with the case study presented.

KEYWORDS

MEA, CO2 capture, Optimization, Machine Learning, LASSO

ACKNOWLEDGEMENTS

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT). (RS-2025-00515836) and by a Korea Institute of Energy Technology Evaluation and Planning (KETEP) grant funded by the Korea government (MOTIE) (RS-2022-KP002700 (20224C10300050).

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POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Carbon neutral bio-methanol production via catalytic pyrolysis using CO_2

Junyoung Park, Dongho Choi, Yongsang An, and Hyungtae Cho*

Department of Chemical Engineering, Kyung Hee University, Korea

ABSTRACT

Bio-methanol is emerging as a practical low-carbon fuel option for decarbonizing the international shipping sector. This work proposed a bio-methanol production process that uses catalytic pyrolysis as a main syngas production step. In particular, CO2-assisted catalytic pyrolysis was employed due to its higher syngas productivity, which was reported in previous work. The resulting process (Strategy B) was modeled and evaluated using 3E (energy, economic, and environmental) analyses. Its performance was compared to the baseline process employing catalytic pyrolysis under N2 condition (Strategy A). Process simulations indicated that Strategy B achieved higher bio-methanol productivity and improved energy performance relative to Strategy A, resulting in a lower LCOP of 524 USD ton-1. Furthermore, integrating a biogas reforming process with Strategy B (Strategy C) further increased bio-methanol productivity while enhancing the energy efficiency of overall process. Although Strategy C required substantially higher overall costs, the merits derived from integrating biogas reforming process reduced the LCOP to 503 USD ton-1. Life cycle assessment (LCA) showed that Strategy C achieved lower net GHG emission than Strategy B, leading to improved eco-efficiency. Overall, these findings suggest that Strategy C could offer a promising option for sustainable bio-methanol production, contributing to decarbonization in the international shipping sector.

KEYWORDS

Bio-methanol, catalytic pyrolysis, CO2 utilization, biogas reforming, techno-economic analysis, life cycle assessment

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POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Optimization of an Induction Heating-Assisted Ammonia Decomposition Reactor for Efficient Hydrogen Production

Juyeon Cho, Chul-jin Lee*

Department of Chemical Engineering, Chung-Ang University, Korea

ABSTRACT

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.

KEYWORDS

Induction-heated reactor design, Ammonia cracking, CFD (thermo-fluid–reaction modeling), Electromagnetic–thermal coupling, Skin effect

ACKNOWLEDGEMENTS

This work(research) was supported by ITECH R&D program of MOTIE/KEIT [project No. RS-2023-00266831, Development of Novel Plasma Process for Hydrocarbon Cracking].

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POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Temporal fusion transformer–based surrogate modeling for adaptive and energy-efficient operation of hybrid semi-batch/batch reverse osmosis

Heun Se Kim and Kiho Park*

Department of Chemical Engineering, Hanyang University, Korea

ABSTRACT

Treatment of hypersaline wastewater generated from lithium-ion battery manufacturing and recycling remains challenging because high water recovery is often accompanied by increased energy demand and severe concentration polarization. This study proposes a temporal fusion transformer (TFT)-based surrogate framework to improve the adaptability and efficiency of a hybrid semi-batch/batch reverse osmosis (HSBRO) process. Bench-scale HSBRO experiments were conducted under varying feed flow rates, semi-batch operation times, purge and refill durations, and feed concentrations, generating a time-series dataset of hydraulic, conductivity, and energy responses. The TFT model was trained to predict cumulative SEC, final brine concentration, and permeate production by integrating static covariates, known operational inputs, and observed process variables. The cumulative SEC model achieved R2 values of 0.99, 0.98, and 0.98 for the training, validation, and test sets, respectively. The trained surrogate was then coupled with pareto-based multi-objective optimization to identify balanced operating conditions that reduce energy consumption and brine concentration while enhancing permeate production. For a representative optimized NaCl case, the model predicted SEC, Brine, and Permeate values of 0.540, 2400.1, and 194.8, respectively. In addition, surrogate-predicted energy results were linked to LCA to evaluate environmental trade-offs among candidate operating strategies under, high-salinity, multi-phase conditions relevant to industrial brines.

KEYWORDS

Hypersaline wastewater, ML, Multi objective optimization, attention score, LCA , HSBRO

ACKNOWLEDGEMENTS

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POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Quantitative Risk Assessment on Liquid hydrogen receiving Terminal

Jeong-Hoon Kim, Hak-Tae Lee, Ju-Eon-Bae, Chul-Jin Lee*

School of Chemical Engineering & Materials Science, Chung-Ang University, Korea

ABSTRACT

This study integrated process design and quantitative risk assessment for a large-scale liquid hydrogen terminal. By modeling 10,000 m^3 tanks under actual operating conditions, we identified that high-pressure pumps and vaporizers are the primary risk contributors. While equipment-specific risks exist, the overall level remains within the ALARP range. These results will serve as essential foundational data for optimizing designs and establishing safety standards for future liquid hydrogen infrastructure

KEYWORDS

Liquified Hydrogen Receiving Terminal, Liquified Hydrogen(LH2), Quantitative Risk Assessment(QRA), Qualitative Risk Assessment, Hazard Identification, , Liquid Hydrogen Infrastructure, Hydrogen Economy

ACKNOWLEDGEMENTS

This work(research) was supported by ITECH R&D program of MOTIE/KEIT [project No. RS-2023-00266831, Development of Novel Plasma Process for Hydrocarbon Cracking].

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POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

CFD-guided Optimization of Rotationally Driven Slurry Dispersion and Homogeneity

Taean Ko[1], Changbeom Shin[1], Hyungtae Cho[2], Jaewon Lee[1,*]

[1]Hanyang University ERICA, Korea
[2]Kyung Hee University, Korea

ABSTRACT

The uniformity and long-term stability of three-phase mixtures in multiphase reactors strongly affect downstream performance and product quality. As industrial-scale operations increasingly demand tighter control of gas–liquid–solid contacting, optimizing three-phase mixing across the reactor height has become essential, yet simulation studies remain limited because resolving interfacial dynamics and phase interactions in large turbulent systems is numerically challenging. In this study, we analyze height-wise distributions of gas holdup, solids concentration, and liquid circulation under various operating conditions to clarify the relationship between process parameters and three-phase mixing quality, and to provide guidance for process optimization. We employed CFD with an Eulerian–Eulerian multiphase framework and interphase momentum transfer/turbulence closures to simulate gas–liquid–solid interactions and quantify vertical mixing characteristics. The results enable prediction of the operating window and the time required to achieve a sufficiently uniform three-phase mixture as a function of gas flow rate, agitation intensity, and inventory. Consequently, this work bridges numerical simulation and industrial practice by linking height-dependent hydrodynamics to actionable mixing and scale-up guidelines for three-phase systems.

KEYWORDS

Battery Slurry Mixing Process, Computational Fluid Dynamics

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POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Predicting Biodegradation Time Profiles by Leveraging the Effectiveness of Molecular Physicochemical Property–Based Classification

Kairi Kato*, Kazuhiro Takeda

Shizuoka University, Japan

ABSTRACT

In biodegradability assessments, biochemical oxygen demand (BOD) time profiles are widely used as an indicator to characterize the degradation behavior of chemical substances by microorganisms. However, these tests require long experimental periods and substantial costs, making it difficult to comprehensively evaluate many compounds and thereby hindering the rapid environmental assessment of new chemicals. In this study, we developed a machine learning model to directly predict BOD time profiles based on molecular structural information. The experimentally obtained BOD curves were approximated using a Gompertz function capable of describing the temporal evolution of microbial degradation processes, and its parameters reflecting biodegradation progress and reaction kinetics were estimated from molecular descriptors. To suppress overfitting arising from the high dimensionality of descriptor space and to ensure model generalizability, an efficient feature selection method was applied to select variables according to their contributions to prediction performance. Furthermore, to account for differences in degradation mechanisms originating from molecular diversity, clustering based on co mbinations of multiple chemical indicators was introduced. By integrating feature selection with structural classification, the proposed method achieves stable predictive performance across diverse molecular groups while simultaneously improving the robustness and interpretability of the model.

KEYWORDS

Biodegradability, BOD, Machine learning, Gompertz function, Feature selection

P-48

POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Explainable AI (XAI) Analysis of Reboiler Heat Duty in a Pilot-Scale MEA CO_2 Capture Process: Identification of Loading- and Thermally-Controlled Regimes

Yinseo Song, Kiho Park*

Department of Chemical Engineering, Hanyang University, Korea

ABSTRACT

Reboiler heat duty is the dominant contributor to energy consumption in monoethanolamine (MEA)-based post-combustion CO2 capture. However, pilot-scale operations frequently exhibit significant variations in heat duty even at similar CO2 capture rates, indicating complex thermal and process interactions that conventional loading-based and steady-state models fail to explain. In this study, an explainable AI (XAI) model is developed to predict and interpret reboiler heat duty using high-resolution time-series data from a pilot-scale MEA CO2 capture plant. Reboiler heat duty was derived from steam and operational data and integrated with key process variables across the absorber, lean/rich heat exchanger, and stripper. The developed models achieve high predictive accuracy, while SHAP analysis reveals the root causes of anomalous and unexpected duty variations under similar capture performance. The results identify two distinct operational regimes: loading-controlled and thermally-controlled. In the thermally-controlled regime, stripper feed enthalpy, heat exchanger performance, and steam conditions dominate energy demand, overriding the influence of CO2 loading. This interpretable, data-driven framework enables precise diagnosis of energy inefficiencies and provides a robust foundation for digital twin development and real-time optimization of CO2 capture processes.

KEYWORDS

CO2 capture, Reboiler heat duty, Explainable AI (XAI), SHAP, pilot-scale process

ACKNOWLEDGEMENTS

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POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Process-Aware Shapley Flow Analysis for Interpretable Fault Diagnosis in Chemical Processes

Kyojin Jang[1,*], Jeongdong Kim[2]

[1] *Samsung Electronics Co., Korea*
[2] *Massachusetts Institute of Technology, USA*

ABSTRACT

Understanding complex interactions among process variables is essential for effective monitoring and diagnosis in chemical processes. While feature attribution methods such as SHAP provide insights into variable importance, they do not capture how contributions propagate through the underlying process structure. In this study, we propose a process-aware interpretation framework by integrating Shapley flow with a directed process graph for the Tennessee Eastman Process (TEP). A subset of representative variables is selected based on process knowledge and data relevance, and a directed graph is constructed to reflect physically plausible dependencies among process units. A tree-based model is trained for binary fault detection, and SHAP values are first used to identify key contributing variables. These contributions are then decomposed along the graph using Shapley flow to reveal how effects propagate across the process. The results show that while SHAP identifies important variables, Shapley flow provides additional insights into the pathways of influence, highlighting critical propagation routes under fault conditions. Comparative analysis between normal and fault scenarios demonstrates that the proposed approach captures structural changes in contribution flow, enabling enhanced process-level interpretability. This framework offers a practical and interpretable tool for analyzing complex industrial process data.

KEYWORDS

Shapley Flow, Process Interpretability, Fault Diagnosis, Graph-based Analysis

ACKNOWLEDGEMENTS

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POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Comparison of Energy Efficiency and Remixing Effects among Various Heat-Integrated Distillation Configurations

Hsin-Hui Liang[1], You-Cheng Jiang[1], Hao-Yeh Lee[1,2,*]

[1]*National Taiwan University of Science and Technology, Taiwan*
[2]*Process Net-Zero Research Center, Taiwan*

ABSTRACT

Distillation columns represent one of the energy-intensive equipment in chemical process, and improving their energy efficiency remains an important issue in process design. In this paper, various heat -integrated configurations are investigated and compare d to observe their energy efficiency and remixing effects. Advanced configurations derived from direct and indirect distillation sequences, such as multi-effect distillation (ME) and thermally coupled distillation with side-streams (TCDS), have been proposed to enhance energy utilization and reduce remixing effects. However, within the context of TCDS, previous studies have primarily focused on vapor side-stream configurations, leaving the energy-saving potential of liquid side -streams systematically unexplored. This study proposes a Hybrid Heat -Integrated Configuration with Liquid side -streams (HHIC-L), using an n -pentane/n-hexane/n-heptane separation system as a benchmark. Developed from both direct and indirect sequences, HHIC -L combines the benefits of ME heat recovery and TCDS efficiency while eliminating the operational problems of vapor streams. Simulation results show tha t the proposed HHIC-L configuration for the direct sequence reduces reboiler energy consumption by 41% and Total Annual Cost (TAC) by 28%. These findings highlight that the HHIC-L configurations offer highly substantial energy-saving potential for sustainable process intensification.

KEYWORDS

Distillation, Thermal Integration, Energy Saving, Remixing Effect

ACKNOWLEDGEMENTS

Authors gratefully acknowledged the support from National Science and Technology Council of Taiwan under grant No: NSTC 114-2637-8-011-006-

P-51

POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Design and Optimization of a Hydrogen Ventilation System Using Transient CFD Dispersion Analysis in SMR Process

Sang Won Lee, Yong Woo H wang, Young Woo Chon*

Program in Circular Economy & Environmental System, Inha University, Korea

ABSTRACT

Driven by carbon-neutral policies and the adoption of zero-carbon fuels, hydrogen demand has surged, leading to a rapid increase in hydrogen production facilities. Due to hydrogen's wide flammability limits and low minimum ignition energy (MIE), accidental leakage can escalate into explosion hazards with severe consequences. This study employs computational fluid dynamics (CFD) to predict hydrogen dispersion under leakage scenarios representative of a steam methane reforming (SMR) process and to develop an optimized ventilation strategy. The simulations were performed as time-accurate transient analyses using the RNG k–ε turbulence model coupled with a species transport model, enabling evaluation of the temporal evolution of hydrogen concentration during venting. A parametric assessment was conducted by varying the vent location and ventilation flow rate, and the resulting hydrogen concentration fields were systematically compared. The results confirm that an upper vent configuration with a ventilation rate of 80.8 m3/min maintains the hydrogen concentration below 1 vol%, remaining below the lower flammability limit (LFL).

KEYWORDS

Computational fluid dynamics (CFD), Hydrogen leak scenario, Steam methane reforming (SMR), Ventilation system

ACKNOWLEDGEMENTS

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POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Techno-Economic and Life Cycle Assessment of Hydrogen and Methanol Production from Nonwoven Polymer Waste Using CO_2-Assisted Pyrolysis

Seyeong Lee[1,2], Jaeho Baek[2], Hyungtae Cho[3], Jaewon Lee[4,*]

[1]Korea Institute of Industrial Technology, Korea
[2]Department of Chemical and Biomolecular Engineering, Yonsei University, Korea
[3]Department of Chemical Engineering, Kyung Hee University, Korea
[4]Department of Materials Science and Chemical Engineering, Hanyang University, Korea

ABSTRACT

The pandemic has sharply increased mask consumption, resulting in approximately USD 468 million of nonwoven polymer waste (NPW) in 2021, with this amount projected to double within ten years. Because high-efficiency particulate air (HEPA) filters cannot be recycled, incineration is commonly employed, leading to the emission of hazardous pollutants. This study explores CO2-assisted pyrolysis of NPW, which produces a CO yield 6.5 times higher than that of conventional N2-assisted pyrolysis. Based on the experimental findings, three process configurations were designed: waste-to-hydrogen (WtH), waste-to-methanol with multi-stage pressure swing adsorption (WtMMPSA), and waste-to-methanol with single PSA (WtMSPSA). In all cases, CO2-assisted pyrolysis served as the syngas source. The WtH process integrated natural gas steam methane reforming and water–gas shift reactions to enhance hydrogen production. For methanol synthesis, syngas purification and conditioning were achieved using PSA, with the WtMSPSA scheme simplifying separation through pre-reforming and selective CO2 removal, verified by dynamic simulation. Techno-economic and life cycle assessments demonstrated that WtMSPSA achieved the lowest LCOE (0.327–0.504 USD/kWh) and net-negative greenhouse gas emissions across grid and renewable scenarios. These results highlight CO2-assisted NPW pyrolysis as a viable and sustainable alternative to incineration.

KEYWORDS

Plastic Recycling, Nonwoven polymer waste (NPW), CO2assisted Pyrolysis, Techno-economic analysis (TEA), Life cycle assessment (LCA)

P-S1

POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Gaussian Process Surrogate Modelling with Electrode Geometry Encoding for Multi-Pollutant Electrocoagulation System using Small Datasets

Lian See Tan[1,*], Mathias Neufang[2], Antonio Del Rio Chanona[2], Nor Ain Mohd Noor Azli[1], Norhuda Abdul Manaf[1]

[1]Malaysia-Japan International Institute of Technology, Universiti Teknologi Malaysia, Kuala Lumpur, Malaysia
[2]Department of Chemical Engineering, Imperial College London, London, UK

ABSTRACT

Electrocoagulation (EC) is an electrochemical wastewater treatment process capable of simultaneously removing multiple pollutants, including chemical oxygen demand (COD), total phosphorus (TP), nitrate (NO3), and total suspended solids (TSS). Optimising EC systems through physical experimentation alone is resource-intensive, motivating the development of data-driven surrogate models. However, small datasets present a significant challenge for machine learning. This work employed Gaussian process (GP) surrogate models for an EC system using 27 observations. Electrode geometry was encoded as a continuous area-to-distance (A/d) ratio, converting a mixed categorical-continuous input space into a two-dimensional representation that improved surrogate model performance over raw categorical inputs. Two GP architectures were compared: independent single-task GP models trained per pollutant, and a joint multi-task GP employing the intrinsic coregionalisation model (ICM) kernel. The single-task GP achieved test R2 values of 0.71 (COD), 0.77 (TSS), 0.53 (NO3), and 0.26 (TP). The multi-task GP yielded 0.40 (COD), 0.57 (TSS), 0.28 (NO3), and 0.55 (TP). The ICM task covariance matrix collapsed to near-zero across all pollutant pairs, indicating that EC removal mechanisms operate as effectively independent processes. For EC systems with limited data, independent single-task GP models with feature encoding offer a practical modelling approach, providing a foundation for subsequent Bayesian optimisation of operating conditions.

KEYWORDS

Gaussian process; electrocoagulation; surrogate modelling; wastewater treatment

ACKNOWLEDGEMENTS

The authors would like to thank the Eric and Wendy Schmidt AI in Science Global Faculty Fellowship (supported by Schmidt Sciences) and Universiti Teknologi Malaysia for providing the financial support that resulted in this work.

P-S2

POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Graphical Approach for Optimal Deployment of Carbon Dioxide Removal (CDR) Methods

Yu Jian Tan[1], Xue Qin Lim[1], Dominic C. Y. Foo[1], Raymond R. Tan[2]

[1]Department of Chemical and Environmental Engineering/Centre of Excellence for Green Technologies, University of Nottingham Malaysia, Selangor, Malaysia
[2]Department of Chemical Engineering, De La Salle University, Manila, Philippines

ABSTRACT

Carbon dioxide removal (CDR) is increasingly required to complement direct emission reductions in achieving net-zero targets, particularly for sectors with unavoidable residual emissions. This study develops a graphical method based on carbon emission pinch analysis (CEPA) to plan the deployment of multiple CDR methods over time. Low-, medium-, and high-durability CDR methods are represented using characteristic time profiles and combined into a supply composite curve, which is then compared with the buyer's cumulative demand composite curve over a common planning horizon. Pinch points are then identified to evaluate supply–demand feasibility and determine the required horizontal or vertical shifting strategies. Two industrial case studies, aviation and cement, are used to demonstrate the shifting strategies from both buyer and supplier perspectives. In both cases, the supplier perspective focuses on adjusting the deployment timing of selected CDR methods. Under oversupply conditions, selected CDR methods can be delayed to avoid premature deployment and unnecessary early capital investment, while under insufficient-supply conditions, selected CDR methods can be advanced to improve supply availability and meet demand on time. In contrast, the buyer perspective evaluates procurement-side adjustments, including reducing low-durability CDR under oversupply conditions, further reducing residual emissions, purchasing immediate CDR credits, or delaying compliance when supply is insufficient. Overall, the results show that CEPA-based graphical analysis can improve the temporal alignment between CDR supply availability and buyer demand.

KEYWORDS

carbon dioxide removal; carbon emission pinch analysis; carbon dioxide removal deployment; net-zero; targeting, process integration

P-S3

POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Fuzzy-Structured Reinforcement Learning for Nonlinear Process Control under Changing Operating Conditions

Mohd Fauzi Zanil[1,2], Zainal Ahmad[2,*], Syamsul Rizal Abd Shukor[2], Agus Saptoro[3], Zulfan Adi Putra[4]

[1] *School of Engineering, Asia Pacific University of Technology and Innovation, Kuala Lumpur, Malaysia*
[2] *School of Chemical Engineering, Universiti Sains Malaysia, Penang, Malaysia*
[3] *Western Australian School of Mines, Curtin University, Kalgoorlie, WA, Australia*
[4] *Process Engineering Specialist, Exiron Baja Pratama, Bandung, Indonesia*

ABSTRACT

Nonlinear process systems operating under changing conditions present significant challenges for control design, as system dynamics vary due to disturbances, aging, and operating point shifts. Conventional controllers such as proportional–integral–derivative (PID) rely on fixed parameters and often suffer performance degradation when process characteristics change. Reinforcement learning (RL) offers a data-driven adaptive alternative; however, most RL-based controllers employ a single global policy that assumes homogeneous dynamics, limiting their ability to represent condition-dependent nonlinear behavior and causing performance deterioration during transitions. This paper addresses this limitation by introducing a fuzzy-structured reinforcement learning framework for nonlinear process control. The proposed approach integrates fuzzy membership functions within the RL architecture to partition the operating space and organize multiple local policies, which are blended to produce a smooth global control action. This structural decomposition enables improved representation of condition-dependent dynamics while avoiding abrupt switching and instability. The approach is evaluated using a nonlinear mathematical model and a laboratory-scale temperature control system. Comparative results against PID and conventional monolithic RL demonstrate up to 21% reduction in integral absolute error (IAE), 26% faster settling time, and 17% reduction in control action variation. These results confirm that fuzzy-structured RL improves adaptive control performance under changing operating conditions.

KEYWORDS

Reinforcement learning; Fuzzy systems; Nonlinear process control; Adaptive control; Temperature control; SDG 9

ACKNOWLEDGEMENTS

N/A

P-S4

POSTER

13:30~14:30 · Poster Session P1 · Engineering Building D

Forecasting-Based Dynamic Dispatch under Process Flexibility Limit Constraints for an Off-Grid Power-to-Methanol System

Mingqi Bai[1], Pengcheng Wang[1], Meng Qi[2], Yi Liu[2], Zhang Bai[1,*]

[1]College of New Energy, China University of Petroleum (East China), Qingdao, 266580, China

[2]State Key Laboratory of Chemical Safety, College of Chemistry and Chemical Engineering, China University of Petroleum (East China), Qingdao, 266580, China

ABSTRACT

Power-to-methanol is a promising pathway for coupling renewable electricity utilization with low-carbon chemical production. However, the inherent intermittency of wind and solar power conflicts with the relatively stable energy demand of chemical processes, requiring the coordinated integration of renewable power forecasting, flexible process operation, and energy-storage management. This study investigates an off-grid power-to-methanol system through an integrated framework that combines AI-driven wind–solar forecasting, process flexibility analysis, and dynamic load dispatch. A CEEMDAN–LSTM model is used for renewable power prediction, K-means++ clustering is applied to identify 12 representative wind–solar scenarios, and Aspen Plus/Aspen Plus Dynamics models are developed to evaluate the flexible operation of the methanol synthesis unit under load variations. The results show that daily forecasting achieves higher accuracy than weekly forecasting, with prediction errors of 1.23% for wind power and 3.09% for solar irradiance. Dynamic simulations indicate that flexible-load operation of the methanol synthesis unit is technically feasible, while compressor outlet temperature is the dominant limiting factor for process flexibility. A minimum load limit of 15% is identified to avoid excessive temperature excursions during low-load transitions. Furthermore, short-term dispatch results for the 12 representative typical days demonstrate that forecast–actual power mismatch is mainly absorbed by the battery system, highlighting the need to incorporate battery state-of-charge regulation into load optimization. This study provides a dynamic modeling and optimization basis for integrating renewable power forecasting with flexible chemical process operation, contributing to the development of intelligent and carbon-neutral process systems.

KEYWORDS

Power-to-methanol; Flexibility Limit; CEEMDAN–LSTM; Dynamic Simulation; Load Dispatch

P-53

POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Computational Synthesis and Techno-Economic Optimization of Intensified Cryogenic Distillation Sequences for Olefin Recovery from Diverse Chemical Recycling Feedstocks

Li-Chin Hsiao and Jeffrey Ward*

Department of Chemical Engineering, National Taiwan University, Taiwan

ABSTRACT

The global plastic waste crisis demands efficient chemical recycling technologies to recover critical monomers like ethylene and propylene. With International Energy Agency projections showing continued plastic demand growth through 2050[1], optimizing energy-intensive cryogenic distillation is essential. This study evaluates two advanced process intensification configurations—stacked side-stream sequences and dividing wall columns—applied to methanol-to-olefins (MTO) and plastic pyrolysis gas feedstocks[2, 3]. Using Aspen Plus and a Simulated Annealing algorithm coded in Python, we conducted rigorous optimization and techno-economic analyses incorporating thermodynamic considerations when operating at cryogenic temperatures and the associated refrigeration requirements. Our comprehensive economic assessment determines the most viable separation strategy for each scenario. Results demonstrate that optimal distillation design is product-specific: for ethylene separation (MTO case), stacked distillation proves optimal due to minimal remixing effects; for the more challenging propylene separation, stacked side-stream sequences consistently outperform across both feedstocks, surpassing dividing wall columns. The findings highlight the significant impact of operating temperature on refrigeration power requirements and overall economics, providing clear guidance for designing sustainable olefin recovery systems and contributing to the circular economy framework for petrochemical production with reduced environmental impact and enhanced resource utilization efficiency across diverse chemical recycling pathways[4].

KEYWORDS

Process intensification; Dividing wall column; Olefin recovery; Chemical recycling; Techno-economic optimization

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Exergy, economic and life cycle assessment of novel cogeneration systems based on chemical heat pumps

Xijun Wang[1,2], Xiaomeng Jiang[1,2], Xingrui Lan[1,2], Shuguang Xiang[1,2,*], Xiaoyan Sun[1,2], **Lili Wang**[1,2,*], Li Xia[1,2], Shaohui Tao[1,2]

[1] *College of Chemical Engineering, Qingdao University of Science and Technology, China*
[2] *Shandong Key Laboratory of Chemical Process Simulation and Optimization Industrial Software, China*

ABSTRACT

The subjects of Process Systems Engineering (PSE) are Carbon Neutrality As global energy and environmental pressures increase, the recovery of industrial low-temperature waste heat (LTWH) has become increasingly important. This study develops four novel cogeneration systems based on chemical heat pumps to simultaneously provide thermal energy and electricity from LTWH. Through system optimization, the internal cogeneration system (NORC-IAH) identified the optimal configuration, NORC-IAH1, which effectively converts LTWH, generating 5.94×105 kWh of electricity and 3.21×106 kWh of high-temperature heat annually. Thermodynamic, economic, and environmental assessments were conducted for NORC-IAH1. Exergy analysis shows the highest exergy loss in the distillation column T1, at 599.85 kW, and the lowest exergy efficiencies for pump P1 and T1, at 37.25% and 41.93%, respectively. Economic analysis reveals a total annual cost of $321,641.8 y-1, with T1 and heat exchanger H1 contributing the most, indicating potential improvements in heat transfer efficiency. Life cycle assessment highlights the carcinogenic risk from sulfidic tailings during stainless steel construction stage, with emissions of 19,861.2 kg 1,4-DCB equivalent. This study provides a foundation for industrial waste heat recovery and environmental sustainability.

KEYWORDS

Cogeneration systems; Chemical heat pumps; Exergy analysis; Economic analysis; Life Cycle Assessment

ACKNOWLEDGEMENTS

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Assessing Feasibility and Consistency in AI-Generated Process Flowsheets

Margareth[1,2] and Ung Lee[1,2,3,*]

[1]Clean Energy Research Center, Korea Institute of Science and Technology, Korea
[2]Division of Energy and Environmental Technology, University of Science and Technology (UST), Korea
[3]Department of Chemical and Biological Engineering, Korea University, Korea

ABSTRACT

Recent advances in large language models (LLMs) suggest their potential for generating chemical process flowsheets from structured design specifications. Realizing this potential in practice requires that generated designs satisfy fundamental engineering constraints, motivating systematic approaches for assessing feasibility and consistency. This work investigates the feasibility and consistency of AI-generated process flowsheets through a structured assessment framework. Multiple flowsheets are generated and translated into formal representations of unit operations and stream variables, enabling systematic evaluation of mass balance closure, streams continuity, unit operation validity, and specification completeness. The analysis identifies recurring patterns of inconsistency, including missing specifications, invalid unit connections, and discontinuities in process conditions. Based on these observations, targeted correction strategies are introduced to resolve common inconsistencies without additional LLM calls. By coupling generative models with a constraint-based assessment layer, the proposed approach supports more reliable use of AI in early-stage process design. This study provides a practical pathway for integrating LLM-generated designs with established engineering workflows.

KEYWORDS

Chemical Process Design, Large Language Model, Process Evaluation, Flowsheet Generation

P-57

POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

GraphSAGE-Based Surrogate Modeling and Optimization of Heating Parameters for Ceramic Firing Process

Minori Noda, Shota Kato, and Manabu Kano*

Department of Informatics, Kyoto University, Japan

ABSTRACT

In ceramic manufacturing, the firing process accounts for about 60% of total CO 2 emissions. Reducing emissions requires redesigning firing conditions; however, optimal design relies on accurate simulation of the internal temperature distribution of the product. Since direct measurement under high-temperature conditions is infeasible, the process is typically modeled using the finite element method (FEM) . Although FEM provides accurate results, its high computational cost limits its use in iterative optimization. In this study, we developed a surrogate model based on Graph Sample and Aggregated Embeddings (GraphSAGE) to predict temperature in a cylindrical ceramic product . We conducted FEM simulations under 83 firing conditions to generate training and test data. For the test data, the root mean squared error (RMSE) was 0.987 K with a coefficient of determination of 1.00. Using the trained model, we solved an optimization problem based on Powell's method to minimize heating time subject to a maximum temperature difference constraint of 50 K. The optimal solution was verified by FEM and satisfied the constraint. The proposed approach required about 3 minutes, whereas optimization based on FEM was estimated to require approximately 140 hours. These results demonstrate that the proposed method enables accurate and computationally efficient optimization of firing conditions.

KEYWORDS

Graph Neural Network, surrogate model, finite element method, optimization, ceramic manufacturing

ACKNOWLEDGEMENTS

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Chemical Reaction Pathway Synthesis to Recover Value Added Chemicals from Crude Bio-Oil

Yen Qin Lee[1], Xiao Syuen Lim[2], and **Nishanth Chemmangattuvalappil**[2,*]

[1]*Department of Chemical & Environmental Engineering, University of Nottingham Malaysia, Malaysia*
[2]*School of Engineering, Sunway University, Malaysia*

ABSTRACT

Bio-oil produced from hydrothermal liquefaction (HTL) is a complex mixture of several organic components. The organic layer contains significant quantities of phenol and various phenolic derivatives. If these phenolic derivatives can be converted to phenol, the recovery process will be simpler, and the resulting product will have higher value. In this work, computer-aided molecular design (CAMD) tools have been developed to identify reactants capable of converting phenolic derivatives into phenol, along with possible reaction pathways and the conditions that favour this conversion. The structures of chemical compounds that can convert phenolic derivatives into phenol in a thermodynamically feasible manner have been estimated using CAMD tools. Since the identity of reactant and byproducts are unknown at the beginning, the molecular groups that constitute the reactants and products are introduced into a mathematical programming framework in the form of variables that needs to be estimated. Process conditions to obtain the optimal conversion have also been identified. The output from the programme is a collection of molecular groups that constitute reactants and byproducts formed in the thermodynamically feasible reactions. The developed algorithm can be used as a screening tool before performing experimental verification on the potential pathways. .

KEYWORDS

Chemical reaction pathways, computer aided molecular design, solvent design, thermodynamic feasibility studies

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Large Language Model Assisted Workflow Automation for Distillation Process Simulation and Optimization

Po-Chia Chiu, Yu-Sheng Chen, Hao-Yeh Lee, Yan-Ling Yang*

Department of Chemical Engineering, National Taiwan University of Science and Technology, Taiwan

ABSTRACT

An interactive decision-support framework utilizing Python-based automation via the COM interface to interact with Aspen Plus is proposed. By integrating rule-based logic and domain knowledge-based strategies, the system develops specialized Modular Components (MCPs) and skills. This dual-layered structure enables a Large Language Model (LLM) to function as an intelligent co-pilot, translating engineering goals into executable sequences within a human-in-the-loop (HITL) workflow, validated through methanol and isopropyl alcohol (IPA) dehydration cases involving non-ideal behaviors. Results show the LLM-assisted system successfully achieves product purities above 99.9% for methanol and 99.7 wt% for IPA. These outcomes demonstrate the potential of LLM-driven automation to enhance the success rate of process synthesis and optimization, offering a powerful tool for digital transformation in the chemical industry.

KEYWORDS

Large language models, Aspen Plus, COM interface, Human-in-the-loop, Process workflow automation, Process optimization

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

An exploratory attempt on integrating anaerobic digestion fundamentals with machine learning concepts in Indian and European Chemical Engineering Academic Classrooms

Pragya Singh[1], Sara Marchini[2], Asad H. Sahir[1], Markus Schubert[2]

[1]Indian Institute of Technology Ropar, India
[2]Technische Universität Dresden, Germany

ABSTRACT

Chemical Engineering Education needs to respond to current major transitions in process industries owing to digitalization and a shift towards sustainable energy sources. There is a great need to integrate data-driven modelling tools in addressing achievement of sustainable development goals since complex, variable, and uncertain process conditions demand adaptive , data informed optimization beyond traditional models. Within this context, the authors recognize the need to enrich students' ability to apply machine learning (ML) in real process systems scenarios particularly addressing sustainability. Following the 2024 Digital Green Talents Award conferred by the German Federal Ministry of Education and Research (BMBF) to the principal author (PS), this work was advanced through participation in the ERASMUS+ InnoLAB (Innovative Learning Across Borders) framework. Within this framework, a case study-based chemical engineering education module was designed to integrate anaerobic digestion fundamentals with ML modelling of biogas systems. The module focused on predicting CO2 content using correlation analysis and Random Forest regression. The delivery of the education module was explored during classroom interactions at IIT Ropar (India) and TU Dresden (Germany). A mixed-method pre-post academic evaluation conducted with 40 international participants revealed improved understanding of regression modelling and increased confidence in ML-based process analysis.

KEYWORDS

Bioenergy, Digitalization, Engineering Education research, Sustainability

P-61

POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Decarbonizing Fluid Catalytic Cracking via Multi-Objective Optimization of a Plant-Calibrated Kinetic Riser Model

Priyam Nayak*, Sanjay Mahajani and Kannan Moudgalya

Department of Chemical Engineering, Indian Institute of Technology Bombay, India

ABSTRACT

Fluid catalytic cracking (FCC) units present a critical challenge in modern refineries by simultaneously governing petrochemical production and contributing significantly to CO2 emissions through coke combustion. This work develops a unified and industrially grounded framework that integrates detailed kinetic modeling, plant-data-driven parameter estimation, and multi-objective optimization for sustainable FCC operation. A novel twelve-lump kinetic scheme is proposed with explicit representation of gasoline sub-fractions and light olefins (propylene and butenes), enabling improved resolution of product selectivity compared to conventional lumped models. The kinetic parameters are estimated using industrial plant data, ensuring direct relevance to real operating conditions. The calibrated model is coupled with an NSGA-II-based optimization framework to systematically quantify trade-offs between competing objectives. Two multi-objective optimization problems are formulated: (i) maximizing economic benefits while minimizing CO2 emissions, and (ii) maximizing propylene production while minimizing CO2 emissions to reflect petrochemical-oriented refinery operation. The resulting Pareto fronts reveal strong nonlinear trade-offs; in particular, increasing propylene yield from 13,000 to 42,000 kg/h results in CO2 emissions rising from 47,000 to 57,500 kg/h. A well-defined knee region is identified, providing optimal operating conditions with maximum marginal gains. The proposed framework establishes a rigorous pathway for decarbonizing FCC units while enabling flexible transition toward petrochemical-centric refinery operation.

KEYWORDS

Fluid catalytic cracking (FCC) , Multi-objective optimization , NSGA-II, Kinetic modeling , CO2 emissions, Propylene production , Decarbonization , Refinery optimization

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Machine Learning Surrogate with Cascade Architecture for Wax Hydro-Cracking and -Isomerization

Pyeong-Gon Jung and Joonjae Ryu*

Department of Chemical Engineering, University of Seoul, Korea

ABSTRACT

Hydro-cracking and -isomerization (HDK-ISO) of Fischer-Tropsch wax are critical steps in producing high-quality lubricant base oils and middle distillates. Although Aspen Plus rigorously simulates these processes, its high computational cost limits its use in optimization and real-time control. This study presents a machine learning surrogate model that replicates carbon-number product distributions predicted by Aspen Plus with significantly reduced computation time. The proposed surrogate adopts a mechanistically decomposed forward cascade architecture comprising three gradient boosting models. First, an isomerization conversion model predicts the normal-to-isomer conversion for each carbon number. Second, a regime classifier categorizes operating conditions as either severe or mild cracking based on feed properties and process variables. For severe conditions, a sigmoid cracking model predicts two shape parameters (the inflection point n50 and steepness log k) that define the carbon-number-dependent cracking conversion profile. Product fragments are distributed downstream using the Gambaro stoichiometric scheme. A key contribution is the introduction of feed-range filtering prior to sigmoid fitting, which eliminates low-signal artifacts and substantially improves prediction accuracy for distillate-type feeds. Five-fold cross-validation yields R2 = 0.998 for isomerization, 98.8% classification accuracy, and R2 = 0.994/0.935 for n50 and log k, respectively, demonstrating reliable interpolation across diverse operating conditions.

KEYWORDS

Surrogate model, Hydroisomerization, Hydrocracking, Gradient boosting, Forward cascade, Fischer-Tropsch wax

ACKNOWLEDGEMENTS

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Advanced Control of Cracking Furnaces in Ethylene Plants Based on Soft Sensing Technology

Qun Wu[1], Yaoming Wu[2], and Wenli Du[1,*]

[1]*East China University of Science and Technology, China*
[2]*Sinochem Quanzhou Petrochemical Co., China*

ABSTRACT

The cracking furnace is the core equipment of the ethylene unit, with cracking depth serving as a critical quality indicator that determines product distribution and economic efficiency. This paper designs an advanced control scheme for cracking depth and conducts industrial validation. First, historical industrial data (feedstock load, temperature, cracked gas composition, etc.) were collected and preprocessed through steps such as outlier removal, smoothing, and shifting to train a soft-sensing model for predicting cracking depth. Then, cracking depth was used as the quality indicator to control the Cracking Furnace Outlet Temperature (COT). Simultaneously, real-time industrial data were utilized to perform online correction of the cracking depth model, ensuring model accuracy and thereby guaranteeing control effectiveness. Finally, the proposed method was implemented through configuration in the DCS system of the enterprise's ethylene unit. The results show that fluctuations in cracking depth were significantly reduced after the deployment of the advanced control algorithm, indirectly generating economic benefits of 7 million RMB for the ethylene facility with an annual capacity of 1 million tons.

KEYWORDS

Advanced control, Soft-sensing model, Cracking furnace, COT

ACKNOWLEDGEMENTS

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Multi-Objective Optimization and Integrated Process Intensification for Sustainable and Low-Carbon Methyl Propionate Production

Ronghua Liang, Ruru Ma, Chunfa Miao, Peizhe Cui, Xin Li, Yinglong Wang*

College of Chemical Engineering, Qingdao University of Science and Technology, Qingdao, China

ABSTRACT

In this study, a new process was proposed that combines reactive-extractive distillation, pervaporation, and heat integration. This process addresses the complex azeotropic system and high energy consumption in methyl propionate preparation. Glycerol was selected as the optimal extractant after analysis of biological toxicity, relative volatility, and σ-profile. Based on these results, a process flow was designed, and NSGA-II was used for multi-objective optimization. The three-column reactive-extractive distillation was determined as the best structure. It reduced total annual cost and gas emissions by 66.35 % and 62.23 %, respectively, compared to the five-column process. Additionally, the pervaporation membrane replaced the high-energy recovery column, and a heat integration scheme was designed. The final process combined heat integration and pervaporation. Compared to the initial five-tower process, it reduced annual total cost by 81.57 %, gas emission by 83.65 %, and total energy consumption by 81.20 %. This study provides a feasible technical solution for green, efficient methyl propionate production, and sets an example of “screening-optimization-integration” process intensification for complex systems.

KEYWORDS

Reactive-extractive distillation; Pervaporation; Intensification strategy; Comprehensive performance analysis

ACKNOWLEDGEMENTS

N/A

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Reliability-Aware Plastic Waste-to-Hydrogen Supply Chain Optimisation Considering Spatial Heterogeneity

Selena Kian Yii Song[1], Jean Pimentel[2], Ákos Orosz[3], Viknesh Andiappan[1], Ferenc Friedler[2], Bing Shen How[1,*]

[1]Faculty of Engineering, Swinburne University of Technology, Malaysia
[2]Department of Systems Science, Széchenyi István University, Hungary
[3]Department of Computer Science and Systems Technology, University of Pannonia, Hungary

ABSTRACT

There is a growing interest in seeking alternative hydrogen production pathways to meet rising demand. Recently, plastic waste-to-hydrogen has emerged as a promising option. Existing studies have sought to optimise its supply chain design, but they typically rely on fixed process parameters (e.g., a pre-fixed feedstock-to-product conversion ratio) while neglecting the impact of spatial heterogeneity of the plastic waste feedstock on the optimality of supply chain design. Note that incorporating this variability is essential to ensure that proposed solutions remain robust and applicable under dynamic real-world conditions. This study, therefore, addresses this gap by developing a hybrid optimisation framework that integrates a random forest regression model to predict hydrogen yield and purity as a function of the elemental composition of the plastic waste feedstock (carbon, hydrogen, nitrogen, oxygen, and sulphur content). To ensure long-term feasibility, the framework determines the optimal plastic waste allocation and site selection through the simultaneous consideration of economic performance and supply chain reliability, where location-specific hazard risks are considered. The effectiveness of the model is demonstrated through an illustrative case study in Selangor, Malaysia.

KEYWORDS

Uncertainty management, waste valorisation, circular economy, turquoise hydrogen

ACKNOWLEDGEMENTS

The authors would like to acknowledge the financial support from Swinburne University of Technology Sarawak Campus in the form of a student scholarship.

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Spray-reliquefaction using subcooled LH2 tanks in import hydrogen terminals

S. W. Park, C. J. Lee*

Department of Chemical Engineering, Chung-Ang University, Korea

ABSTRACT

BOG generation increases with liquid level due to the larger heat transfer area, while pressure sensitivity is higher at low liquid levels because of the larger vapor space. Application of subcooled LH2 spray effectively suppresses BOG accumulation and maintains tank pressure within allowable limits when the spray flow rate exceeds the BOG generation rate. Compared with conventional compressor-based BOG management systems, the proposed method significantly improves energy efficiency by eliminating gas compression and refrigeration. The results demonstrate that spray-reliquefaction using subcooled LH2 tanks provides a simple and energy-efficient solution for BOG control in LH2 import terminals.

KEYWORDS

BOG, Pressurizing, Subcooled tank, Import hydrogen terminals, Integrated process

ACKNOWLEDGEMENTS

This work is supported by the Korea Agency for Infrastructure Technology Advancement (KAIA) grant funded by the Ministry of Land, Infrastructure and Transport (Grant RS-2022-00155807).

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Photothermal Membrane Distillation: Theoretical Analysis of Photothermal Layer Placement Effects in DCMD and SGMD

Sunyoung Oh, Boram Gu*

School of Chemical Engineering, Chonnam National University, Korea

ABSTRACT

The intensifying water-energy-environment (WEE) nexus has heightened the demand for efficient solar-driven strategies for clean water production. Photothermal enhancement converts absorbed solar energy into localized interfacial heating, strengthening evaporation and promoting thermally induced vapor pressure gradients that drive mass transport. This approach enables effective utilization of solar energy through heat-driven processes. Operation under liquid phase conditions, however, remains limited by catalyst instability, ionic interference, and bubble-induced transport resistance, which disrupt thermal driving force stability and reduce system performance. Membrane distillation (MD) mitigates these limitations by selectively delivering salt-free vapor and sustaining a stable vapor pressure gradient across the membrane. This study presents a numerical analysis of thermal driving force formation in direct contact membrane distillation (DCMD) and sweep gas membrane distillation (SGMD) with photothermal layer placement on the feed and permeate sides. The two configurations differ in permeate side phase conditions, leading to distinct thermal resistance structures and driving force development. Photothermal layer location regulates vapor pressure formation at the evaporation interface and internal temperature distribution, resulting in configuration-dependent driving force behavior. The present mechanistic analysis establishes quantitative design principles for optimizing configuration and coating placement in solar-driven photothermal MD systems.

KEYWORDS

Membrane distillation, Photothermal evaporation, Photothermal membrane distillation, Desalination

ACKNOWLEDGEMENTS

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P-68 **POSTER**
13:30~14:30 · Poster Session P2 · Engineering Building D

Development of a Real-time Detection and Suppression Method for Sequential Alarms in Plant Operations

Saki Inoue, Masaru Noda*

Department of Chemical Engineering, Fukuoka University, Japan

ABSTRACT

Advances in plant monitoring systems within the chemical industry have significantly increased the volume of alarms managed per operator. However, many industrial sites have yet to adequately evaluate the necessity and scope of alarm management, leading to a proliferation of nuisance alarms. These alarms often fail to provide novel diagnostic information while increasing the operator's verification workload, which may lead to the oversight of critical alarms and potential industrial accidents. Consequently, reducing nuisance alarms is essential for enhancing operational safety. This study focuses on developing a real-time suppression method for sequential alarms, a specific type of nuisance alarm. Conventional methods primarily rely on databases constructed from historical data, which limits their ability to handle previously unknown sequential alarms. To address this limitation, we propose an improved detection and suppression methodology by integrating and refining existing dot matrix analysis (Wang et al., 2015) and redundancy analysis (Butters et al., 2015). The proposed method predicts the occurrence of unknown sequential alarms from real-time data and dynamically updates the database. Preliminary results suggest that this approach effectively identifies unknown sequential alarms that were difficult to extract using conventional dot matrix analysis alone. This research is expected to provide an integrated framework for various alarm analysis methods, facilitating the identification of sequential alarms and advancing future alarm suppression techniques.

KEYWORDS

Logical Processing; Sequential Alarm; Dot matrix Analysis; Redundancy Analysis; Plant Operation Data

ACKNOWLEDGEMENTS

This work was supported by JSPS KAKENHI Grant Number 23K04491.

P-69

POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Exploration of flexible syngas production pathways via superstructure-based optimization of chemical looping process

Sang-Hyeok Jeon and Joonjae Ryu*

Department of Chemical Engineering, University of Seoul, Korea

ABSTRACT

By facilitating the inherent separation of H2O and CO2 from combustion exhausts, chemical looping reforming (CLR) offers a highly efficient and economical approach to carbon capture. The composition of the final product in such systems is strongly governed by the redox pathways of the oxygen carrier (OC), making them essential variables in process design. Despite their importance, previous research has largely been confined to a narrow range of predetermined reaction routes. To address this limitation, we present a novel superstructure-based optimization model utilizing Fe2O3 as the OC. This approach concurrently evaluates operating temperatures, reactant selection, and all possible oxidation and reduction stages. By systematically analyzing various combinations of these parameters, our framework successfully derives both primary and alternative reaction pathways tailored to different syngas compositions. The results confirm that the proposed methodology serves as a highly adaptable platform for designing syngas production processes with flexible compositions.

KEYWORDS

Chemical looping, Superstructure, Global optimization, Syngas

ACKNOWLEDGEMENTS

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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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Life Cycle Assessment-based Optimization of Amine Blends for Blue Hydrogen Production via Carbon Capture from Steam Methane Reforming Flue Gas

Seungjun Choi[1], Yoonjae Lee[1], Gayoung Lee[1], Shinhyeon Kim[1], Hyunshik Yoon[2], Jaebong Kim[2], Jeehoon Han[1,*]

[1]*Department of Chemical Engineering, Pohang University of Science and Technology, Korea*
[2]*ENIS INC, Korea*

ABSTRACT

While blue hydrogen serves as a vital bridge to a carbon-neutral economy, its environmental viability depends on the efficiency of carbon capture unit integrated with steam methane reforming (SMR). This study proposes a CO2 absorption framework employing a synergistic blend of methyldiethanolamine (MDEA) and piperazine (PZ) to overcome the performance limits of conventional single-amine systems. Utilizing actual industrial SMR flue gas data, we developed a rate-based model in Aspen Plus. Life cycle assessment (LCA) was subsequently conducted to evaluate the overall environmental performance, incorporating energy-intensive regeneration, direct emissions from uncaptured CO2, and the environmental burdens with wastewater treatment and solvent consumption. Our analysis identifies an optimal MDEA/PZ mixing ratio that achieves a 90% capture rate while minimizing the carbon footprint. These results provide a comprehensive guideline for the deployment of environmentally sustainable and energy-efficient blue hydrogen infrastructure.

KEYWORDS

Carbon Capture, Blue Hydrogen, Process Simulation, Life Cycle Assessment

ACKNOWLEDGEMENTS

This work was supported in part by the National Research Foundation of Korea (NRF) grants funded by the Korea government (MSIT) (RS-2025-23323940, RS-2026-25480561).

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Integrated design of ammonia-based solid oxide fuel cell system preventing nickel nitride degradation

Je-Woo Shim, Dong-Kyoung Shin, Chul-Jin Lee*

Department of Chemical Engineering, Chung-Ang University, Korea

ABSTRACT

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.

KEYWORDS

Hydrogen, Ammonia, Solid oxide fuel cell (SOFC), Nitridation prevention, Gas separation process, Power generation

ACKNOWLEDGEMENTS

This work was supported by the Korea Institute of Energy Technology Evaluation and Planning(KETEP) and the Ministry of Climate, Energy & Environment(MCEE) of the Republic of Korea (No. RS-2025-02653278).

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Neural Network-Based Design of Low-Temperature Selective Catalytic Reduction Catalysts for NOx After-Treatment

Shinjae Kim and Yeonsoo Kim*

Department of Chemical Engineering, Kwangwoon University, Korea

ABSTRACT

Zeolite-based catalysts for the selective catalytic reduction (SCR) of nitrogen oxides (NOx) can deactivate after hydrothermal aging, and predicting post-aging durability remains challenging. We developed a neural network (NN) model to predict NOx conversion under aging conditions. We used a publicly available dataset of 4,289 records compiled from 83 publications. The dataset includes catalyst composition, synthesis and processing details, zeolite type, and reaction and aging conditions. After removing physically impossible NOx conversions that were below zero or above one hundred percent, 4,172 records remained. To focus on hydrothermally aged performance, we selected 1,419 records in which aging temperature, aging time, and H2O fraction were all above zero. The data were split into training and test sets at an 80–20 ratio, and stratified splitting was applied to mitigate distributional bias between the splits. After hyperparameter optimization, the final model achieved test performance with R2 above 0.90. This model enables rapid assessment of durability across diverse aging conditions and supports the design of robust SCR catalysts for low-temperature NOx after-treatment.

KEYWORDS

Selective catalytic reduction, Hydrothermal aging, Zeolite catalyst, Neural Network, NOx conversion

ACKNOWLEDGEMENTS

This work is supported by the Specialized Graduate School Program in the (field of support) funded by the Government of the Republic of Korea (Ministry of Climate, Energy and Environment) and administered by the Korea Environment Corporation.

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Evaluating Circular Economy and Policy Pathways for a Sustainable Transition in the Indian PET Sector

Shubham Sonkusare, Yogendra Shastri*

Department of Chemical Engineering, Indian Institute of Technology Bombay, India

ABSTRACT

Growing environmental and regulatory pressure on plastic waste management is accelerating the transition of the PET (polyethylene terephthalate) sector toward more sustainable alternatives such as recycled PET (rPET), bio-based PET (bPET), and PLA. This study develops an integrated system dynamics model to examine long-term transition pathways in the Indian PET sector over 2021–2045. The model captures material flows, market competition among options, and the effects of circular economy (CE) interventions, as well as Extended Producer Responsibility (EPR) and carbon credit (CC) policies. A multinomial LOGIT framework is used to allocate market share. Results indicate that under business-as-usual conditions, vPET remains the dominant with 70% market share, while rPET penetration is limited to 28%. In contrast, aggressive CE reduces the vPET market share from 60% to 30% by 2045, while cumulative GHG emissions decrease by 5.8%. A 50% collection rate, phased EPR CC implementation, and moderate reuse provide the most robust pathway toward an rPET-led system. This improves landfill diversion by about 73% and yields cumulative savings of nearly 2 billion USD by 2045. The findings highlight the importance of strengthening recycling infrastructure and well-calibrated policy support to achieve a sustainable, economically balanced transition to a PET sector.

KEYWORDS

PET, circular economy, recycling, EPR, carbon credits, system dynamics

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Multi-period co-optimization of vertical thermosyphon reboilers for seasonal operation in amine-based carbon capture

Shuhao Zhang[1], Zekun Yang[2]

[1]*School of civil Engineering, Chongqing University, China*
[2]*Department of Chemical Engineering, University of Manchester, UK*

ABSTRACT

In amine-based Post-Combustion Carbon Capture (PCC) systems, the stripping process is highly energy-intensive, with the reboiler acting as the primary energy-consuming component. Consequently, optimizing reboiler design and operation is essential for reducing the overall energy penalty and cost of carbon capture. Among various types, Vertical Thermosyphon Reboilers (VTRs) are widely applied in the petrochemical industry because of low fouling tendency and investment cost. However, a major challenge in practical PCC applications is the significant fluctuation of upstream flue gas loads caused by seasonal variations, which directly affects the reboiler's heat duty requirements. Building upon previous research that developed an automated optimization design model for VTRs, this study proposes a multi-period co-optimization framework tailored for seasonal operation. A high-fidelity mathematical model of the VTR is established, incorporating complex hydraulics and thermodynamics. By employing a Mixed-Integer Nonlinear Programming (MINLP) approach, the model considers multiple seasonal operating scenarios as simultaneous constraints. In this framework, varying flue gas feed rates are translated into different heat duty targets that the reboiler must satisfy across all periods. The optimization model, implemented using the SCIP solver in GAMS, simultaneously determines the optimal geometric variables to satisfy the full spectrum of seasonal heat duty targets. The results indicate that this multi-period design approach provides a more robust equipment configuration compared to conventional single-period designs. By accounting for fluctuating operational demands, the proposed method ensures stable performance and improves the overall economic efficiency of the carbon capture process throughout its life cycle. This research provides a theoretical basis and practical design guidelines for enhancing energy efficiency in carbon capture systems under variable seasonal conditions.

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Process Design for Fuel-Grade DME production from Biomass

Songho Lee, Junyoung Park, Dongho Choi and Hyungtae Cho*

Department of Chemical Engineering, Kyung Hee University, Korea

ABSTRACT

Dimethyl ether (DME) has gained attention as a low-carbon fuel due to its fuel properties comparable to liquefied petroleum gas (LPG). However, the global warming potential of DME strongly depends on the feedstock used and the production pathways. It is noteworthy that waste-derived biogas routes (e.g., landfill gas) can markedly reduce greenhouse gas emissions relative to fossil natural-gas pathways. In this work, three biomass-to-DME configurations were developed. Among the unit operations, syngas generation is a key step. Accordingly, the three processes are distinguished primarily by their syngas production routes: (1) biogas upgrading and reforming, (2) catalytic pyrolysis of biomass, (3) a hybrid integration of routes ((1) and (2)). These syngas production configurations are coupled with reverse water-gas shift (RWGS) or low-temperature water-gas shift (LTS) to achieve the stoichiometry requirement for DME synthesis (M = (H2-CO2)/(CO+CO2) ≈ 2.05), followed by DME synthesis. We then performed a comparative techno-economic analysis (TEA) across the three Bio-DME pathways. Based on the best-performing pathway, techno-economic scale sensitivity determined the optimal production capacity for the process, validating the feasibility of modular implementation. Conclusively, this research provides a strategic blueprint for robust waste-derived fuel production, contributing to industrial sustainability and the realization of a circular economy.

KEYWORDS

Renewable DME; Biogas; Biomass Pyrolysis; Syngas Conditioning; Techno-Economic Analysis; Modular Implementation

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Enumeration of Multiperiod Heat Recovery Networks with Integrated Sensible Heat Storage for Energy Intensive Industrial Symbiosis

Tiffany Jia Ning Ang[1], Jean Pimentel[2], Ákos Orosz[3], Ferenc Friedler[2], Viknesh Andiappan[1], Bing Shen How[1,*]

[1]*Faculty of Engineering, Swinburne University of Technology, Malaysia*
[2]*Department of Systems Science, Széchenyi István University, Hungary*
[3]*Department of Computer Science and Systems Technology, University of Pannonia, Hungary*

ABSTRACT

Energy-intensive industries contribute substantially to greenhouse gas emissions. To address this issue, industrial symbiosis schemes have gained significant attention for minimising energy use across multiple facilities through thermal energy storage (TES). Nevertheless, a systematic approach to selecting the optimal TES configuration and integrating it into the heat exchanger network (HEN) design for multi-period operations remains underexplored. Accordingly, this work develops a sequential approach for synthesising feasible multiperiod HEN configurations for industrial symbiosis with consideration of sensible heat storage (SHS). In the first stage, the heat cascade model is applied to determine the optimal capacity flow rate (CP) of a two-tank heat storage system by minimising utility and storage costs. In the second stage, P-HENS, a graph-theoretical-based software for HEN synthesis, is used to generate a list of feasible multiperiod HENs that maximise energy recovery. The resulting HENs are ranked by total annualised cost (TAC), which includes utility, heat exchanger, and storage costs. A case study involving a steel mill and a cement plant, considering three SHS options, is conducted to demonstrate the effectiveness of the proposed method. The generation of alternative HENs enables decision-makers to select a preferred solution by considering practical aspects rather than focusing only on economic criteria.

KEYWORDS

Interplant heat integration, Flexible heat exchanger network, Waste heat utilisation, near best, eco-industrial park

ACKNOWLEDGEMENTS

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Large Language Model Assisted Automation for Reactor Process Simulation, Synthesis, and Optimization

Ting-Yen Chiang, Yu-Sheng Chen, Hao-Yeh Lee, Yan-Ling Yang*

Department of Chemical Engineering, National Taiwan University of Science and Technology, Taiwan

ABSTRACT

Chemical process simulation often requires extensive manual interaction, creating bottlenecks in iterative design workflows and relying heavily on operator expertise. This study presents an automated framework for Aspen Plus process simulation using a large language model (LLM) integrated with the Model Context Protocol (MCP). The framework employs a structured six-phase workflow supported by more than 60 MCP tools with verified COM node paths and validated parameter constraints. To address COM API limitations in reaction set creation, a practical workaround using backup file text manipulation is implemented, supporting multiple reaction types with proper unit conversion handling. The framework also incorporates a process engineering knowledge base and safety guards to prevent erroneous operations. Validation through case studies covering representative unit operations — including stream mixing, heating, flash separation, distillation, and a continuous stirred-tank reactor with power-law kinetics — confirms correct functionality across all workflow phases. The results indicate strong potential for workflow acceleration, engineering decision support, and AI-assisted process design applications in chemical engineering practice.

KEYWORDS

Large language model, Process simulation automation, Aspen Plus, Model Context Protocol, Reactor process design, Engineering decision support

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Catalyst Performance Prediction Using LLM-Based Feature Selection

Takahiro Sakashita, Shota Kato, and Manabu Kano*

Kyoto University, Japan

ABSTRACT

The development of high-performance catalysts requires efficient discovery and optimization, but these processes are often hindered by high cost of experiments and limited availability of experimental data. Catalyst performance prediction typically involves high-dimensional descriptors derived from material composition, structure, and operating conditions, while the amount of available data remains small. Under such circumstances, constructing predictive models that are both accurate and interpretable is a critical challenge. Feature selection plays an important role in addressing this issue by reducing model complexity and improving generalization performance. However, while data-driven feature selection methods are widely used, systematically integrating accumulated domain knowledge from electrochemistry and catalysis science remains a challenging task. In this study, we propose a feature selection framework based on large language models (LLMs) to incorporate domain knowledge into the modeling process. The LLMs are utilized to evaluate the relevance and physical plausibility of candidate features, which enables informed selection of descriptors prior to model training. We applied the proposed method to the prediction of catalyst performance and compared its performance with conventional feature selection techniques. The results demonstrated that the LLM-based feature selection can improve prediction accuracy under limited data conditions.

KEYWORDS

Catalyst design, Feature selection, Knowledge-guided modeling, Large language models, Data-scarce systems (Font: Times New Roman, 12pt, Italic)

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Estimation and Attribution Analysis of Alzheimer's Disease Progression Indicators Based on MRI Images Using Deep Learning

Takumi Sekiya, and Keigo Matsuda*

Nagoya University, Japan

ABSTRACT

Alzheimer's disease (AD) is a progressive disorder where early detection is crucial due to the difficulty of recovery. While MRI-based atrophy assessment is standard, identifying subtle early changes remains challenging. Existing machine learning studies predominantly focus on classification, lacking exploration into the regression of continuous progression indicators and medical interpretation. This study proposes a framework to regressively estimate multiple AD progression indicators. The framework incorporates hierarchical input refinement and attribution analysis using 3D Grad-CAM to identify key regions and verify their medical validity. A 3D CNN with skip connections was developed. Using MRI images processed with region extraction and spatial normalization, the model estimates cognitive scores (MMSE, HDSR) and atrophy. After training on whole -brain images, regional importance was quantified using 3D Grad-CAM. Input regions were hierarchically narrowed to important areas for re-training. The model was evaluated using five -fold cross-validation, and the mean and standard deviation of the coefficient of determination were calculated. Results identified the superior frontal gyrus, hippocampal CA1, and hippocampal tail as critical regions. These regions are medically associated with cognitive function and atrophy, consistent with established medical knowledge.

KEYWORDS

Alzheimer's disease, MRI analysis, Deep learning, Regression, Explainable AI

ACKNOWLEDGEMENTS

This work was supported by Health Labour Science Research Grants from the Ministry of Health, Labour and Welfare, Japan (Grant Number 23GB1003).

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Integrating Process Simulation with Large Language Models for Automated Life Cycle Inventory Generation: A Case Study of Reactive Distillation

Tsai-Wei Wu*, Chun-Wei Chen

Department of Chemical Engineering, National Cheng Kung University, Taiwan

ABSTRACT

In the process design phase of a sustainable process, LCA can serve as an important tool for evaluating or optimizing the process. Reactive distillation (RD), combining two functions in one unit operation, offers significant potential for process intensification and energy savings. However, quantifying its environmental benefits via Life Cycle Assessment (LCA) remains challenging due to the labor-intensive nature of Life Cycle Inventory (LCI) data collection. This study proposes a novel framework integrating Aspen Plus simulation with Large Language Models (LLMs) to streamline LCI generation. We utilize a Python-based parser to automatically extract rigorous mass and energy balance data from Aspen Plus reports. Beyond simple data extraction, an LLM framework enhanced by RAG is employed to contextualize simulation outputs. It assists in defining the LCA goal and scope (e.g., cradle-to-gate scope) and rationalizing methodological choices (e.g., allocation rules, cut-off criteria) by retrieving and analyzing relevant standards from scientific literature. A case study on the production of butyl acetate is conducted to validate the framework. We want to demonstrate the feasibility of this workflow in reducing manual data entry errors and efficiently bridging simulation parameters with environmental impact assessment. This approach provides a digitalized pathway for assessing sustainable chemical processes.

KEYWORDS

LLM, LCA, Process intensification, PSE automation

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Adaptive Organosilicon Optimization via Supervised Contrastive and Condition-Aware Safe Reinforcement Learning

Jiyang Xiao, Zhongmei Li*, Qinhao Sun, Jionghao Lou, Shiming Wu, Enbo Feng

Key Laboratory of Smart Manufacturing in Energy Chemical Process, East China University of Science and Technology, China

ABSTRACT

Organosilicon materials are essential in modern industry, yet their synthesis involves complex dynamics that challenge process control. Process optimization requires maximizing the M2 monomer yield while enforcing a minimum CH3Cl conversion constraint to prevent hazardous byproduct accumulation. However, current practice faces three barriers: multi-rate data heterogeneity between high-frequency sensors and sparse lab assays; ill-defined operating regimes due to shifting catalyst activity; and the inability of traditional methods to guarantee zero-violation safety. To address these, we propose an end-to-end framework integrating supervised contrastive learning with condition-aware safe reinforcement learning (CA-SRL). First, to align asynchronous data, a dual-branch encoder combines Temporal Convolutional Networks and Multi- Layer Perceptrons via cross-attention, with supervised contrastive loss enhancing feature discriminability across process conditions. Second, a Gaussian Mixture Model probabilistically partitions the latent space into interpretable condition clusters, learning a high-precision surrogate of process dynamics. Third, a dual safety mechanism—Lagrangian relaxation for soft guidance and hard action projection for zero-violation execution—ensures inherent safety during exploration. Validated on three months of actual industrial data, the framework achieves a 1.56% higher M2 yield while guaranteeing strict constraint satisfaction and real-time computational efficiency, offering a deployable paradigm for safe optimization in complex chemical processes.

KEYWORDS

Organosilicon Synthesis; Safe Reinforcement Learning; Supervised Contrastive Learning; Condition Recognition; Multi-rate Data Fusion

ACKNOWLEDGEMENTS

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Stochastic Robust Optimal Scheduling of Industrial Utility Systems Coupled with Green Ammonia under Multiple Uncertainties

Xiaoya Cao, **Liang Zhao***

Key Laboratory of Smart Manufacturing in Energy Chemical Process, Ministry of Education, East China University of Science and Technology, China

ABSTRACT

This paper develops an integrated modeling and optimization framework that couples Life Cycle Assessment (LCA) with Two-Stage Stochastic–Robust Optimization (TSRO) to address the pronounced randomness and multi-scale uncertainties in renewable wind–solar generation and industrial steam demand, enabling optimal scheduling of an industrial utility system (IUS) integrated with green ammonia production. On the supply side, a Copula-based approach is employed to capture the joint dependency structure between wind and photovoltaic outputs, and representative renewable energy scenarios are generated using K-Means clustering. On the demand side, the non-convex distribution characteristics of steam load are analyzed using Support Vector Data Description to extract boundary structures, and a data-driven non-convex uncertainty set is constructed via polyhedral complex robust modeling to enhance robustness under extreme load fluctuations. A TSRO model minimizing annual total cost (ATC) and global warming potential (GWP) is then formulated and efficiently solved through a nested Column-and-Constraint Generation (C&CG) algorithm for mixed-integer optimization. Case studies demonstrate that the proposed framework yields a clear Pareto trade-off between economic performance and environmental impact, and outperforms deterministic and conventional stochastic programming approaches in uncertainty characterization, solution robustness, and computational efficiency.

KEYWORDS

Stochastic–robust optimization, Industrial utility systems, Green ammonia integration, Renewable energy uncertainty, Life cycle assessment

ACKNOWLEDGEMENTS

This work was supported by National Natural Science Foundation of China (62373154, 22178103).

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Fast data and theory fusion modeling method for dynamic distillation systems based on the Physics-constrained dynamic mode decomposition

Xing Qian[1], Haotong Wu[1], Yuhui Yin[2,3], Shengkun Jia[2,3], Yiqing Luo[2,3], Xigang Yuan[2,3,*]

[1] *College of Information Science and Technology, Beijing University of Chemical Technology, China*
[2] *School of Chemical Engineering and Technology, Tianjin University, China*
[3] *State Key Laboratory of Chemical Engineering and Low-carbon Technology, China*

ABSTRACT

In the research of dynamic distillation systems, modeling methods based on theoretical models (such as thermodynamics and fluid mechanics) hold significant research and application value. However, the large computational scale, complex physical or chemical formulas, and lengthy calculation times have limited its application in many scenarios. Contrasting with theoretical models, data -driven models based on historical production data have faster solution speeds, and there is no need to consider complex varia ble relationships when constructing the models. However, the output results from the data model fail to match the basic derivation of the theoretical model. Integrating the two modeling approaches mentioned above has become a cutting -edge research focus. Currently, the hybrid model based on Physics-Constrained Dynamic Mode Decomposition (PCDMD), proposed by the authors[1], has demonstrated its excellent model performance in the field of fluid dynamics. Facing dynamic distillation systems in the chemical engineering field, this work makes partial improvements to the algorithm framework as shown in Figure 1. It employs Dynamic Mode Decomposition with control method (DMDc) to rapidly build a data-driven model that incorporates the changes in input signals of the dynamic distillation system. Additionally, it integrates the theoretical model of the dynamic distillation system (s uch as equations of material balance, phase equilibrium, mole fraction summations, and heat balance) using a non -intrusive filtering and correction method. Case of two multistage separation processes —absorption and distillation systems—demonstrate that PCDMD can effectively handle high -dimensional and strongly nonlinear dynamic distillation systems. Moreover, the PCDMD method shows a certain degree of physical interpretability for its output results and achieves a balance between data and theory. Figure 1: The framework of Physics-constrained dynamic mode decomposition for dynamic distillation systems.

References [1] Yuhui Yin, Chenhui Kou, Shengkun Jia, et al. PCDMD: Physics -constrained dynamic mode decomposition for accurate and robust forecasting of dynamical systems with imperfect data and physics. Computer Physics Communications, 2024, 304, 109303.

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

A Comparative Study of Reinforcement Learning and Model Predictive Control in Isopropanol Dehydration Process

Yu-Cheng Chao[1], Yan-Ling Yang[2], Hao-Yeh Lee[1,*]

[1] *Department of Chemical Engineering, National Taiwan University of Science and Technology, Taiwan*
[2] *Department of Chemical Engineering, National Taiwan University, Taiwan*

ABSTRACT

This study evaluates hierarchical control strategies for the isopropanol–water extractive distillation process using ethylene glycol as an entrainer. A lower-layer cascade PI controller provides a stable foundation, while the upper layer employs either a Seq2Seq-based Model Predictive Control (MPC) or Reinforcement Learning (RL) algorithms, including PPO, SAC, and TD3. The Seq2Seq model forecasts dynamic trajectories to optimize tray temperatures, while the RL agents are tested against various reward structures and action space constraints to ensure operational stability. The findings reveal that while PPO maintains consistent stability, SAC and TD3 are prone to oscillations under disturbances. These instabilities are effectively mitigated by utilizing asymmetric reward functions that penalize purity undershooting and by narrowing action space constraints to enforce smoother adjustments. Quantitative analysis shows that both Seq2Seq-based MPC and RL controllers significantly outperform the PI baseline in tracking precision and recovery during feed disturbances. This research underscores the critical importance of reward shaping and action space design, proving that AI-driven hierarchical control can achieve robust, high-purity, and energy-efficient solutions for complex chemical processes.

KEYWORDS

Extractive distillation; Sequence-to-Sequence-based Model Predictive Control; Reinforcement learning control

P-85 **POSTER**

13:30~14:30 · Poster Session P2 · Engineering Building D

A comparative analysis of process flexibility for pressure-swing and extractive distillation systems

Yu-Ying Chen[1], Zong Yang Kong[2], Vincentius Surya Kurnia Adi[3,4], Hao-Yeh Lee[1,*]

[1]*Department of Chemical Engineering, National Taiwan University of Science and Technology, Taiwan*

[2]*School of Engineering, Sunway University, Malaysia*

[3]*Department of Chemical Engineering, National Chung Hsing University, Taiwan*

[4]*Department of Chemical Engineering, National Cheng Kung University, Taiwan*

ABSTRACT

In chemical process design, optimization often focused solely on minimizing total annual cost, which usually leads to insufficient flexibility against feedstock fluctuations. This study utilizes the Flexibility Index (FI) to quantify a system's capacity to maintain performance in the face of unexpected disturbances. Through multi-objective optimization, Pareto optimal solution sets are identified to compare the process flexibility and cost of pressure-swing distillation (PSD) and extractive distillation (ED) for acetone-methanol separation. PSD achieves separation by exploiting the shifts in azeotropic composition at different operating pressures. On the other hand, ED utilizes an entrainer to alter the relative volatility of the components, thereby eliminating the azeotrope. While most literature focuses primarily on the economic performances of comparing PSD and ED systems, this research evaluates both flexibility and cost simultaneously. Furthermore, an efficient method for rapid FI analysis in dual-column systems is developed, identifying key factors that influence flexibility in each architecture. It is believed that these findings provide a new perspective on the performance of ED and PSD, offering insights that contrast with traditional cost-centered conclusions.

KEYWORDS

Process design; Process optimization; Process simulation; Separation; Aspen Plus

ACKNOWLEDGEMENTS

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Process design and multi-objective optimization for the separation of methyl acetate/vinyl acetate/water azeotrope by extractive distillation based on mixed entrainer

Yang Zhang, Zhaoyou Zhu, Xin Li, Peizhe Cui, Yinglong Wang*

Qingdao University of Science and Technology, China

ABSTRACT

Vinyl acetate, a widely used industrial monomer, forms a ternary azeotropic system with methyl acetate and water during production. Residue curve mapping characterized this azeotrope and established its separation sequence. Relative volatility then identified the optimal entrainer, with efficacy validated through σ-profile and electrostatic potential analysis. We designed single and multiple processes using mixed entrainer for extractive distillation. Multi-objective genetic algorithm optimization of critical variables calculated the optimal operating parameter set. Building on this, a heat-integrated process was designed. Comprehensive evaluation covered economic, environmental, energy, and utilization perspectives. Compared with the original process, the heat-integrated process reduced energy consumption by 36.1% and gas emissions by 37.6%, while thermodynamic efficiency improved to 39.36%, enhancing economic and environmental benefits. This study establishes an optimization method for extractive distillation to efficiently separate the Methyl acetate/Vinyl acetate/Water ternary azeotropic system, offering systematic theoretical and practical frameworks for integrated energy utilization, cost reduction, and process intensification.

KEYWORDS

Vinyl acetate; Extractive distillation; Mixed entrainer; Multi-objective optimization; Heat integration.

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Simulation and technoeconomic analysis for low-carbon coal-to-liquids process coupling renewable energy and green hydrogen

Yao Jiashu, Liu Yurong, and Du Wenli*

East China University of Science and Technology, China

ABSTRACT

The subjects of Process Systems Engineering (PSE) are Carbon Neutrality. Conventional coal-to-liquids (CTL) technology is challenged by high carbon emissions and low efficiency. Two innovative low-carbon CTL routes coupled with renewable electricity are proposed: RE-CTL and RE-GH-CTL (with green hydrogen). A detailed comparison with the conventional process, based on modeling and simulation, was conducted from carbon, thermodynamic, and economic perspectives. The RE-GH-CTL process significantly improves carbon utilization efficiency from 58.79% to 95.82% and reduces carbon emissions to 1.02 tCO2/t liquids, compared to 5.17 tCO2/t liquids in conventional CTL. Thermodynamically, energy and exergy efficiencies show slight improvement. Economically, RE-GH-CTL exhibits higher production costs due to electrolysis electricity demand, making its profitability highly sensitive to electricity price. It becomes profitable only below 0.34 CNY/kWh and outperforms the alternatives below 0.29 CNY/kWh. The payback period for RE-GH-CTL ranges from 8 years (at 0.2 CNY/kWh) to 15 years (at 0.4 CNY/kWh), while conventional processes break even around year 13. Overall, the proposed process offers an environmentally and potentially economic route supporting carbon neutrality and sustainable development goals.

KEYWORDS

Coal-to-liquids; Green hydrogen; Process simulation; Performance analysis

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Techno-Economic Analysis of Amine-Based Carbon Capture for Maritime Liquefied Natural Gas Engines and Solid Oxide Fuel Cells

Yeji Choi, Jeehoon Han*

Department of Chemical Engineering, Pohang University of Science and Technology (POSTECH), Korea

ABSTRACT

To meet the IMO's 2050 net-zero emission strategy, the maritime sector requires onboard carbon capture and storage (OCCS). Although solid oxide fuel cells (SOFCs) offer high efficiency, comparative studies on their integration with OCCS are limited. This study evaluates the techno-economic feasibility of integrating amine-based OCCS with liquefied natural gas (LNG) engines and LNG-SOFC systems. Engine exhaust profiles are modeled using general technical data, while the SOFC system is simulated using Aspen Plus and Aspen Custom Modeler. The amine-based carbon capture processes for both routes are rigorously modeled in Aspen Plus to determine mass and energy balances. A techno-economic analysis is then conducted to assess capital expenditure (CAPEX), operating expenditure (OPEX), levelized cost of energy, and carbon capture costs. Although the SOFC system incurs a higher initial CAPEX due to stack investments, its superior electrical efficiency and optimal exhaust characteristics reduce carbon capture OPEX. This advantage effectively offsets the initial costs, resulting in a highly competitive life cycle carbon capture cost. Transitioning to LNG-SOFC systems with amine-based OCCS provides a strategic economic advantage over conventional LNG engines and offers a financially viable roadmap for shipowners to comply with stringent IMO net-zero targets.

KEYWORDS

Solid Oxide Fuel Cell, Onboard Carbon Capture, Techno-Economic Analysis, Maritime Decarbonization

ACKNOWLEDGEMENTS

This work was supported in part by the National Research Foundation of Korea (NRF) grants funded by the Korea government (MSIT) (RS-2025-23323940, RS-2026-25480561).

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Design of an Iron Powder–Based Energy Carrier Supply Chain

Yi-Hung Lin, Cheng-Liang Chen*

Department of Chemical Engineering, National Taiwan University, Taiwan

ABSTRACT

Iron powder has emerged as a promising energy carrier for net-zero energy systems, offering a safe and scalable option for storing renewable energy and transporting it over long distances. Compared with direct electrification and hydrogen-based pathways, iron powder provides high volumetric energy density, solid-state handling, non-flammability, and compatibility with existing industrial infrastructure. Renewable electricity can be used to reduce iron oxides in fluidized bed reactors, storing energy in metallic iron, while energy can later be released through iron oxidation in circulating fluidized bed combustors. By integrating renewable iron reduction, energy release, and oxide recovery, iron powder enables a closed-loop, low-carbon energy supply chain. Because of its potential in long-duration energy storage, dispatchable power generation, and high-temperature industrial heating, iron powder is regarded as a promising system-level energy carrier for future low-carbon energy systems.

KEYWORDS

Net-zero emissions, Iron powder energy carrier; Long-duration energy storage; Low-carbon energy supply chain

ACKNOWLEDGEMENTS

The author would like to thank Professor Cheng-Liang Chen and colleagues in the Department of Chemical Engineering for their support and helpful suggestions in completing this study

P-90 **POSTER**

13:30~14:30 · Poster Session P2 · Engineering Building D

Techno-economic Analysis and Life Cycle Assessment of Sustainable Aviation Fuel Production via CO_2 Fisher-Tropsch Synthesis

Seonuk Yu, Seungjun Choi, Jeehoon Han*

Department of Chemical Engineering, Pohang University of Science and Technology, Korea

ABSTRACT

Sustainable aviation fuel (SAF) is regarded as being pivotal to the decarbonization of the aviation sector. Among emerging routes, CO2 Fischer-Tropsch (CO2-FT) synthesis offers a direct pathway from captured CO2 and low-carbon hydrogen to jet-range hydrocarbons. However, comprehensive process-level assessments remain scarce because CO2-FT is still relatively immature and integrated flowsheet models are rarely available. In this study, a modelling framework is developed, which couples a MATLAB-based kinetic model of single-reactor CO2-FT system, in which reverse water gas shift and Fischer-Tropsch reactions proceed simultaneously, with an Aspen Plus flowsheet for separation, recirculation and upgrading to jet fuel. The impact of the recycle ratio on overall CO2 conversion and the quantification of its implications for utility demands and product yields was explored. Techno-economic analysis and life cycle assessment were performed to evaluate the feasibility of the process, with sensitivity analyses covering CO2 and hydrogen sources and electricity mixes. The results identify the supply and operating conditions that are most critical to performance, informing the design of credible CO2-to-SAF routes.

KEYWORDS

sustainable aviation fuel, CO2 Fischer-Tropsch, process modeling, techno-economic analysis, life cycle assessment

ACKNOWLEDGEMENTS

This research was supported in part by the program of Development of Eco-friendly Chemicals as Alternative Raw Materials to Oil (No. 2022M3J5A1085257) through the National Research Foundation of Korea (NRF) funded by the Ministry of Science and ICT and in part by the National Research Foundation of Korea(NRF) grant funded by the Korea government(MSIT)(RS-2026-25480561)

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Investigating the Influences of Electrochemical Kinetic Parameters on the Operating Voltage of PEM Water Electrolysis Cells

Yu-Da Hsiao*, Chia-Kai Wang and Shi-Hsuan Lu

Department of Chemical Engineering and Biotechnology, National Taipei University of Technology, Taiwan

ABSTRACT

Proton exchange membrane (PEM) water electrolysis has shown its advantages for operations at high and transient current densities, which highlights its superiority over the conventional alkaline water electrolyzers (AWE). Nevertheless, the influences of PEM water electrolysis cell voltage to kinetic characteristics have rarely been systematically investigated, resulting in an incomplete understanding of their relative significance and combined effects. Therefore, in this study, a numerical model of PEM water electrolysis cell voltage was used to perform sensitivity analysis, yielding quantitative insights into the effects of electrochemical kinetic parameters on electrolysis cell voltage. The results quantitatively indicated that the PEM water electrolysis cell voltage is predominantly governed by the charge transfer coefficients, exchange current densities and activation energies of oxygen and hydrogen evolution reactions taking place at anode and cathode respectively, which mainly affect the activation overpotential of PEM cells. On the other hand, geometric and operating parameters, particularly the operating current density, cell temperature and membrane thickness, were found to be relatively minor factors but posing direct effects on the ohmic overpotential.

KEYWORDS

Proton exchange membrane water electrolysis (PEMWE); Sensitivity analysis; Numerical modeling; Electrochemical kinetic parameters;

ACKNOWLEDGEMENTS

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Numerical Modeling of Ion Transport in Nanofiltration Membranes Using the DSPM-DE Model

Yunju Kim, and Kiho Park*

Department of Chemical Engineering, Hanyang University, Korea

ABSTRACT

Nanofiltration (NF) membranes have gained attention as a cost-effective alternative to reverse osmosis (RO) for removing organic matter and ions from industrial wastewater, achieving comparable separation performance at lower operating pressures. In this study, the DSPM-DE (Donnan Steric Pore Model with Dielectric Exclusion) model was applied to predict ion transport within NF membranes. The model quantitatively describes membrane–ion–solution interactions by incorporating steric hindrance, Donnan equilibrium, and dielectric exclusion effects into the extended Nernst–Planck equation. However, solving the coupled nonlinear equations along the membrane thickness (1D) is often hindered by numerical divergence and oscillatory behavior. To address this, thermodynamic constraints were incorporated into the computational approach to ensure numerical stability. The model predicted an ion rejection of approximately 80% for a single-salt (NaCl) aqueous solution using a commercial NF 270 membrane at pH 7, in quantitative agreement with the manufacturer's specifications. This validates the capability of the proposed modeling approach to capture ion separation behavior under practical operating conditions. With further extension to multi-ion systems and novel membrane materials, this work can serve as a computational reference for industrial process design in applications such as valuable metal recovery and semiconductor wastewater treatment, where precise ion selectivity is critical.

KEYWORDS

Nanofiltration, Membrane, DSPM-DE, Modeling

ACKNOWLEDGEMENTS

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Surrogate Model for Joint Prediction of Local Fields and Process-Level KPIs in Ethane Cracking Reactors

Yunyue Shang, Wenli Du*, Yichun Li**

State Key Laboratory of Industrial Control Technology, East China University of Science and Technology, China

ABSTRACT

Reaction, heat transfer, and flow are strongly coupled in ethane cracking reactors, making accurate prediction of local fields and process-level key performance indicators (KPIs) important for reactor analysis and evaluation. Existing surrogate models often focus on outlet variables or single prediction tasks, while integrated learning across local-field, species-concentration, derived-composition, and process-level KPI prediction tasks is hindered by gradient conflicts among tasks. To address this issue, a multi-task surrogate model is developed for joint prediction of local fields and process-level KPIs in ethane cracking reactors. Built on a dual-decoder low-rank U-Net, the model combines separate decoders for local-field and species-related prediction, low-rank residual modules for efficient feature refinement, a local-field-prioritized gradient coordination strategy, a global fusion module based on decoded feature summaries, and gradient detachment under a fixed single-stage training protocol. Compared with the single-decoder U-Net baseline model, the proposed model preserves KPI prediction quality while improving predictions of four local-field variables, key-species concentration fields, and species-derived composition fractions. For these three variable groups, mean R2 values all exceed 0.994, while NRMSE decreases by 35.97%, 43.93%, and 49.85%, and NMAE decreases by 43.88%, 48.01%, and 50.24%, respectively. These results demonstrate integrated high-fidelity prediction of reactor states and process-level KPIs.

KEYWORDS

Ethane cracking reactor; Multi-task learning; Surrogate model; Local field prediction; KPI prediction

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

A Parallel Column Generation Algorithm for Two-Dimensional Two-Stage Guillotine Cutting Problem with Multiple Stock Sizes

Zheng Xinya[1], Liu Changxin[1], Li Zhongmei[1], Li Yichun[1], Yang Minglei[1,2,*]

[1]Key Laboratory of Advanced Control and Optimization for Chemical Processes, East China University of Science and Technology, China

[2]Engineering Research Center of Process Systems Engineering, East China University of Science and Technology, China

ABSTRACT

This paper addresses a complex two-dimensional cutting problem in modern steel manufacturing. Based on actual production processes, the problem is formulated as a non-rotational, multi-sized, two-dimensional two-stage guillotine cutting problem subject to industrial constraints. Due to these process-specific limitations, classical two-stage solution methods are not directly applicable. To tackle this challenge, we developed a parallel column generation algorithm. Specifically, complex process constraints were embedded and solved within the pricing subproblems. Furthermore, a parallel mechanism operating across multiple stock plates was designed to significantly accelerate the dynamic generation of high-quality cutting patterns. Integrating an overproduction penalty mechanism to optimize the trade-off between total stock plate usage and overproduction, the algorithm rapidly generated high-quality cutting patterns under continuous relaxation, followed by an integer recovery phase to obtain practical feasible solutions. The algorithm was comprehensively evaluated using benchmark datasets of various scales derived from historical orders of a steel enterprise. Computational results demonstrate that the proposed approach not only achieves high-quality near-optimal solutions for small-scale instances but also exhibits superior computational efficiency and stability in large-scale industrial scenarios.

KEYWORDS

column generation, cutting stock problem, two-stage guillotine cutting, integer programming

ACKNOWLEDGEMENTS

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Multi-Rate Fusion of Acoustic and Vibration Signals for Soft Sensing of Ball Mill Internal States: A Lab-scale Study in Bayer Process

Xiangyang Zhu, Zhongmei Li*, Tinghang Zhao, Jingrui Wang, Enbo Feng

Key Laboratory of Smart Manufacturing in Energy Chemical Process, East China University of Science and Technology, China

ABSTRACT

In the Bayer alumina production process, ball mills are critical for bauxite grinding to prepare slurry for downstream dissolution. Real-time knowledge of internal states — such as fill level, grinding concentration, and media wear—is essential for optimizing energy efficiency and ensuring stable operation. However, industrial practice faces three major challenges: (1) manual assays with 2–4 hour intervals cause severe feedback lag; (2) motor current alone fails to distinguish between overfilled and underfilled conditions due to similar current drops; (3) intense mechanical noise and limited sensor accessibility hinder reliable feature extraction. To address these limitations, this paper proposes a multi-modal soft sensing framework based on multi-rate fusion of acoustic and vibration signals. A temporal alignment module based on adaptive resampling synchronizes continuous acoustic features with sparsely sampled (5 –10 min intervals) vibration data. A hybrid CNN-LSTM architecture extracts robust time-frequency features from acoustic signals while capturing temporal dependencies from vibration sequences. Furthermore, an attention-based fusion mechanism adaptively weights modality contributions to enhance robustness under varying conditions. Validated on a laboratory-scale ball mill platform, the proposed method achieves significantly higher accuracy in inferring fill level and grinding concentration compared to single-modal approaches, effectively overcoming the lag and ambiguity of conventional methods. This study provides a theoretical and experimental foundation for intelligent monitoring and advanced control in industrial alumina refineries.

KEYWORDS

Ball Mill; Soft Sensing; Multi-rate Data Fusion; Acoustic Emission; Vibration Analysis; Bayer Process

ACKNOWLEDGEMENTS

This work was supported by National Natural Science Foundation of China under Grant 62394343, Shanghai Rising-Star Program(24QA2706100).

P-96 **POSTER**

13:30~14:30 · Poster Session P2 · Engineering Building D

Accelerating Catalyst Discovery for CO_2 hydrogenation via an ML-Driven Cascade Framework and Genetic Algorithm

Hyunjin Kang[1], Hyundo Park[2], Insoo Ro[3,*], Hyungtae Cho[1,*], Jaewon Lee[4,*]

[1] *Department of Chemical Engineering, Kyung Hee University, Korea*
[2] *Department of Chemistry, Northwestern University, USA*
[3] *Department of Chemical and Biological Engineering, Korea University, Korea*
[4] *Department of Materials Science and Chemical Engineering, Hanyang University, Korea*

ABSTRACT

Methanol synthesis via CO2 hydrogenation is pivotal for carbon neutrality, yet optimizing both catalytic activity and stability remains a significant challenge. This study proposes a machine learning-driven cascade framework to tackle this dual challenge. We constructed two independent NGBoost models using literature data: (1) methanol yield model (R2=0.89, RMSE=1.09) and (2) stability (Time-on-Stream) model (R2=0.94, RMSE=0.76), both providing uncertainty quantification. The framework follows a sequential strategy: a Genetic Algorithm (GA) first screens for high-activity candidates, which are subsequently evaluated for long-term performance by the stability model. This approach effectively filtered out candidates with high initial activity but rapid deactivation risks, efficiently identifying a high-confidence cluster of catalysts that satisfy both yield and stability requirements.

KEYWORDS

CO2 hydrogenation, Machine Learning, High-Throughput Screening, Genetic Algorithm

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Comparative Analysis of CO_2-to-SAF Pathways via Integrated Process Design and Optimization

Jeongmin Lee and Joonjae Ryu*

Department of Chemical Engineering, University of Seoul, Korea

ABSTRACT

The aviation industry accounts for approximately 2–3% of global CO2 emissions, and the transition to sustainable aviation fuel (SAF) is increasingly recognized as a critical pathway toward carbon neutrality. CO2-to-SAF production routes, which directly convert captured CO2 into jet fuel, enable simultaneous greenhouse gas reduction and resource circularity; when integrated with renewable energy, carbon-negative operation becomes achievable. However, the efficiency and competitiveness of different SAF production pathways vary considerably depending on the conversion technology, energy supply, and techno-economic conditions, necessitating systematic comparative analysis. This study develops a rigorous process model for an integrated reverse water-gas shift (RWGS) and Fischer-Tropsch (FT) synthesis pathway as a representative CO2-to-SAF route. Each unit operation is modeled based on reaction kinetics, and kinetic parameters are estimated through mathematical optimization. A process simulator is coupled with optimization algorithms to conduct sensitivity analysis and process optimization over key operating variables—including reaction temperature, pressure, and feed ratio—evaluating their effects on SAF production efficiency and economic performance. The results identify optimal operating conditions for the RWGS-FT pathway and provide a systematic decision-making framework for CO2 utilization and power-to-liquid processes.

KEYWORDS

Sustainable Aviation Fuel, CO2 utilization, RWGS, Fischer-Tropsch synthesis, process optimization

ACKNOWLEDGEMENTS

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Design Optimisation of Baffle Geometry for Mitigating Acceleration-Induced Boil-Off Gas in Liquid Hydrogen Tankers

Jingyeong Im[1,2], Boram Gu[1,*] and Wangyun Won[2,*]

[1] *School of Chemical Engineering, Chonnam National University, Korea*
[2] *Korea University, Korea*

ABSTRACT

This study investigates acceleration-induced flow effects on boil-off gas (BOG) generation during liquid hydrogen road transport using three-dimensional computational fluid dynamics (CFD). Vehicle acceleration intensity and internal baffle design were examined to characterise transient flow behaviour under realistic driving conditions. Furthermore, a parametric optimisation framework was introduced to explore structural configurations that could reduce BOG under dynamic loading. Simulations were conducted for acceleration scenarios reaching 40 km/h and 80 km/h. A transient multiphase model with vapour-liquid mass transfer was applied to analyse interphase transport and BOG within a cryogenic hydrogen tank. Different acceleration magnitudes were imposed at identical terminal speeds to isolate acceleration effects. Three configurations were assessed: unbaffled, permeable baffled, and centre-hole baffled. Porous baffle permeability and centre-hole diameter were varied to evaluate their influence on flow damping and evaporation behaviour. Results show that acceleration intensity and baffle configuration strongly influence internal flow structures and evaporation rates. Baffles mitigate large-scale sloshing and reduce interfacial renewal compared with the unbaffled case. The parametric analysis demonstrates the sensitivity of BOG behaviour to baffle permeability and hole size under transient driving conditions. These findings demonstrate the importance of integrating driving dynamics with internal structural design in optimising liquid hydrogen transport systems.

KEYWORDS

Liquid hydrogen, Computational fluid dynamics, Sloshing damping, Boil-off-gas

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Mechanistic-Informed Data-Driven Framework for Generalized Reaction Yield Prediction Across Novel Chemical Spaces

Zhe Li, and Jingyi Lu*

East China University of Science and Technology, China

ABSTRACT

The subjects of Process Systems Engineering (PSE) are evolving toward universal machine learning frameworks for cross-category reaction yield prediction. Reaction yield is central to synthetic efficiency. However, constructing universal models is severely constrained by the inherent sparsity of experimental data. Existing methodologies are predominantly tailored for specific high-throughput experimentation (HTE) datasets. While effective in data-rich environments, these models lack the transferability required to generalize across diverse reaction classes. To address these limitations, we propose a transferable framework leveraging heterogeneous reaction data extracted from Reaxys. The architecture employs Graph Convolutional Networks (GCNs), pre-trained on selected yield-critical features, to encode generalized molecular representations. These structural embeddings are subsequently integrated with reaction-center atomic features computed derived from GFN2-xTB. This integration synthesizes topological and quantum determinants into a cost-effective representation of underlying reaction mechanisms. To bolster robustness in low-data regimes, the framework employs a kernel-based distance metric to evaluate chemical proximity within the latent feature space. Validated against Suzuki and Buchwald-Hartwig benchmarks, this approach consistently outperforms established baselines. More significantly, the framework maintains over 70% accuracy on Heck reactions, confirming its robust capability to generalize into novel chemical spaces.

KEYWORDS

Reaction Predict, Graph Neural Network, Metric Learning, Deep Learning .

ACKNOWLEDGEMENTS

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Effects of Photoacid Generator Composition on Proton Transport, Deprotection Kinetics, and Line Edge Roughness in Chemically Amplified Resists: A Reactive Molecular Dynamics Study

Sangdeok Kim[1], Jaehyun Ryu[1], Seungtae Kim[1], Sangwoo Kwon[1], Claire S. Adjiman[2], and Won Bo Lee[1,*]

[1] *School of Chemical and Biological Engineering, Seoul National University, Korea*
[2] *Department of Chemical Engineering, Imperial College London, UK*

ABSTRACT

Line edge roughness (LER) is a primary limitation of extreme ultraviolet (EUV) lithography for sub-7 nm patterning. It depends on how the photoacid produced by the photoacid generator (PAG) diffuses through the resist during post-exposure bake (PEB). Classical molecular dynamics (MD) cannot represent the proton directly, so we substitute Li+ as a proxy, following Bottoms et al. [19,20] who validated an inert ionic surrogate for acid diffusion. We compare three PAG combinations: triphenylsulfonium triflate (TPS-TFO), diphenyliodonium triflate (DPI-TFO), and triphenylsulfonium perfluorobutanesulfonate (TPS-PFBS). Reactive MD with a 0.5-nm Li+-carbonyl distance criterion is used to model deprotection. For TPS-TFO, three activation levels (50%, 75%, 100%) are simulated in both homogeneous (bulk) and heterogeneous (bilayer) configurations. In the bulk, Li+ diffusivity is similar across PAGs, but TPS-PFBS yields a notably larger simulation box at all conversions because PFBS interacts more strongly with the polymer. The expanded matrix lowers the effective acid concentration and slows the reaction. In the bilayer, LER decreases monotonically with deprotection. DPI-TFO gives the lowest LER (about 5 nm at 65% deprotection), TPS-TFO is intermediate, and TPS-PFBS is highest. Higher PAG activation in TPS-TFO also lowers LER at fixed deprotection. The molecular factor that distinguishes the three systems is the ion-polymer interaction, which controls matrix volume and reaction rate. Smaller PAG ions, particularly smaller cations, favor lower LER.

KEYWORDS

extreme ultraviolet lithography, chemically amplified resist, photoacid generator, reactive molecular dynamics, line edge roughness, ion transport

P-101

POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Multi-Agent Debate for Feasibility-Aware Design of CO_2 Electrolysis Systems from Economic and Environmental Perspectives

Youngwon Lee[1], Youlim Chung[1], Juyeon Kim, Minji Kim[2], Jin Ko[2], Junghwan Kim[2], and Jonggeol Na[1,*]

[1]*Department of Chemical Engineering & Materials Science, Ewha Womans University, Korea*
[2]*Department of Chemical and Biomolecular Engineering, Yonsei University, Korea*

ABSTRACT

Multi-agent debate frameworks are Large Language Model (LLM)-based approaches in which AI agents with different perspectives improve reasoning through iterative argumentation. Recently, these frameworks have been extended to complex decision-making problems, yet their application to process systems engineering remains limited. In this study, we propose a multi-agent debate framework integrating techno-economic analysis (TEA) and life-cycle assessment (LCA) for feasibility-aware design of CO2 electrolysis systems. A LangGraph-based structure coordinates interactions among TEA and LCA specialists, moderator, and decision agent. All discussions are grounded in Aspen Plus simulation results that describe process flows, unit operation, and stream data. A key feature is the instegration of hidden constraints, including operating limits and performance boundaries, into agent reasoning. These feasibility constraints are obtained from a retrieval-augmented generation (RAG) system built on a knowledge graph. This enables the framework to avoid unrealistic process conditions that are not captured by conventional optimization or sensitivity analysis. The framework also provides explicit reasoning behind design choices through agent interactions, improving interpretability. Results show effective exclusion of infeasible design regions while identifying solutions that satisfy both economic and environmental perspectives, demonstrating that multi-agent debate can serve as a practical decision-making framework for process system design.

KEYWORDS

Multi-agent debate, Multi-agent system, Large language models, Techno-economic analysis, Life-cycle assessment, CO2 electrolysis

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Numerical Modeling and Determination of Optimal Catalyst Loading for Ortho-Para Conversion PFHX Reactors in Hydrogen Liquefaction Process

Changseo Lee[1], Suyeon Kim[1], Sungwon.hwang[1,2,3,*]

[1] *Department of Chemistry and Chemical Engineering, Inha University, Korea*
[2] *Education and Research Center for Smart Energy Materials and Process, Inha University, Korea*
[3] *3D Convergence Center, Inha University, Korea*

ABSTRACT

Despite growing interest in hydrogen liquefaction, precise investigations into optimal catalyst loading for ortho-para (o-p) conversion remain limited, particularly for large-scale applications. This study develops a numerical model for a Plate-Fin Heat Exchanger (PFHX) reactor designed for a 50 TPD liquefaction capacity. The system operates at a pressure range of 20–25 bar and employs a multi-stage cooling configuration consisting of six heat exchange zones to reduce the temperature from 308 K to 20 K, while strictly adhering to a maximum allowable pressure drop constraint of 0.15 bar per zone to optimize process efficiency. By coupling reaction kinetics with cryogenic hydrogen properties, the model determines the minimum catalyst loading required to achieve target conversion rates of 95–98% while suppressing exothermic boil-off. Furthermore, it evaluates the complex trade-offs between conversion efficiency, catalyst-induced pressure drop, equipment sizing, and operational expenditure (OPEX). The findings provide critical design indicators to minimize flow resistance while ensuring economic feasibility. Ultimately, this research offers a comprehensive design guideline for the industrial-scale implementation of efficient and stable PFHX reactors in liquid hydrogen systems.

KEYWORDS

Hydrogen Liquefaction, Ortho-Para (o-p) Conversion, PFHX, Catalyst Loading , Trade-off Analysis

ACKNOWLEDGEMENTS

GS E&C, CEPI(Clean Energy Process Integration Lab)

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Dynamic Life Cycle Assessment of Steel Industry Electrification Pathways

Gayoung Lee[1], Myungsuk Son[2], Jongil Bae[1], Jinsu Kim[3] and Jeehoon Han[1,*]

[1]*Department of Chemical Engineering, Pohang University of Science and Technology, Korea*
[2]*Korea Testing Laboratory, Korea*
[3]*Department of Petrochemical Materials, Chonnam National University, Korea*

ABSTRACT

The steel industry is a hard-to-abate sector that emits significant amounts of CO2 due to energy-intensive processes and the use of coke as a reducing agent in iron ore reduction. Decarbonizing is crucial for achieving carbon neutrality goals. Consequently, a transition to hydrogen-based steelmaking, in which hydrogen serves as a reducing agent, is underway. Life cycle assessment (LCA) is used to evaluate climate change impacts from greenhouse gas (GHG) emissions, and global warming potential over a 100-year time horizon is widely used as a representative impact category. However, time-independent characterization of static LCA limits its ability to reflect temporal changes associated with the timing of emissions and atmospheric concentrations. To address these limitations, this study applied a dynamic LCA framework that incorporates time-dependent characterization factors and GHG concentrations. A cradle-to-gate system boundary was established. Steel production processes transitioning to electrification were modeled to produce 1 tonne of crude steel with an increasing share of renewable electricity. The transition to an electrification process not only reduces total GHG emissions but also lowers the proportion of CO2. Therefore, accurately evaluating decarbonization pathways for the steel industry requires a dynamic LCA approach that reflects temporal dynamics.

KEYWORDS

dynamic life cycle assessment, steel industry, electrification, global warming potential

ACKNOWLEDGEMENTS

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Uncertainty-Based Cost Optimization of Hydrogen Production Using Dynamic LNG and CEPCI Forecasts

Dong Guk Kim, Yoo Ri Kim, Seong Bin Ga, Dong Hwi Jeong*

Department of Chemical Engineering, University of Ulsan, Korea

ABSTRACT

This study presents an uncertainty-based economic evaluation of blue hydrogen production using the Levelized Cost of Hydrogen (LCOH). Liquefied natural gas (LNG) price and the Chemical Engineering Plant Cost Index (CEPCI) were selected as key uncertain inputs, both exhibiting time-varying stochastic behavior. CEPCI was modeled using a log-return-based break-point AR(1) framework, with residuals fitted to a skewed Student-t distribution to reflect structural changes and asymmetric heavy-tailed behavior. LNG prices were modeled using a mean-reverting framework, with residuals fitted to a logistic distribution to represent stochastic deviations around the long-run equilibrium. Process-level economic factors were obtained from Aspen simulations, and these were combined with the simulated LNG and CEPCI paths to estimate the future distribution of LCOH. Risk was assessed using both central and tail-based metrics, including P95 and Conditional Value at Risk (CVaR), to identify economically stable operating conditions under uncertainty.

KEYWORDS

Blue hydrogen, Process simulation, Probabilistic forecasting, Uncertainty analysis, Monte Carlo simulation

ACKNOWLEDGEMENTS

This work was supported by the Industrial Technology Innovation Program (RS-202400507471, “Development and Demonstration of an Operations Optimization Platform for AI-Driven Autonomous Manufacturing in Refinery and Petrochemical Processes”) funded by the Ministry of Trade, Industry & Energy (MOTIE, Korea). This result was supported by the "Regional Innovation System & Education (RISE)" through the Ulsan RISE Center, funded by the Ministry of Education (MOE) and the Ulsan Metropolitan City, Republic of Korea.(2025-RISE-07-001) This work was supported by the National Research Foundation of Korea(NRF) grant funded by the Korea government(MSIT) (No. RS-2023-00217778)

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

External Coupling-Based Multi-objective Optimization Framework for DMR Processes in Aspen Plus

Jeong Cheol Lee, Nguyen Minh Tan, Dong Hwi Jeong*

Department of Chemical Engineering, University of Ulsan, Korea

ABSTRACT

Dry methane reforming (DMR) is a promising process for CO2 utilization and syngas production. However, the application of multi-objective optimization (MOO) to Aspen Plus-based DMR processes is often limited by restricted degrees of freedom, particularly when reactor models are defined by fixed operating conditions or simplified kinetics. This results in a constrained design space, making it difficult to obtain meaningful Pareto-optimal solutions. To address this limitation, this study proposes an external coupling framework that integrates Aspen Plus with a Python-based optimization environment. Process variables are manipulated externally via COM automation, enabling systematic exploration of an expanded design space. The Aspen model is treated as a black-box simulator, where input variables are iteratively updated and output performance metrics are extracted. The MOO problem is formulated to consider process-level performance indicators, including energy-related and system-level efficiency metrics. A black-box optimization strategy is adopted to handle the nonlinearity and computational complexity of the process. This framework provides a flexible and extensible approach for process optimization and enables future integration with techno-economic analysis (TEA) and life cycle assessment (LCA).

KEYWORDS

Dry methane reforming, Multi-objective optimization, Aspen plus simulation, External coupling framework, Black-box optimization, Process systems engineering

ACKNOWLEDGEMENTS

This work was supported by the Industrial Technology Innovation Program (RS-202400507471, “Development and Demonstration of an Operations Optimization Platform for AI-Driven Autonomous Manufacturing in Refinery and Petrochemical Processes”) funded by the Ministry of Trade, Industry & Energy (MOTIE, Korea). This result was supported by the "Regional Innovation System & Education (RISE)" through the Ulsan RISE Center, funded by the Ministry of Education (MOE) and the Ulsan Metropolitan City, Republic of Korea.(2025-RISE-07-001) This work was supported by the National Research Foundation of Korea(NRF) grant funded by the Korea government(MSIT) (No. RS-2023-00217778)

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

A Single Adsorption-Energy Feature for Accurate Prediction of MOF Gas Uptake with a Residual MLP

Yongsang An[1], Nahyeon An[2], Junyoung Park[1], Hyungtae Cho[1] and Seongbin Ga[3,*]

[1]*Department of Chemical Engineering, College of Engineering, Kyung Hee University, Korea*
[2]*School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, USA*
[3]*School of Chemical Engineering, University of Ulsan, Korea*

ABSTRACT

Metal–organic frameworks (MOFs) are promising tunable porous materials for gas storage and separation, and the rapid growth of publicly available databases—now exceeding hundreds of thousands of structures—has created a growing demand for efficient computational screening. Grand canonical Monte Carlo (GCMC) simulations remain the standard for evaluating adsorption performance, but their cost makes exhaustive assessment at this scale impractical. Machine-learning surrogate models can accelerate the process; however, most rely solely on geometric descriptors such as pore diameter, surface area, and void fraction, which quantify available space without encoding adsorbent–adsorbate interactions. We propose augmenting these structural features with a single physically grounded descriptor: the minimum adsorption energy obtained from a machine-learning interatomic potential (MLIP), which captures adsorbent–adsorbate affinity with higher accuracy than classical force fields at a fraction of the cost. A residual MLP will be trained on approximately 7,000 MOFs to predict argon uptake at 1 bar and 293 K, with targeted treatment of underrepresented high-uptake structures. We expect the largest accuracy gains for high-uptake candidates most relevant to screening, and the framework is readily extensible to other adsorbates by recomputing the energy descriptor for the target gas.

KEYWORDS

Metal-Organic Frameworks, Gas Adsorption, Uptake Prediction, Machine Learning Interatomic Potential, Adsorption Energy

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Spatio-Temporal Techno-Economic Assessment of Power-to-Olefins Production

Hira Mahmood, Jay Liu*

Department of Chemical Engineering, Pukyong National University, Korea

ABSTRACT

Methanol-mediated Power-to-Olefins (PtO) systems represent a promising pathway capable of reducing emissions by ~60% depending on electricity carbon intensity. However, their techno-economic performance depends on geographic renewable resource quality and technological progress. This study presents combined spatial and temporal techno-economic assessment of PtO pathway across three countries. Detailed process model is developed using commercial simulator, incorporating polymer electrolyte membrane electrolyzer-based hydrogen production powered by hybrid renewable electricity. Spatial variability is captured using country-specific electricity prices, financial parameters and resource conditions to quantify production costs, energy requirements, and cost drivers. Furthermore, forward-looking temporal analysis is conducted for baseline scenario, 2026, 2030, 2040, and 2050 to evaluate long-term competitiveness under evolving energy system conditions. The minimum olefin selling price ranges from 1.5 to 2.49 $/kg. The United States exhibits the lowest cost due to favorable renewable electricity conditions, while South Korea shows the highest values, reflecting higher electricity costs and lower renewable capacity factors. Temporal projections indicate that declining renewable electricity costs and technology learning effect could reduce production costs by approximately 15–30% by 2050. The results demonstrate that geographic deployment and technological evolution determine PtO competitiveness, emphasizing the need for spatially resolved forward-looking strategies for large-scale decarbonization of olefin production.

KEYWORDS

Power-to-Olefins, Techno-economic assessment, Spatio-temporal analysis, Renewable electricity

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

xThermoGNN: An Interpretable Multi-Level Graph Neural Network for Predicting the Decomposition Heat of Reactive Chemicals

Hong Wang[1,2], Meng Qi[1,2], Yi Liu[1,2,*]

[1]*State Key Laboratory of Chemical Safety, China University of Petroleum (East China), China*
[2]*College of Chemistry and Chemical Engineering, China University of Petroleum (East China), China*

ABSTRACT

The heat of decomposition (ΔH_d), a core parameter characterising energy release intensity during decomposition reactions, is critical for hazard identification, safety classification, and reaction risk assessment. However, conventional experimental determination is costly, time-consuming, and poses safety risks for high-energy samples, failing to meet high-throughput screening demands in early-stage R&D. Although traditional Quantitative Structure-Property Relationship (QSPR) methods offer a feasible prediction approach, linear models struggle to capture complex nonlinear structure-decomposition heat relationships and exhibit insufficient generalisation across multiple substance categories (e.g., nitro compounds, high-energy non-nitro compounds, organic halides). This study proposes xThermoGNN, an interpretable Graph Neural Network for end-to-end prediction of decomposition heat from molecular structures. The model employs multi-level representation learning on molecular graphs, extracting structural information from atoms, chemical bonds, and molecular fragments, with adaptive hierarchical feature fusion via graph attention mechanisms. Based on 482 exothermic reactive chemicals from DSC experiments, xThermoGNN achieved high-precision predictions on an independent multi-category test set. Furthermore, attention-weight-based interpretability analysis reveals that atom-level representations identify element types, bond-level representations characterise chemical bond types, and fragment-level representations aggregate functional group features. These complementary, multi-granularity representations provide scientific insights into intrinsic structure-property relationships governing decomposition heat.

KEYWORDS

reactive chemicals; decomposition heat; graph neural network; explainable artificial intelligence; thermal safety assessment

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POSTER

13:30~14:30 · Poster Session P2 · Engineering Building D

Machine Learning Aided Performance Prediction of Biomass Gasificaiton

Xin Du[1,2], Junghwan Kim[3,*], Yi Liu[1,2,*]

[1] *State Key Laboratory of Chemical Safety, China University of Petroleum (East China), China*
[2] *College of Chemistry and Chemical Engineering, China University of Petroleum (East China), China*
[3] *Department of Chemical and Biomolecular Engineering, Yonsei University, Korea*

ABSTRACT

Biomass gasification is an effect approach for sustainable syngas production and carbon-neutral energy conversion. However, conventional chemical process simulation methods often require complex reactor modeling and extensive parameter calibration, which limits its applicability for rapid evaluation of different biomass feedstocks. In this study, a machine learning-based framework was developed to predict gas yields from biomass gasification as a supplement or alternative to traditional kinetic modeling. Experimental data from literature, including biomass proximate and ultimate analyses, gasification temperature, equivalence ratio, and steam-to-biomass ratio, were used as model inputs, while the volume fraction yields of H2, CO, CO2, and CH4 were selected as prediction targets. Ensemble models including Random Forest (RF), eXtreme Gradient Boosting (XGBoost) and Categorical Boosting (CatBoost), and kernel-based machine learning method Support Vector Machine (SVM) were employed. The proposed model enables rapid estimation of syngas composition with different operation conditions and various biomass sources while maintaining satisfactory prediction accuracy. SHAP analysis was used to interpret the positive or negative impact of each input feature to output gas yield. An Aspen Plus gasification model was also developed as a comparison to the machined learning method. Result shows that the machine learning approach outperformed the baseline Aspen Plus model.

KEYWORDS

Biomass gasification, syngas yield, machine learning, data-driven prediction, process simulation

PSE ASIA 2026 · PART III

Proceedings

Full Papers

Nine full papers contributed to the PSE ASIA 2026 proceedings, presented alongside the corresponding oral and poster sessions of the symposium.

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- **OS-A3-02** Abhishek Kumar Pandey
- **OS-B4-02** Qingqing Zhang
- **OS-B4-03** Tian Qiu
- **OS-B4-04** Rohit Kumar Yadav
- **OS-C4-01** Sungmin Lee
- **P-13** Chonghyo Joo
- **P-15** Cuimei Bo
- **P-49** Kyojin Jang
- **P-100** Sangdeok Kim

OS-A3-02

SESSION

A3 · July 6 (Mon) 10:15~10:30

PRESENTER

Abhishek Kumar Pandey

Targeting CO2 emission in a Carbon Capture and Utilisation facility with epistemic uncertainty in the parameters

Abhishek Kumar Pandey*, Santanu Bandyopadhyay

Indian Institute of Technology Bombay, India

The full paper follows on the next page.

Research Article - Peer Reviewed Conference Proceeding
PSE ASIA 2026 - 12th Asian Symposium on Process System Engineering
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Targeting CO_2 emission in a Carbon Capture and Utilisation facility with Epistemic Uncertainty in the parameters

Abhishek K. Pandey[a]*, Santanu Bandyopadhyay

[a] Indian Institute of Technology Bombay, Department of Energy Science and Engineering, Mumbai, Maharashtra, India
[b] Indian Institute of Technology Bombay, Department of Energy Science and Engineering, Mumbai, Maharashtra, India
* Corresponding Author: abhishek.pandey@iitb.ac.ina

ABSTRACT

Mitigating CO_2 emissions from industries is the 13th Sustainable Development Goal (SDG) set by the United Nations. Carbon capture and utilisation (CCU) is an emerging technology that significantly reduces CO_2 emissions from industries by capturing CO_2 and utilising it for economic benefits. The CCU facility in industrial parks is designed to maximise CO_2 capture with exact parameters using pinch techniques. Lack of system knowledge and unavailability of past data at the design stage introduce epistemic uncertainty in parameters. The existing literature reports the incorporation of epistemic uncertainty with the pinch technique to minimise resource requirement. This work focuses on minimising CO_2 emissions from a CCU facility. The mathematical formulation presented in this paper incorporated epistemic uncertainty in parameters using interval numbers. The Best-Worst approach and pinch analysis are used to determine the minimum CO_2 emission from a CCU facility. The best-case and the worst-case for CO_2 minimisation are identified, and the pinch technique is applied to obtain the solution. The highest and lowest values of minimum CO_2 emission are the two extreme solutions and define the interval for CO_2 emission from the CCU facility. The optimisation approach is demonstrated through an illustrative case study on the CCU facility.

Keywords: CCU, Epistemic uncertainty, Pinch Analysis, Interval linear programming,

INTRODUCTION

CO_2 emissions from the industries are a major contributor to climate change, but industries like cement, iron and steel, and refineries are the main drivers of the economy in developing countries. For example, 3.92% of global CO_2 is released through cement production (Crippa et al., 2023), petrochemical refineries released around 4-10% of global CO_2 emissions (Pivac et al., 2024), 2.8 billion tons of CO_2eq to global GHG emissions came from the iron and steel industry in 2019 (Ren et al., 2025). Technologies like Carbon Capture and Utilisation (CCU) aim to mitigate CO_2 emissions by capturing flue gases from the process industries and utilising the captured CO_2 for the synthesis of marketable chemicals. A CCU facility is a sustainable approach as it reduces industrial CO_2 emissions and increases revenue by selling other products which are synthesised from captured CO_2. A CCU facility is a pipeline network which connects industries which emit flue gas, mainly CO_2, with a CO_2 capturing unit and the industries where CO_2 is required. A CCU facility is a source-sink network, which is also referred to as a CO_2-integration network.

Pinch analysis is used in industries to promote sustainability. A typical pinch application on a deterministic CO_2-integration network increases CO_2 reutilisation and flue gas emission. Pinch analysis was initially developed to optimise the utility of heat exchanger networks in process industries (Linhoff and Flower, 1978). The application of pinch analysis is extended to different domains, and different pinch techniques were developed. For example, the Limiting Composite Curve (Wang and Smith, 1994), Material Reuse Pinch Diagram (El-Halwagi et al., 2003), and Source Composite Curve (Bandyopadhyay, 2006) were developed for different applications. In the context of the CO_2-integration network, the Source Composite Curve (SCC) is a tabular method that provides the minimum unutilised flue gas released into the atmosphere from a network with deterministic parameters.

The lack of knowledge and unavailability of past data about system parameters require the designers to deal with parameters with epistemic uncertainty. Targeting the CO_2-integration network under epistemic conditions is important due to the possibility of multiple solutions to proceed further with network design. The applied methodology to identify the target values in CO_2-integration network also produces different result. Epistemic uncertainty in linear programming problem was addressed using fuzzy linear optimisation approach to provide an interval of freshwater requirement in a fictitious source-sink network (Tan, 2011). The freshwater minimisation problem was modelled using the fuzzy representation of parameters. The epistemic uncertainty was incorporated in modelling of optimisation problem of source-sink network using interval numbers (Bandyopadhyay, 2020). An Interval Linear Programming (ILP) problem was mathematically formulated, which was solved using the Best-Worst method and the Pinch analysis. The existing literature focuses on the minimisation of resource requirement under epistemic conditions. This work emphasizes on the minimisation of waste generation in a source-sink network while accommodating epistemic uncertainty in parameters. Waste generated in source-sink network is equivalent to release of unutilised flue gas from the CO_2-integration network.

The outline of the remaining part of this paper is as follows. A CO_2-integration network is explained, and the mathematical formulation of optimisation problem is presented in the next section. A graphical representation of a CO_2-integration network with epistemic parameters is shown in Figure 1. The solution methodology is explained using mathematical analysis of water reuse. The proposed approach is demonstrated through a case study on a CCU facility. The results from this case study are reported with their physical significance. Summary of this work and possible future research investigations are discussed in the conclusion section.

PROBLEM STATEMENT AND MATHEMATICAL FORMULATION

A CO_2-integration network has four elements: CO_2-sources, CO_2-sinks, a resource and atmosphere. Every element is characterised by two parameters, which are flow and quality. In a CO_2-integration network, a CO_2-source is an industrial plant which emits flue gas, mainly containing CO_2. The flow parameter of CO_2-sources is the rate of emission of flue gas in tonnes per hour. The quality parameter of CO_2-sources is defined as the composition of non-CO_2 gases in the flue gas. CO_2-sources provide flow to the network, and the CO_2-sinks in the network utilise this flow to synthesise their chemical product, urea and dimethyl ether. The flow parameter in CO_2-sinks is tonnes of flue gas per hour required to synthesise its chemical products, and the quality parameter is the acceptable limit to the composition of non-CO_2 gases in the stream of flue gas. A CO_2-integration network is designed for optimal demand and supply match between CO_2-sources and CO_2-sinks. When CO_2-sources are not able to fulfil demands at CO_2-sinks, a resource is utilised. A resource in the CO_2-integration network is an industrial plant from which a stream with a high concentration of CO_2 has to be imported, like a hydrogen production facility. The flow and quality parameter of the resource is the same as CO_2-sources, but a cost is associated with it. The atmosphere in the CO_2-integration network absorbs unutilized flue gas and does not impose any limit on the flow and quality of absorbed flue gas. The flow and quality parameter of CO_2-sources and sinks are functions of production rate, operating life, economic viability, and market demand. These factors introduce epistemic uncertainty in the flow and quality parameter of sources and sinks in the CO_2-integration network. Figure 1 presents the CO_2-integration network with epistemic parameters.

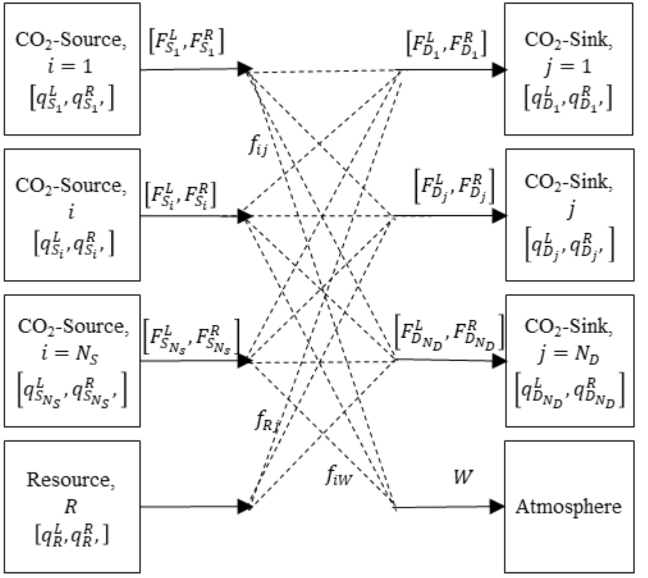

Figure 1: General structure of CO_2-integration network with epistemic parameters

For the CO_2-integration network, the quality is typically represented using an inverse numerical scale. It means that a higher numerical value indicates a low proportion of CO_2.The purpose of the CO_2-integration network is to reduce the environmental impact due to emissions from the CO_2-sources, and hence it is designed to minimise the release of unutilized flue gas into the atmosphere. The optimisation problem can be stated as follows:

- A set of N_S CO_2-sources exists to provide streams with associated quality and flow. Quality of i_{th}

CO₂-source is defined by an interval number $[q^L_{S_i}, q^R_{S_i}]$. Similarly, the flow provided by i_{th} CO₂-source is defined as $[F^L_{S_i}, F^R_{S_i}]$.

- A set of N_D CO₂-sinks needs to be fulfilled with quality and flow. The quality interval that j_{th} CO₂-sink can accept is $\left[q^L_{D_j}, q^R_{D_j}\right]$. The flow provided to j_{th} CO₂-sink must fall within given limits, i.e. $\left[F^L_{D_j}, F^R_{D_j}\right]$.
- A resource R acts as an external source. The resource is also required to meet the CO₂-sinks quality and flow requirements. The quality interval of resource is $[q^L_R, q^R_R]$.
- The atmosphere W is the last structural element of the CO₂-integration network. All the unutilised flow is directed toward the atmosphere. It does not have any restriction on the flow and quality of the stream it can accept and act as an external CO₂-sink.
- The objective is to optimise the CO₂-intergation network for minimum release of unutilized flue gas into the atmosphere and to reduce the environmental impact of CO₂-sources.

The mathematical formulation of the optimisation problem for the CO₂-intergation network, presented in Figure 1, is as follows:

$$Min \sum_{i=1}^{N_S} f_{ij} \quad (1)$$

Subjected to the following constraints:

$$\sum_{j=1}^{N_D} f_{ij} + f_{iw} = \left[F^L_{S_i}, F^R_{S_i}\right] \forall i \quad (2)$$

$$\sum_{i=1}^{N_S} f_{ij} + f_{Rj} = \left[F^L_{D_j}, F^R_{D_j}\right] \forall j \quad (3)$$

$$\sum_{i=1}^{N_S} f_{ij}\left[q^L_{S_i}, q^R_{S_i}\right]. + \left[q^L_R, q^R_R\right] \times f_{Rj} \leq \left[F^L_{D_j}, F^R_{D_j}\right] \times \left[q^L_{D_j}, q^R_{D_j}\right] \quad \forall j \ (4)$$

The objective function of this formulation is to minimise the total emission of unutilized CO₂ into the atmosphere in Eq(1). This objective function is subjected to flow-balance constraints, which are Eq(2) and Eq(3), and a quality-load balance constraint, i.e., Eq(4). f_{ij} is the flow from CO₂-source i to CO₂-sink j, f_{iW} is defined as the flow from CO₂-source i to the atmosphere, and f_{Rj} is the flow from resource R to CO₂-sink j. $F^L_{S_i}$ and $F^R_{S_i}$ represent the lower and upper flow limit from the CO₂-source i, respectively. The summation of all the flows from CO₂-source i has to be within $F^L_{S_i}$ and $F^R_{S_i}$. Similarly, the total flow CO₂-sink j can accept has to fall within $F^L_{D_j}$ and $F^R_{D_j}$, where $F^L_{D_j}$ is the lower limit, and $F^R_{D_j}$ is the upper limit of the flow for CO₂-sink j. $q^L_{S_i}$ represents the lower limit of quality provided by CO₂-source i, and $q^R_{S_i}$ is the upper limit of that quality. All the streams, from CO₂-source i, must have quality value between $q^L_{S_i}$ and $q^R_{S_i}$. Similarly, all the flow streams from any resource R have quality in the range of $[q^L_R, q^R_R]$. Likewise, for any sink j, the maximum quality it can accept must be in the range$\left[q^L_{D_j}, q^R_{D_j}\right]$. Where $q^L_{D_j}$ is the lower limit, and $q^R_{D_j}$ is the upper limit of allowable quality any CO₂-sink j can accept. This problem is solved using the proposed methodology.

SOLUTION METHODOLOGY

In this work, the stated problem is approached through a sequential combination of two methods: the Best-Worst method and the Source Composite Curve (SCC), respectively. The optimisation problem shown in Eq(1-4) is an interval linear programming problem. Among multiple methods, the Best-Worst approach is one of the methods to reduce an interval linear programming problem into a linear programming problem (Saocheng, 1994). The Best-Worst approach identifies the most favourable and most hostile conditions in which the objective functions can be optimised. The most favourable condition to minimise the release of unutilized flue gas into the atmosphere is when the CO₂-sources emit flue gas at a low rate with a low amount of non-CO₂ gases into the flue gas stream, and the CO₂-sinks demand CO₂ at a high flow rate with a high proportion of non-CO₂ gases in the flue gas stream. Similarly, the most hostile conditions in which the release of unutilized flue gas can be minimised is when the flue gas is emitted at a high rate from the CO₂-sources with a high amount of non-CO₂ gases in the flue gas stream, while CO₂-sinks require flue gas at a low flow rate and with low composition of non-CO₂ gases in the flue gas stream. The most favourable condition is referred to as best-case, and the most hostile one is called worst-case, to minimise the release of unutilized flue gas into the atmosphere. The identification of best and worst cases reduces interval linear programming into two linear programming problems. Each of them is solved using SCC separately. SCC is a graphical pinch technique which determines the minimum waste generation in a source-sink network. In the CO₂-integration network, the extended application of SCC would provide the minimum unutilized CO₂ released into the atmosphere for each case. The solution provided by SCC in the best-case is the minimum among minima in all possible combinations of parameter values. The best-case solution for the CO₂-integration network is the lowest value of minimum unutilized flue gas released into the atmosphere. Mathematically, solving the worst-case with SCC provides the maximum among minima in all linear programming problems possible due to an infinite combination of parameter values. In the CO₂-integration network, the highest value is the release of the minimum unutilized flue gas into the atmosphere. The necessary tools, which constitute the proposed methodology, and their relevant significance are discussed. The proposed methodology is explained in the following steps:

Step 1: Set the flow and quality parameter of CO_2-Sources to the lower limit of the given interval value. The flow and quality parameter of each CO_2-Sinks is set to its upper limit.

Step 2: Solve the parameter combination set in Step 1 for the minimum release of unutilised flue gas using SCC. This provides the lowest value of minimum unutilized flue gas from the network.

Step 3: Set the flow and quality parameter of CO_2-Sources to the upper limit and that of CO_2-Sinks to the lower limit.

Step 4: The parameter combination, arranged in Step 3, is solved for the minimum release of unutilized flue gas by SCC. This provides the worst-case solution for the CO_2-integration network.

The proposed methodology is demonstrated through an illustrative example.

ILLUSTRATIVE EXAMPLE

Capturing CO_2 from flue gas and utilising it to further synthesise other marketable products is a sustainable way to mitigate flue gas emissions. A case study is adapted from Li et al (2024). The presented case study includes a CO_2-integration network comprising four industrial plants that act as CO_2-sources, three chemical synthesis units that act as CO_2-sinks, an imported CO_2 stream that is a resource, and the atmosphere, which accepts unutilised flue gas from the network. This CO_2-integration unit acts as a Carbon Capture and Utilisation (CCU) unit. The flow and quality data are deterministic in the case study presented in Li et al (2024). A hypothetical margin is introduced in the data while adapting to account for epistemic uncertainty in the parameters. Table 1 and 2 shows the complete data for the case study.

Table 1: Process data for CO_2-sources in the illustrative example

CO_2-Sources	**Quality (Wt%)**	**Flow(t/h)**
Ammonia Plant	[0.018, 0.020]	[100.0, 110.0]
Ethanol Plant	[0.045, 0.050]	[34.2, 37.62]
Cement Palnt	[0.630, 0.700]	[193.0, 212.3]
Coal-fired Power Plant	[0.774, 0.860]	[921.0, 1013.1]

Table 2: Process data for CO_2-sinks in the illustrative example

CO_2-Sinks	**Quality (Wt%)**	**Flow(t/h)**
Urea Plant	[0.010, 0.011]	[113.400, 126.000]
Methanol Plant	[0.015, 0.017]	[219.285, 243.650]
Dimethyl EtherPlant	[0.140, 0.154]	[139.140, 154.600]

Imported CO_2 is available with 100% purity. The proposed methodology is applied to this example. The flow and quality parameters of CO_2-sources are set to their lower limit, and those of CO_2-sinks are set to their upper limit to obtain the best-case solution in this problem. The SCC is applied to this combination of parameters, and the minimum flue gas released into the atmosphere, provided by LCC, is 1072.928 t/h. The total flue gas emitted by CO_2-sources is 1248.200 t/h, and total flue gas required at CO_2-sinks is 524.25 t/h under best-case conditions. 1072.928 t/h is the lowest among all minima for unutilized flue gas released into the atmosphere. No other value of flue gas emission from the network lower than 1072.928 t/h is possible without bringing flow and quality dissatisfaction at CO_2-sinks. 1072.928 t/h is the best-case solution for minimum unutilised flue gas release from the CO_2-integration network. The best case presents the most optimistic scenario as CO_2-sources provide their least flow with the purest quality, and CO_2-sinks also demand the highest flow and the worst quality.

The most pessimistic conditions for minimum release of unutilised flue gas are when the rate of providing flue gas to the network by CO_2-sources is the highest, with the worst available quality, and CO_2-sinks are consuming the least flow at the purest quality. These are the worst conditions to minimise the release of unutilised flue gas from the CO_2-integration network. The parameters are set to the values corresponding to the worst-case condition. The unutilised flue gas optimisation problem, with worst-case conditions, is a linear optimisation problem which is solved using SCC. 1197.083 t/h is the minimum unutilised flue gas released from the CO_2-integration network under worst-case conditions. The total flue gas requirement at CO_2-sinks is 471.825 t/h, and the CO_2-source produces 1373.020 t/h corresponding to worst-case conditions. The presented unutilised flue gas problem is an ILP, in which an infinite number of linear programming problems are possible with the objective function of minimising flue gas emission from the CO_2-integration network; 1072.928 t/h is the least and 1197.083 t/h is the highest of all the optima possible. This solution signifies that no CO_2-integration network can have a value of minimum unutilised flue gas less than 1072.928 t/h and that is higher than 1197.083 t/h while satisfying flow and quality demands at all CO_2-sinks.

CONCLUSION

CO_2-integration in process industries promotes their economic viability, mitigates flue gas emissions and reduces air pollution. CO_2-integration is a type of source-sink networks which are designed using Pinch techniques.

Parameters like operating life, flue gas emission, and production rate are epistemic in nature as they are controlled by market forces, and previous data is ineffective in the accurate estimation of these parameters. The epistemic uncertainty in these parameters results in epistemic flow and quality at CO_2-Sources and CO_2-Sinks. The design of a CO_2-integration network, employed in an epistemic environment, is done using the Pinch technique with the Best-Worst approach. This work presents a mathematical formulation to minimise the flue gas emission from the CO_2-integration network, which is solved using the Best-Worst approach and LCC. The Best-Worst approach reduces the given ILP problem into two linear optimisation problems which corresponds to two extreme conditions for optimizing objective function. The solution from these two LP problems represents the highest and the least value of minimum flue gas emission. These two extreme LP problems is solved using SCC and then the best-case and worst-case solution is obtained. This methodology is demonstrated using a case study on a CO_2-integration network. The proposed methodology provided the highest and lowest value for minimum flue gas emission, that are 1072.928 and 1197.083 t/h, respectively. The lower limit of minimum flue gas emission shows that no network can exist which emit flue gas less than 1072.928 while fulfilling demands of flow and quality at CO_2-sinks. This is notable that if flue gas emission is decreased further, the constraint satisfaction in CO_2-integration network will be compromised. The upper limit, that is 1197.083 t/h, is the highest value among all minima optimized for any possible combination of parameter values. Any CO_2-integration network, for the given problem, which emits flue gas higher than 1197.083 t/h is operating sub-optimally. The design of CO_2-integration network according to worst-case conditions assures constraint satisfaction for all possible parameter values. This work discussed the physical significance of both extreme solutions with respect to level of uncertainty accommodated. This work enables designer to identify suitable flue gas emission at design stage of the CO_2-integration network. This work leads to a target for network design which brings forward possibilities of future discussion on new scheme of network design.

This work focuses on targeting flue gas emission from the CO_2-integration network with epistemic parameters. The designing of networks in an epistemic environment is the future direction in which research can be done to develop a holistic methodology. Network design in an epistemic environment also poses a challenge in identifying the critical parameters and conditions for the robustness of a network against uncertainty. This work shows the significance of flue gas emission in designing CO_2-integration networks.

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OS-B4-02

SESSION

B4 · July 6 (Mon) 14:45~15:00

PRESENTER

Qingqing Zhang

PINN-based surrogate modeling and configuration optimization of autothermal green ammonia reactors under wide load operation

Qingqing Zhang, Xudong Zhou, Li Zhou*, Xu Ji

Sichuan University, China

The full paper follows on the next page.

PINN-based surrogate modeling and configuration optimization of autothermal green ammonia reactors under wide load operation

Qingqing Zhang, **Xudong Zhou**, **Li Zhou***, **Xu Ji**

School of Chemical Engineering, Sichuan University, Chengdu 610065, Sichuan, China

*Corresponding author: chezli@scu.edu.cn

ABSTRACT

Volatile renewable energy introduces wide load variations into green ammonia synthesis, creating a need for rapid and repeated reactor evaluation that rigorous mechanistic simulations cannot practically meet. To address this computational bottleneck, this study proposes a residual-attention physics-informed neural network (PINN) surrogate for single-bed adiabatic ammonia reactors. The model incorporates an explicit flow reciprocal feature ($1/F_{in}$) to capture non-linear residence time sensitivities across the full load range, and employs a residual-attention architecture to resolve stiff reaction gradients. Trained on high-fidelity ODE-generated data, the surrogate achieves prediction errors below 1% for both outlet temperature and N_2 conversion, while accelerating inference by approximately four orders of magnitude relative to the reference ODE solver. Exploiting this speed advantage, single-bed surrogates are cascaded to evaluate three inter-bed heat integration configurations for three-bed autothermal ammonia reactors (quench-cooled, series indirect-cooled, and series-parallel split) across load levels from 30 to 100%, with inter-bed split ratios optimized at each load. The series-parallel split configuration achieves the highest NH_3 production across all loads, and at 30–50% load effectively prevents catalyst extinction and thermal runaway through adaptive redistribution of inter-bed split ratios. T-X phase diagram analysis shows that this configuration maintains operating trajectories closest to the thermodynamic equilibrium curve, quantitatively explaining its superior single-pass conversion. These results establish the series-parallel split design as the preferred architecture for load-flexible green ammonia plants and demonstrate the viability of feature-augmented PINNs as computationally efficient surrogates for surrogate-based operational optimization.

Keywords: *Green Ammonia; Physics-Informed Neural Networks (PINN); Autothermal Reactor; Process Intensification*

1. Introduction

Ammonia synthesis via the Haber-Bosch process accounts for approximately 1.3% of global CO_2 emissions [1]. Interest in green ammonia, produced by electrolytic hydrogen from intermittent renewable electricity, has grown substantially as a route to decarbonize both fertilizer production and long-distance energy transport [2,3]. Unlike conventional plants optimized for steady-state baseload operation, green ammonia facilities must accommodate load variations on minute-to-hour timescales, operating across 30 to 100% of rated capacity while maintaining catalyst integrity and conversion efficiency [4,5].

Operational setpoint adjustment across load levels requires repeated reactor evaluations to identify feasible and near-optimal operating conditions. Rigorous one-dimensional pseudo-homogeneous plug-flow models provide accurate predictions but require iterative ODE integration, typically on the order of seconds per simulation [5]. When embedded in optimization loops requiring hundreds of function evaluations, the cumulative computation time becomes a practical bottleneck. Data-driven surrogates offer microsecond-scale inference but may violate physical constraints under extrapolation, particularly when applied to multi-bed cascades spanning wide load ranges [7,8]. Physics-informed neural networks (PINNs) address these limitations by embedding governing differential equations as soft constraints during training [9,10], improving generalization with limited data. PINNs have been applied to CO_2 methanation [11] and plug-flow reactor control [12]. A concurrent study [13] applied PINNs to ammonia synthesis CFD but focused on single-bed fluid dynamics at fixed load; systematic configuration comparison under wide load ranges has not been reported.

This paper makes two contributions. First, a residual-attention PINN surrogate is developed for a single adiabatic ammonia catalyst bed, incorporating an explicit flow reciprocal input feature ($1/\mathrm{F}_{\mathrm{in}}$) to resolve residence time sensitivity across the full 30 to 100% load range. Second, single-bed surrogates are cascaded to compare three inter-bed heat integration configurations (quench-cooled, series indirect-cooled, and series-parallel split) through surrogate-based optimization of split ratios at each load level, with T-X phase diagram analysis providing a thermodynamic basis for interpreting performance differences.

2. Methodology

2.1 Single-bed reactor model

The adiabatic catalyst bed is modeled as a steady-state one-dimensional pseudo-homogeneous plug-flow reactor. The governing equations are the $\mathrm{N_2}$ mass balance,

$$\frac{d\alpha}{dV} = \frac{0.5 \cdot r_{\mathrm{NH_3}}}{F_{\mathrm{N_2},0}} \tag{1}$$

and the energy balance,

$$\frac{dT}{dV} = \frac{-\Delta H_r \cdot 0.5 \cdot r_{\mathrm{NH_3}}}{\sum_i F_i \cdot C_{p,i}} \tag{2}$$

where $\alpha \in [0,1]$ is the dimensionless fractional $\mathrm{N_2}$ conversion, V is catalyst volume ($\mathrm{m^3}$), $r_{\mathrm{NH_3}}$ is the volumetric $\mathrm{NH_3}$ formation rate ($\mathrm{mol \cdot m^{-3} \cdot h^{-1}}$) computed from a modified Temkin-Pyzhev expression consistent with the Keestra et al. [14] calibration, $F_{\mathrm{N_2},0}$ is the inlet $\mathrm{N_2}$ molar flow ($\mathrm{mol} \cdot$

h^{-1}), T is temperature (K), ΔH_r is the reaction enthalpy ($J \cdot mol^{-1}$), where $\Delta H_r < 0$ for the exothermic ammonia synthesis reaction, such that $dT/dV > 0$ for positive reaction rate $r_{NH_3} > 0$. And $C_{p,i}$ are species molar heat capacities evaluated from standard polynomial correlations [15]. Boundary conditions are $\alpha(0) = 0$ and $T(0) = T_{\text{in}}$.

2.2 PINN surrogate formulation

The PINN takes nine input features: $\boldsymbol{x} = \left[V, F_{\text{in}}, T_{\text{in}}, P, y_{\text{H}_2}, y_{\text{N}_2}, y_{\text{NH}_3}, y_{\text{Ar}}, 1/\text{F}_{\text{in}}\right]$. The explicit inclusion of $1/\text{F}_{\text{in}}$ feature is physically justified as follows. In Eq. (1), the conversion gradient scales inversely with molar flow at fixed kinetics. Without this feature, the network must learn a division relationship from output-input data alone, which is poorly constrained at low loads where F_{in} drops by an order of magnitude. Including $1/\text{F}_{\text{in}}$ directly provides residence time scaling information and substantially reduces prediction error at 30 to 50% load, as confirmed by an ablation study not shown for brevity.

The network consists of five fully-connected residual blocks with 512 neurons each, Tanh activation, LayerNorm, and a multi-head self-attention module (8 heads), as illustrated in Fig. 1. The total training loss is

$$L = \lambda_{\text{data}} L_{\text{data}} + \lambda_{\text{PDE}} L_{\text{PDE}} + \lambda_{\text{IC}} L_{\text{IC}} \tag{3}$$

where L_{data} enforces agreement with 40 steady-state ODE-generated training samples, L_{PDE} penalizes violation of Eqs. (1) and (2) at 32,768 Sobol collocation points, and L_{IC} enforces inlet boundary conditions. Loss weights are $\lambda_{\text{data}} = 1.0$, $\lambda_{\text{PDE}} = 0.2$, and $\lambda_{\text{IC}} = 5.0$. The high weight on L_{IC} suppresses inlet drift accumulated through the volume coordinate. Training uses AdamW with with a learning rate of 10^{-4} over 1500 epochs with ReduceLROnPlateau scheduling. Table 1 summarizes the full architecture and training configuration.

Table 1. PINN architecture and training hyperparameters.

Category	Hyperparameter	Setting
Architecture	Residual blocks × neurons	5 × 512
	Activation function	Tanh
	Attention heads	8
	Normalization	LayerNorm
Training	Optimizer	AdamW, lr = 1e-4
	Epochs	1500
	Data batch / physics batch	40/ 3200
Loss weights	λ_{data} / λ_{PDE} / λ_{IC}	1.0 / 0.2 / 5.0
Input features	V, F_{in}, T_{in}, P, y_{H_2}, y_{N_2}, y_{NH_3}, y_{Ar}, $1/\text{F}_{\text{in}}$	9
Outputs	α (N_2 conversion), T_{out}	2

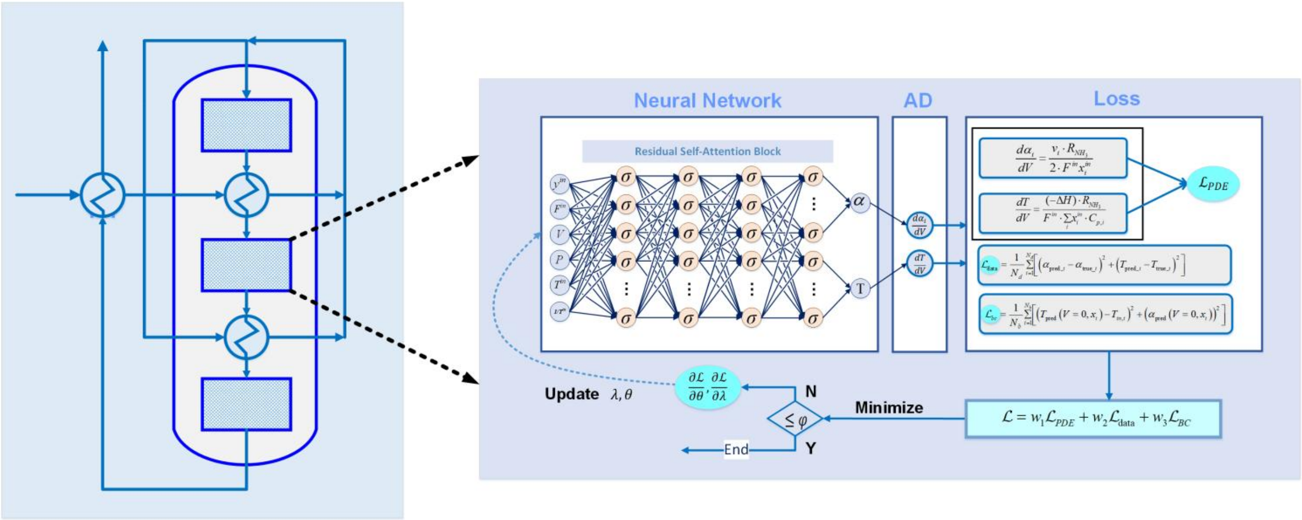

Fig. 1. Architecture and training framework of the residual-attention PINN, including the reactor physics constraints, network structure, and composite loss function.

2.3 Three-bed system assembly and configuration definitions

Three catalyst beds of equal volume ($V_{bed} = 6.9\text{m}^3$ each, $V_{total} = 20.7\text{m}^3$) are assembled with inter-bed heat exchangers. Three heat integration configurations are compared, as illustrated in Fig. 2.

Config A (quench-cooled): The main feed is preheated in a feed-effluent heat exchanger. Cold bypass streams at split ratios R_1 and R_2 are injected between successive beds to reduce inter-bed temperature.

Config B (series indirect-cooled): The full process stream flows sequentially through all heat exchangers and beds without bypass. This configuration has no inter-bed flow control degrees of freedom.

Config C (series-parallel split): Two additional bypass branches decouple feed preheating and inter-bed cooling heat duties. Bypass fraction R_B controls flow through inter-bed exchangers HX_1 and HX_2; bypass fraction R_C controls flow through feed preheater HX_3. This decoupling provides independent thermal management at each load level.

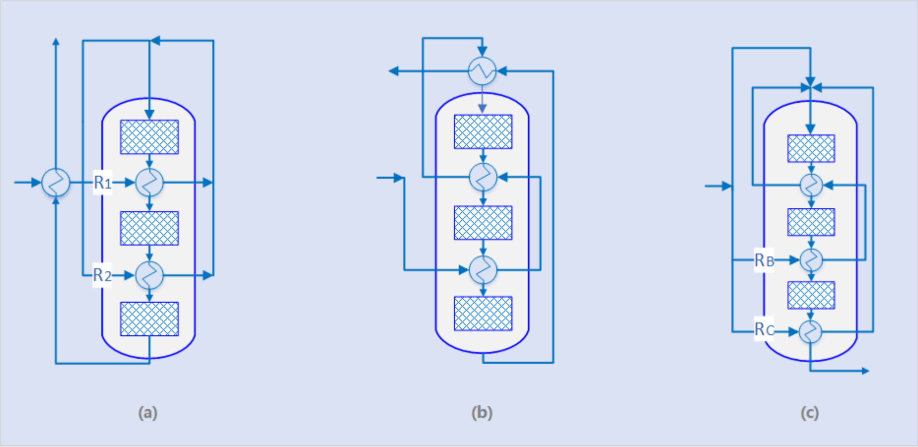

Fig. 2. Three inter-bed heat integration configurations: (a) quench-cooled (Config A); (b) series indirect-cooled (Config B); (c) series-parallel split (Config C).

Single-bed PINN surrogates are cascaded with NTU-ε heat exchanger models and Newton-Raphson enthalpy-balance stream mixing nodes to simulate the three-bed system. The split ratios (R_1, R_2 for Config A; R_B, R_C for Config C) enter the cascade as system-level decision variables that determine each bed's inlet temperature, flow rate, and composition; they are not direct PINN inputs but act through the bed-level boundary conditions. For each configuration and load level, a differential evolution global search followed by SLSQP local refinement maximizes NH_3 production subject to a bed inlet temperature lower bound of 550 K (ignition constraint) and a bed outlet temperature upper bound of 850 K (catalyst sintering constraint) [16].

3. Results and Discussion

3.1 Surrogate model validation

The PINN surrogate is validated against SciPy-BDF stiff ODE reference solutions across load levels from 30 to 100%, using 256 operating conditions sampled by Sobol sequences not included in the training set. Table 2 summarizes the validation metrics. The PINN achieves R^2 of 0.9913 for N_2 conversion and 0.9931 for outlet temperature, with mean absolute errors of 0.0021 (dimensionless) and 2.3 K respectively. These errors fall within the tolerance of industrial process simulation practice, and inference time of 0.03 ms per sample represents a speedup of approximately four orders of magnitude relative to the SciPy-BDF solver (approximately 250 ms per evaluation). This computational advantage enables the multi-start global optimization sweeps described in Section 3.2.

Table 2. Validation metrics of the PINN surrogate on 256 Sobol-sampled test conditions across 30–100% plant load.

Configuration	R^2 (α)	R^2 (T_{out})	MAE (α)	MAE (T(K))	Inference time (ms)
PINN (proposed)	0.9913	0.9931	0.0021	2.3	0.03
ODE solver (SciPy-BDF)	Reference	Reference	-	-	~250

Fig. 3 shows the predicted axial profiles of N2 conversion and outlet temperature against the SciPy-BDF reference for a representative operating condition ($T_{\text{in}} = 623.5\ K$, $P = 120.4\ bar$). The PINN trajectory tracks the reference closely throughout the reactor volume for both outputs, confirming that the embedded mass and energy balance constraints enforce physically consistent spatial derivative profiles, rather than merely interpolating between endpoint values.

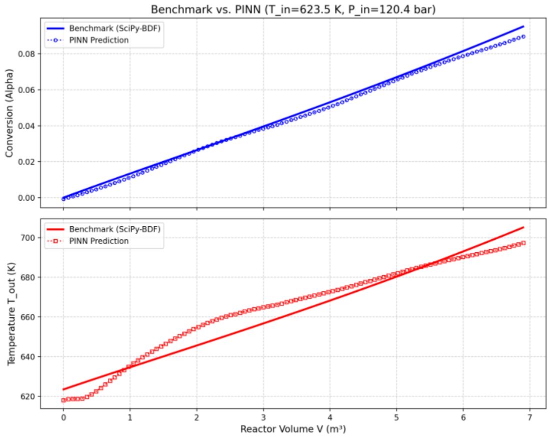

Fig. 3. Predicted axial profiles of N_2 conversion (top) and outlet temperature (bottom) from the PINN surrogate compared with ODE reference solutions at $T_{\text{in}} = 623.5\ K, P = 120.4\ bar$.

Fig. 4 presents violin plots of the absolute prediction error at 30, 50, 70, and 90% plant load. Conversion and temperature errors remain tightly concentrated near zero at 70 and 90% load, where training data coverage is densest. At 30% load, distributions broaden moderately, consistent with increased extrapolation from the training set at low molar flow rates. Critically, errors at 30% load remain bounded, indicating that the physics constraints prevent the physically divergent predictions that unregularized data-driven models exhibit in low-coverage regions [7].

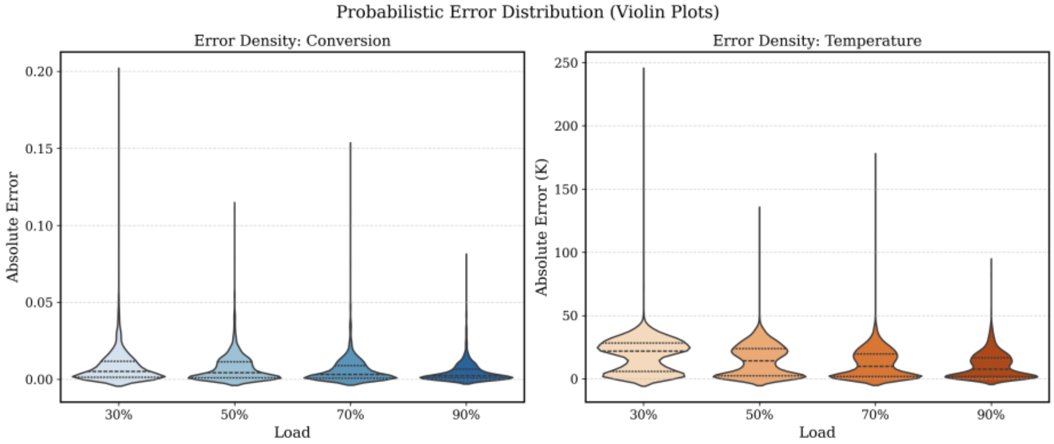

Fig. 4. Distributions of absolute prediction error for N_2 conversion (left) and outlet temperature (right) at 30, 50, 70, and 90% plant load.

Fig. 5 presents parity plots of predicted versus reference N_2 conversion and outlet temperature at all four load levels, with load-specific R^2 and RMSE values annotated in each panel.

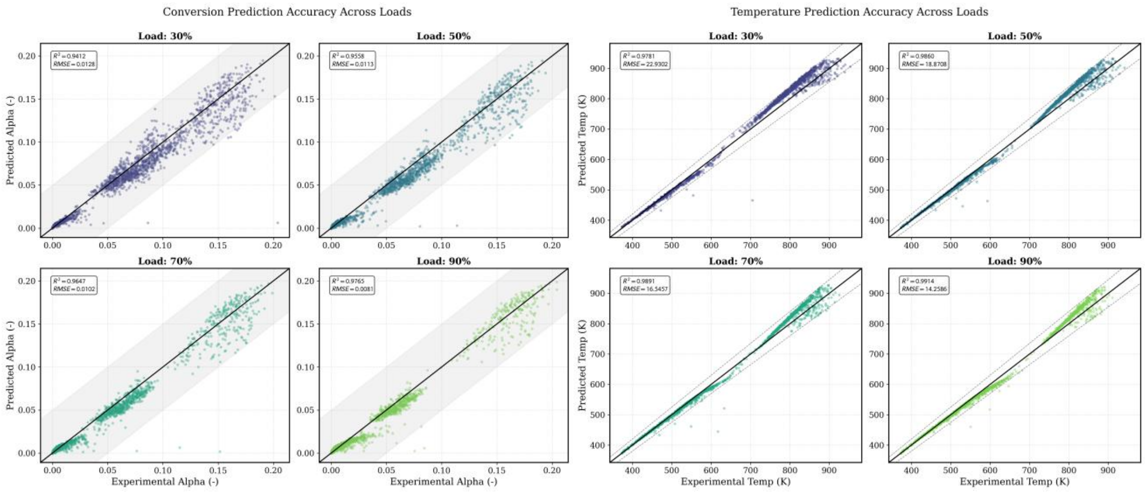

Fig. 5. Parity plots of PINN-predicted versus ODE-reference values for N_2 conversion (left) and outlet temperature (right) at 30, 50, 70, and 90% plant load.

3.2 Configuration comparison: axial temperature profiles and T-X trajectories

Fig. 6 compares axial temperature profiles for the three configurations at 100% load following surrogate-based optimization of available split ratios. Config B exhibits a runaway temperature excursion in Bed 1 that exceeds the 850 K sintering limit, because the absence of inter-bed bypass prevents rejection of the full reaction exotherm. Config A maintains temperatures within bounds but requires a reduced Bed 1 inlet temperature to balance downstream heat loads, leading to underutilization of the Bed 1 catalyst volume in the low-temperature regime. Config C enters Bed 1 at approximately 660 K and maintains a flat-topped temperature plateau near the sintering constraint, which is the physical consequence of the optimizer driving the split fraction to its bound constraint and directing maximum flow through the inter-bed exchanger to reject heat while sustaining the highest allowable reaction temperature. This operating mode maximizes the spatially-averaged reaction rate within Bed 1 subject to the thermal safety constraint.

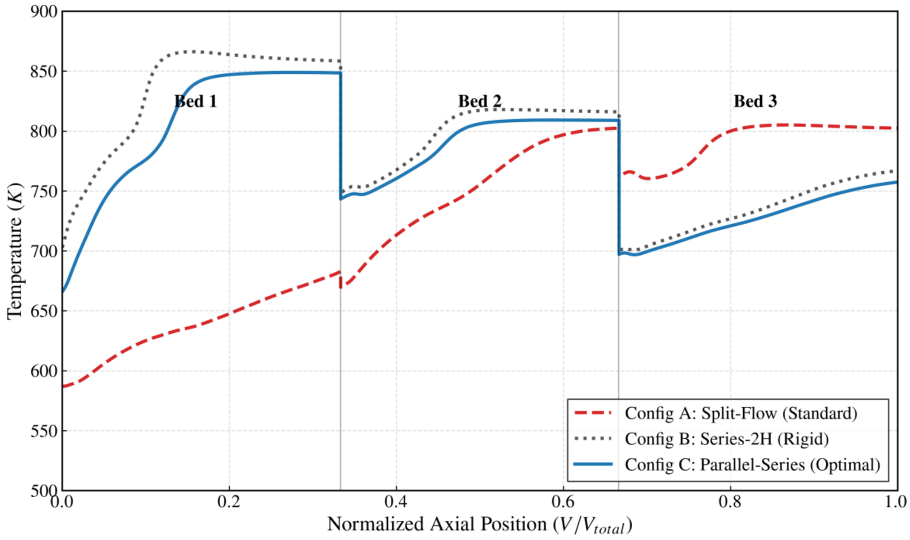

Fig. 6. Axial temperature profiles for Configs A, B, and C at 100% load after surrogate-based optimization. The dashed horizontal line marks the 850 K sintering limit.

Fig. 7 shows the cumulative N_2 conversion profiles along the normalized reactor volume. Config B exhibits a kinetically limited zone in Bed 2 where the trajectory approaches thermodynamic equilibrium and conversion rate falls to near zero. Config C eliminates this plateau through optimized heat integration, achieving productive conversion contributions from all three beds.

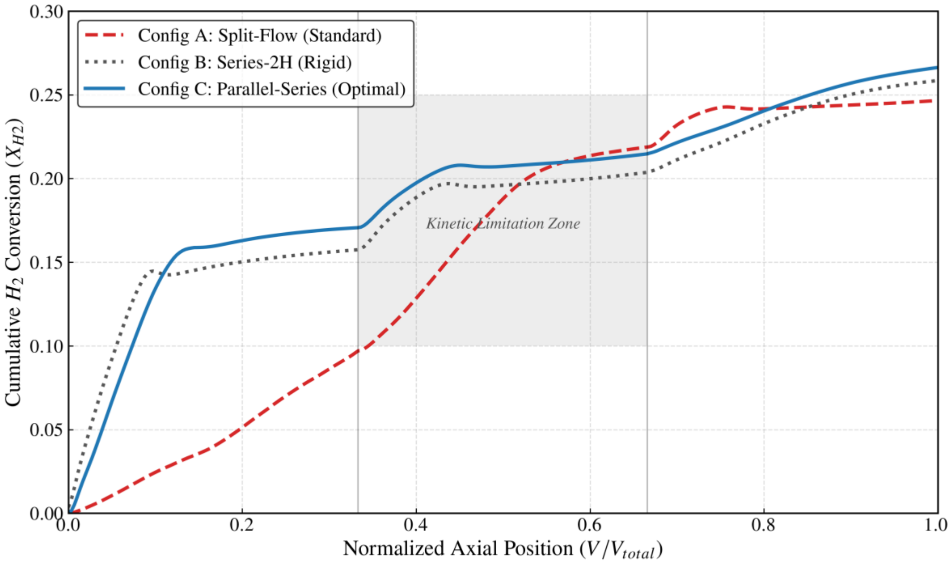

Fig. 7. Cumulative N_2 conversion profiles along the normalized reactor volume for Configs A, B, and C at 100% load. The shaded region in Bed 2 indicates the kinetically limited zone of Config B.

Fig. 8 presents the T-X phase diagram trajectories for all three configurations overlaid on the thermodynamic equilibrium curve at 200 bar. In an autothermal multi-bed reactor, the ideal operating path approaches the equilibrium curve to exploit reaction driving force and then retreats to lower temperature via inter-bed cooling before each successive bed, producing a sawtooth pattern [5,17]. Config A trajectories remain well below the equilibrium curve with narrow sawtooth amplitude, because quench gas injection dilutes both temperature and conversion simultaneously, reducing thermodynamic efficiency. Config B contacts the equilibrium curve prematurely in Bed 2 and Bed 3, arresting further conversion by equilibrium limitation. Config C produces wide, regularly-spaced sawtooth excursions in which Bed 3 tracks closely along the equilibrium curve and retreats sharply upon entering HX_3, before re-entering the final bed section at a point that maximizes further conversion. This behavior quantitatively explains the superior single-pass conversion of Config C.

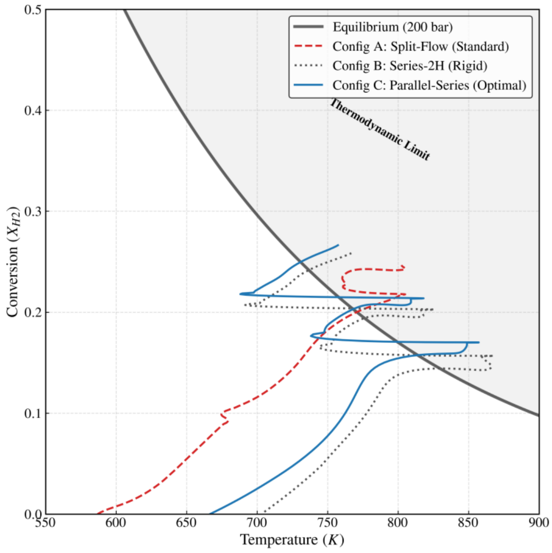

Fig. 8. Temperature–conversion (T–X) phase diagram trajectories for Configs A, B, and C at 200 bar, overlaid on the thermodynamic equilibrium curve.

3.3 Load flexibility comparison

Fig. 9 compares NH_3 production across load levels from 30 to 100%. At loads above 70%, Configs A and C perform comparably, as the available split ratios in Config A have sufficient compensation capacity to approach near-optimal operation. Config B exceeds the sintering constraint at high load without active bypass and is infeasible above approximately 80% load.

At 30 to 50% load, Config C maintains approximately linear production scaling, whereas Config B undergoes a production collapse approaching extinction. The physical mechanism follows directly from the energy balance. At low feed flow rates, the exothermic heat release per unit time decreases substantially. In Config B, whose heat exchanger sizing targets near-nominal flow conditions, inter-bed heat recovery becomes insufficient to preheat the feed to the ignition temperature, triggering thermal collapse of the autothermal loop. Config A partially mitigates this because the cold bypass can be reduced toward zero, but the quench architecture retains a residual preheating deficit because some bypass fraction must remain to maintain bed-to-bed temperature control. Config C decouples these two heat duties: by setting R_B near unity and R_C near zero at 30% load, the optimizer routes essentially all feed flow through the inter-bed exchangers, maximizing heat recovery from Bed 1 and Bed 2 effluents while withholding flow from HX_3 to prevent overcooling of the Bed 3 effluent. This adaptive redistribution maintains bed inlet temperatures above the ignition threshold at all tested loads.

At 100% load, Config C achieves approximately 11,000 kg/h NH_3 production, approximately 10% above Config A. For a commodity chemical produced at scale, this margin represents meaningful improvements in both economic return and energy efficiency [4,18].

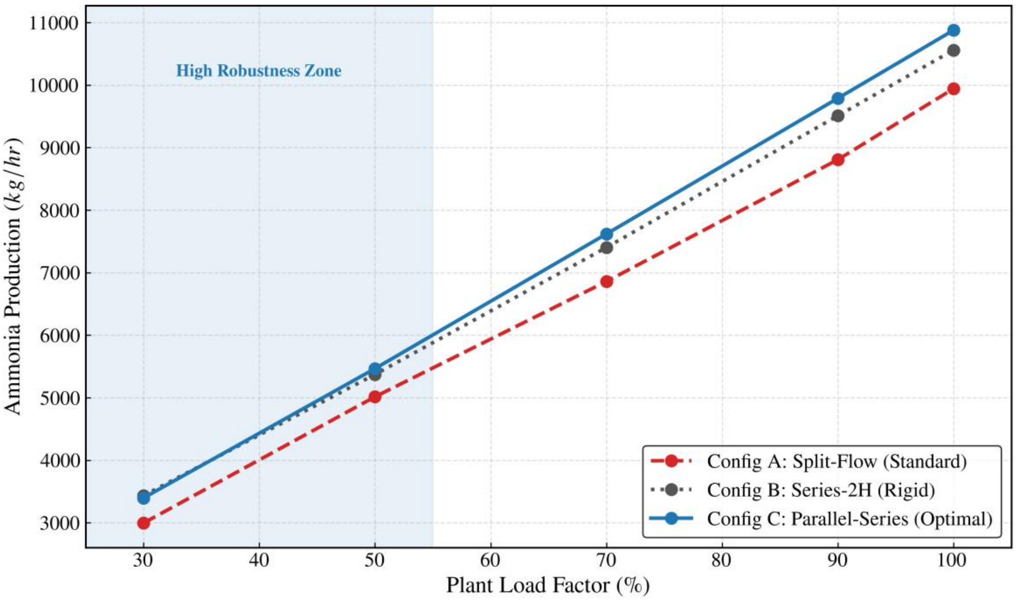

Fig. 9. Ammonia production rate versus plant load factor for Configs A, B, and C. The shaded region highlights the stable operating range of Config C.

Fig. 10 shows the load-dependent optimal split ratios for Config C. At 30% load, R_B approaches 1.0 and R_C approaches 0, indicating maximum recycling of inter-bed heat and minimum diversion to the feed preheater. As load increases beyond 70%, R_B decreases and R_C rises as the reactor transitions from a heat-deficit to a heat-surplus regime. The smooth, monotonic character of these optimal trajectories suggests that a simple scheduled feed-forward control strategy, rather than online real-time optimization, could reproduce the optimizer output to within acceptable tolerance, substantially reducing the control implementation burden in practice [6].

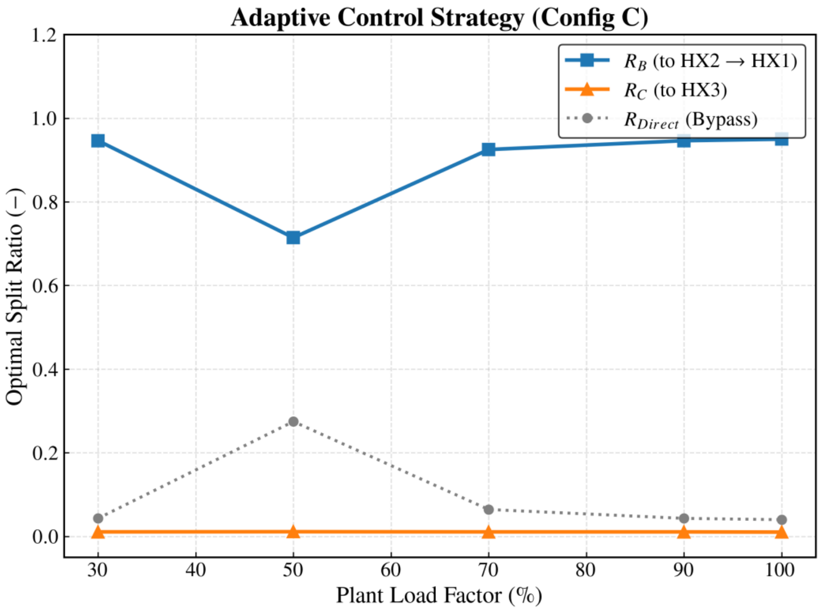

Fig. 10. Optimal split ratios for Config C as a function of plant load, obtained by surrogate-based optimization. $\mathbf{R}_B$: flow fraction through inter-bed exchangers $\mathbf{HX}_1$/$\mathbf{HX}_2$; $\mathbf{R}_C$: flow fraction through feed preheater $\mathbf{HX}_3$; $\mathbf{R}_{direct}$: direct bypass fraction.

3.4 Physical consistency verification

A sensitivity analysis on Config C at 100% load confirms that the PINN surrogate reproduces physically correct parameter responses. A 10% increase in operating pressure raises NH_3 production by approximately 3.0% at the nominal operating pressure of 200 bar, consistent with Le Chatelier's principle for a volume-reducing gas-phase reaction. A 20 K increase in feed inlet temperature reduces production by approximately 2.7%, because the equilibrium constant K_{eq} decreases with temperature faster than the forward rate constant increases under near-equilibrium industrial operating conditions. These responses confirm that the surrogate has internalized the thermodynamic constraints embedded in the physics loss, rather than merely fitting a statistical response surface.

4. Conclusions

A residual-attention PINN surrogate was developed for a single adiabatic ammonia catalyst bed and deployed within a three-bed multi-configuration optimization framework. The surrogate achieves R^2 above 0.99 on the validation set, with an inference speed nearly four orders of magnitude faster than the reference ODE solver, enabling surrogate-based global optimization that would be computationally intractable with mechanistic models alone. Comparison of three inter-bed heat integration configurations showed that the series-parallel split design (Config C) achieves the highest NH_3 production from 30 to 100% load, prevents catalyst extinction at low load through adaptive redistribution of inter-bed heat between the two independent bypass branches, and produces T-X phase diagram trajectories that approach the thermodynamic equilibrium curve most closely. The quench-cooled design remains a viable option at high load but degrades at low load due to an architectural constraint that prevents full decoupling of feed preheating and inter-bed cooling. The series configuration is thermally infeasible at high load without pressure-side control. Future work will extend the surrogate to dynamic formulations and incorporate plant-model mismatch quantification against Aspen Plus reference simulations.

5. Acknowledgments

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OS-B4-03

SESSION

B4 · July 6 (Mon) 15:00~15:15

PRESENTER

Tian Qiu

Capacity Configuration of Power-to-Methanol Systems: A Bi-level Optimization Approach Based on Bayesian and Clustering Algorithms

Yi Wang, Tian Qiu, Miao Yang, Qingqing Zhang, Xu Ji, Li Zhou*

Sichuan University & CPECC, China

The full paper follows on the next page.

12th Asian Symposium on Process Systems Engineering July 5-8, 2026, Seoul, Republic of Korea

Capacity Configuration of Power-to-Methanol Systems: A Bi-level Optimization Approach Based on Bayesian and Clustering Algorithms

Yi Wang[1], Tian Qiu[2], Miao Yang[1], Qingqing Zhang[2], Xu Ji[2], Li Zhou[2,*]

[1]*China Petroleum Engineering & Construction Co. Ltd. southwest branch, Chengdu 610095, P. R. China*

[2]*School of Chemical Engineering, Sichuan University, Chengdu 610065, P. R. China*

* chezli@scu.edu.cn (Corresponding author)

Abstract: Decarbonizing methanol production via renewable integration is crucial for achieving carbon neutrality, yet this transition faces a fundamental challenge. The inherent intermittent of renewables can render the process cost-prohibitive if not properly addressed. This study proposes a Bayesian-enhanced, interactive bi-level optimization approach for the capacity configuration of off-grid wind-solar-driven methanol systems. The upper level optimizes the capacities of key components (renewable power, electrolyzer, hydrogen storage, and methanol synthesis), while the lower level evaluates the annual economic performance of each configuration through a scenario-based stochastic programming model for operation scheduling. To reduce computational burden, K-means clustering is applied to abstract representative scenarios with occurrence probabilities from the annual renewable profile of the targeted location. These scenarios enable rapid estimation of key operational performance indicators (annual methanol yield and operational cost) for various configurations. These estimated indicators are then fed into a Bayesian optimization algorithm, guided by a Gaussian process surrogate model on the upper level, to efficiently map the configuration-economic response surface and navigate the non-convex design space. Applied to a case study in Northeast China targeting 300,000 tons of annual green methanol production from captured CO_2, the method proves effective in optimizing system capacities while enhancing both economic performance and computational efficiency. Findings reveal that while wind-solar hybrids smooth operational fluctuations, they do not necessarily minimize the levelized cost of methanol (LCOM) due to substantially higher capital costs. In certain cases, configurations dominated by a single renewable source may offer superior economic outcomes.

Keywords: Green Methanol; Capacity Configuration; Bi-level Optimization; Bayesian Optimization; K-means Clustering; Mixed-Integer Linear Programming (MILP)

1. Introduction

In recent years, the massive emission of greenhouse gases has caused severe climate change (Li et al., 2025). To achieve the goal of carbon neutrality, renewable energy sources such as wind and solar power have been widely developed globally. However, the inherent intermittency and volatility of renewable energy bring huge challenges to the stable operation of the power grid (Qi et al., 2023). To address this issue, Power-to-X (PtX) technology has been proposed as a promising solution for the long-term storage and transport of renewable energy (Kong et al., 2025).

Among various PtX pathways, the Power-to-Methanol (PtM) system has attracted increasing attention. Methanol is not only an important chemical raw material but also an excellent liquid fuel with high energy density, making it easy to store and transport (Zhang et al., 2025). Therefore, converting renewable energy into green methanol is an effective way to promote the decarbonization of the chemical industry.

However, unlike traditional chemical production, the PtM system is characterized by flexible, time-varying operational characteristics to accommodate the inherent fluctuations of renewable energy while maximizing overall economic performance (Mucci et al., 2023). Since the capacity scales directly influence the operational states of each component, which in turn dictate the scheduling strategy and system economics, the optimal capacity configuration and operational scheduling of the PtM system are inherently coupled and intertwined (Allman et al., 2019; Liu et al., 2025). To address these challenges and improve the economic efficiency of PtM systems, reasonable capacity configuration and operation scheduling are required. Many researchers have studied the optimization of PtM systems. For example, Jiang et al., (2025) developed a mathematical optimization model for a wind-solar-methanol system, emphasizing the integration of flexible operation and hybrid energy storage systems including battery, hydrogen, and methanol tanks to reconcile the contradiction between stable chemical production and intermittent renewable supply. Researchers like Bai et al. (2025) and Zhang et al. (2024) converted the annual scheduling problem into multi-period scheduling by selecting typical days. Some other studies also used clustering methods to reduce data dimensions (Mucci and Bongartz, 2025).

Although previous studies have made progress, the coordinated optimization of system capacity and dynamic scheduling in PtM systems under renewable energy fluctuations still needs further research. Therefore, this paper presents a preliminary capacity configuration and operation scheduling model for a wind-solar-methanol system. The main objective is to minimize the Levelized Cost of Methanol (LCOM) while meeting the production demand.

2. Problem statement

Figure 1 illustrates the conceptual diagram of the proposed green methanol production system. For a PtM system, the objective of capacity sizing is to determine the optimal scales for all critical components. The decision variables of the system include the installed capacities of wind turbines, PV panels, proton exchange PEM electrolyzers, hydrogen storage tanks (HST), and methanol synthesis units. The ultimate goal is to achieve safe and economically viable production of green methanol while deriving the optimal scheduling strategy, subject to engineering requirements and equipment operational constraints.

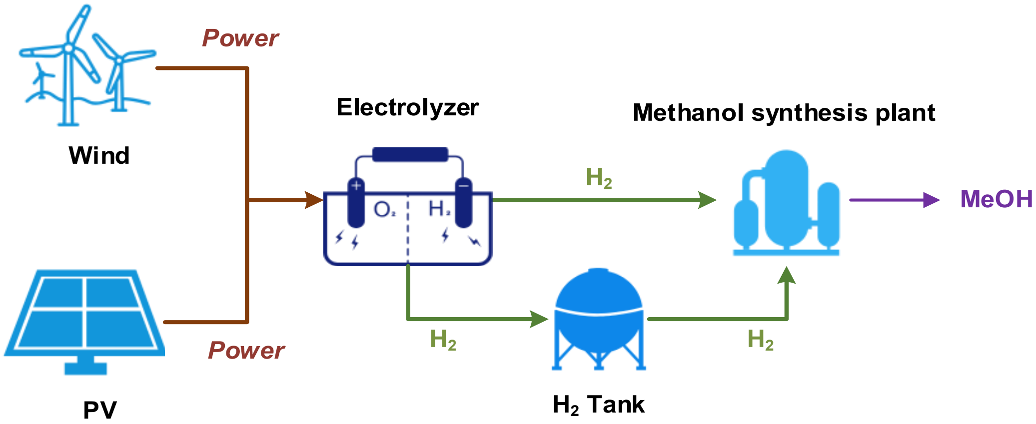

Fig. 1. Schematic diagram of an off-grid green methanol production system driven by renewable energy.

3. Methodology

A bi-level optimization framework is constructed to coordinate the capacity sizing and operational scheduling of the green methanol system. The upper level employs Bayesian optimization as the design layer, determining the installed capacities of system components and providing them as physical boundaries to the lower level. To improve computational efficiency, the lower-level model applies a K-means clustering algorithm to reduce the annual meteorological data into typical operational scenarios. Based on the capacity parameters received from the upper level, the lower level performs dynamic scheduling optimization and calculates the total system cost. These economic results are then fed back to the upper level to guide the Bayesian algorithm's iterative search for the optimal capacity configuration. This interactive framework effectively manages the coupling between long-term investment and short-term operation, ensuring the economic feasibility of the system under renewable energy fluctuations.

Following the bi-level framework, the lower-level operational scheduling is formulated as a scenario-based Mixed-Integer Linear Programming (MILP) problem. To evaluate the comprehensive economic performance, LCOM is generalized as a function of both the upper-level capacity sizing variables $\mathbf{x}$ and the lower-level dynamic scheduling variables $\mathbf{y}_s$ under typical scenarios s:

$$LCOM = \frac{F_{CAPEX}(\mathbf{x}) + \sum_{s \in \mathcal{S}} \pi_s \cdot F_{OPEX}(\mathbf{x}, \mathbf{y}_s)}{\sum_{s \in \mathcal{S}} \pi_s \sum_{t \in \mathcal{T}} M_{\mathrm{MeOH}}\,(\mathbf{x}, \mathbf{y}_s, t)} \qquad (1)$$

where $F_{CAPEX}(\cdot)$ and $F_{OPEX}(\cdot)$ map the decision variables to the annualized capital investment and operational costs, respectively. π_s denotes the probability or temporal weight of the clustered scenario s, where $s \in \mathcal{S}$ and $\mathcal{S}$ is the set of clustered typical scenarios; $t \in \mathcal{T}$, where $\mathcal{T}$ is the set of time steps within each scenario. M_{MeOH} represents the methanol yield.

Renewable Energy Subsystem

To ensure stable operation, the integrated system must maintain a strict real-time power balance between energy generation and consumption at any given time step t. The constraint is formulated as:

$$P_{s,t}^{\mathrm{Wind}} + P_{s,t}^{\mathrm{PV}} = P_{s,t}^{\mathrm{ELE}} + P_{s,t}^{\mathrm{Curt}}, \quad \forall s \in \mathcal{S}, \forall t \in \mathcal{T} \qquad (2)$$

This equation dictates that the total power generated by wind and solar ($P_{s,t}^{\mathrm{Wind}}, P_{s,t}^{\mathrm{PV}}$) must equal the power supplied to the electrolyzer ($P_{s,t}^{\mathrm{ELE}}$) plus the curtailed renewable power ($P_{s,t}^{\mathrm{Curt}}$).

Electrolyzer Hydrogen Production Subsystem

The mass flow rate of hydrogen produced by the proton exchange membrane (PEM) electrolyzer is determined by the electrical power input and the electrolysis efficiency:

$$m_{s,t}^{\mathrm{H_2}} = \eta^{\mathrm{ELE}} \frac{P_{s,t}^{\mathrm{ELE}}}{\mathrm{HHV}^{\mathrm{H_2}}}, \quad \forall s \in \mathcal{S}, \forall t \in \mathcal{T} \qquad (3)$$

$m_{s,t}^{\mathrm{H_2}}$ denotes the hydrogen production, η^{ELE} signifies the hydrogen production efficiency, and $\mathrm{HHV}^{\mathrm{H_2}}$ represents the higher heating value of hydrogen.

Hydrogen Storage Subsystem

The hydrogen storage tank acts as a crucial buffer between upstream hydrogen production and downstream chemical synthesis. To properly characterize the inventory state throughout the scheduling horizon, the mass balance is formulated to account for the initial inventory condition:

$$S_{s,t}^{\mathrm{H_2}} = \begin{cases} S_0^{\mathrm{H_2}} + (m_{s,t}^{\mathrm{H_2},to\mathrm{HST}} - m_{s,t}^{\mathrm{H_2},out\mathrm{HST}})\Delta t, & \forall s \in \mathcal{S}, t = 1 \\ S_{s,t-1}^{\mathrm{H_2}} + (m_{s,t}^{\mathrm{H_2},to\mathrm{HST}} - m_{s,t}^{\mathrm{H_2},out\mathrm{HST}})\Delta t, & \forall s \in \mathcal{S}, \forall t \in \mathcal{T}, t > 1 \end{cases} \qquad (4)$$

$S_{s,t}^{\mathrm{H_2}}$ denotes the dynamic hydrogen inventory, while $S_0^{\mathrm{H_2}}$ signifies the given initial inventory before scheduling. The current inventory is updated by adding the net charging amount (inflow $m_{s,t}^{\mathrm{H_2},to\mathrm{HST}}$ minus outflow $m_{s,t}^{\mathrm{H_2},out\mathrm{HST}}$) over the time interval Δt.

Methanol Synthesis Subsystem

Based on the stoichiometric ratio, the methanol production is directly linked to the actual hydrogen consumed during the catalytic synthesis process:

$$m_{s,t}^{\mathrm{MeOH}} = \frac{\lambda m_{s,t}^{\mathrm{H_2,MeOH}} \mathrm{Mr}^{\mathrm{MeOH}}}{3\mathrm{Mr}^{\mathrm{H_2}}}, \quad \forall s \in \mathcal{S}, \forall t \in \mathcal{T} \qquad (5)$$

$m_{s,t}^{\mathrm{MeOH}}$ is the methanol yield, and $m_{s,t}^{\mathrm{H_2,MeOH}}$ indicates the hydrogen directly supplied to the synthesis unit. $\mathrm{Mr}^{\mathrm{MeOH}}$ and $\mathrm{Mr}^{\mathrm{H_2}}$ denote the relative molecular masses, and λ represents the comprehensive synthesis yield.

4. Case study

A case study was conducted based on the annual meteorological data from a site in Northeast China. This region exhibits excellent renewable energy endowments, with annual capacity factors of 38.11% (3,338 full-load hours) for wind power and 13.48% (1,181 full-load hours) for solar power. The detailed temporal profiles of the renewable capacity factors are illustrated in Fig. 2.

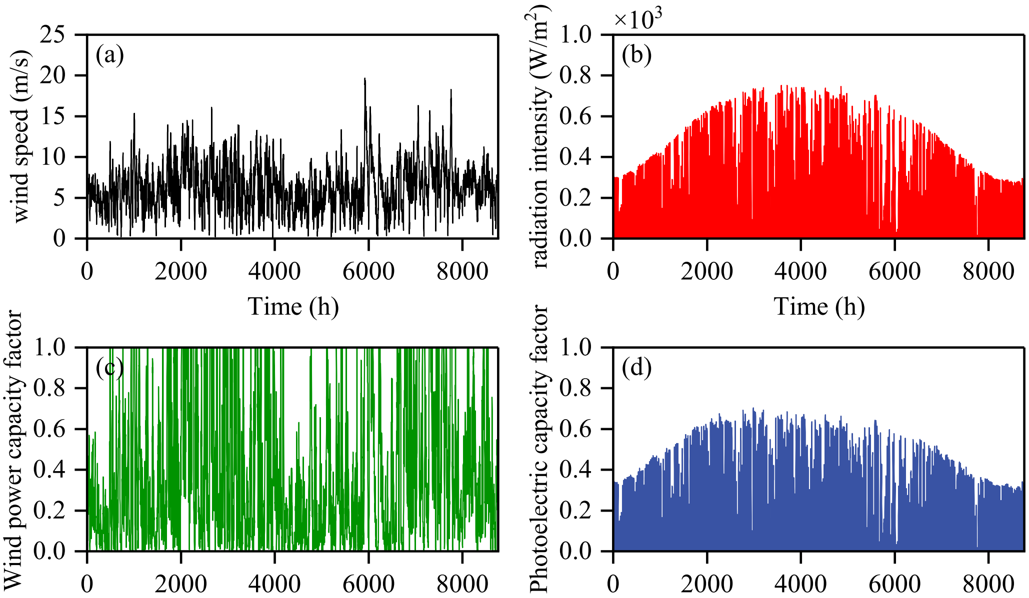

Fig. 2. Local annual meteorological data and corresponding wind and solar capacity factors: (a) wind speed data; (b) solar irradiance data; (c) wind power capacity factor; (d) solar power capacity factor.

To explore the economic potential of PtM systems under different renewable energy configurations and identify the optimal capacity sizing, three cases covering pure wind, pure PV, and wind-solar hybrid systems were established under a fixed annual methanol production target of 300,000 tons.

The proposed optimization framework was implemented in Python via the Pyomo modeling environment and solved using Gurobi 13.0.0 on a high-performance workstation (Intel Core i9-14900KF, 64 GB RAM).

5. Results and Discussion

Table 1 presents the optimal capacity configuration and key performance metrics across the three cases. Fig. 3 further illustrates the economic performance of each case in terms of equipment investment breakdown and LCOM composition. From these optimization results, several key findings regarding the economic feasibility and capacity configuration of the off-grid green methanol system are summarized as follows.

The capacity configuration of wind and solar installations significantly impacts the overall economic performance of the off-grid green methanol system, with capital expenditures (CAPEX) primarily driven by the renewable generation units and the electrolyzer, constituting the dominant share of the total LCOM.

The pure wind system achieves the lowest LCOM (0.562 USD/kg), demonstrating clear economic superiority over the other configurations. This advantage is primarily attributed to the excellent wind resource endowment of the target region, where high equivalent full-load hours ensure sustained electrolyzer utilization and stable hydrogen supply. Although wind turbines carry a relatively higher unit investment cost, their continuous temporal output profile inherently aligns with the long-term steady-state operational requirements of downstream chemical synthesis. This reveals a core economic logic: in wind-abundant regions, a high-utilization-driven configuration strategy significantly outperforms a low-unit-cost-driven strategy in minimizing the LCOM.

Table 1 Optimal system sizing and performance metrics across various cases

	Unit	Different cases		
		Pure Wind	Pure PV	Wind-Solar Hybrid
W^{Wind}	MW	1174	0	1016
W^{PV}	MW	0	3450	363
W^{ELE}	MW	862	1287	948
W^{HST}	kg	78087	182261	64095
W^{MeOH}	kg/h	95724	100000	95635
AR	wt	31.590	32.110	32.222
LCOM	USD/kg	0.562	0.967	0.585

Note: W^{Wind}, W^{PV}, and W^{ELE} denote the installed capacities of wind power, photovoltaic power, and the electrolyzer system, respectively. W^{HST} represents the capacity of the hydrogen storage tank. W^{MeOH} is the nominal capacity of the methanol synthesis unit. AR stands for the annual production of methanol.

Conversely, the pure PV system yields the highest LCOM (0.967 USD/kg) and requires the largest hydrogen storage capacity (182,261 kg) among all cases. This outcome stems from a fundamental temporal mismatch between intermittent daytime generation and the continuous 24/7 demand of the methanol reactor. To bridge this gap, massive long-duration hydrogen storage must be deployed to shift energy across the day-night cycle. Furthermore, to meet the 300,000-ton annual production target under limited solar utilization hours, the upstream PV (3,450 MW) and electrolyzer (1,287 MW) capacities must be drastically oversized to ensure sufficient hydrogen production within the narrow sunlight window. This structural inefficiency, characterized by low energy density and poor time utilization, drastically inflates the initial investment, making the pure PV scenario economically uncompetitive.

The wind-solar hybrid system achieves an intermediate LCOM of 0.585 USD/kg, marginally higher than the pure wind case despite the complementary nature of the two resources. While the hybrid configuration effectively smooths the renewable output profile and reduces hydrogen storage requirements (64,095 kg) compared to the pure PV case, the additional capital investment associated with PV installation offsets these operational benefits. This finding suggests that renewable complementarity does not necessarily translate into economic optimality: when a single resource already offers sufficiently high utilization, introducing a secondary source may increase system complexity and CAPEX without proportional reductions in LCOM.

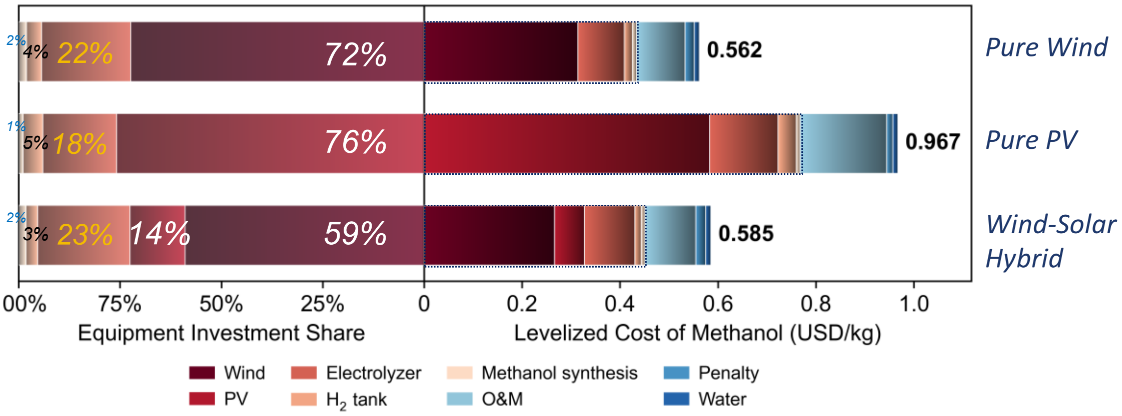

Fig. 3. Economic performance across different cases: (left) percentage stacked bar chart of the equipment investment; (right) stacked bar chart of LCOM breakdown.

6. Conclusions

This study proposes a bi-level optimization framework to evaluate the economic feasibility and optimal capacity configuration of an off-grid green methanol production system. By integrating Bayesian optimization for long-term design with a K-means clustering algorithm for short-term dynamic scheduling, the interactive model effectively manages the coupling between capital investment and operational strategies under renewable energy fluctuations.

The comparative case studies across three renewable configurations reveal several key findings. The annualized capital expenditures, primarily dominated by the renewable generation units and the electrolyzer, constitute the vast majority of LCOM. The pure wind system achieves the lowest LCOM (0.562 USD/kg), demonstrating clear economic superiority driven by high resource utilization. The wind-solar hybrid system yields an intermediate LCOM (0.585 USD/kg), where the additional PV capital investment offsets the benefits of renewable complementarity. The pure PV scenario incurs the highest LCOM (0.967 USD/kg), resulting from severe capacity oversizing caused by the temporal mismatch between intermittent daytime generation and continuous chemical consumption.

These findings collectively demonstrate that temporal utilization, rather than resource diversity or unit equipment cost, is the primary determinant of economic performance in off-grid power-to-methanol systems. A utilization-driven configuration strategy, guided by local renewable resource characteristics, represents the critical pathway to ensuring the economic viability of green methanol production. Furthermore, the quantitative relationship between multi-scale renewable fluctuations and optimal capacity configuration will be further explored in subsequent research.

Acknowledgements

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OS-B4-04

SESSION

B4 · July 6 (Mon) 15:15~15:30

PRESENTER

Rohit Kumar Yadav

Hybrid Auxiliary Heating Optimization for Solar Thermal Integration in Industrial Processes: A Screening Curve Approach

Rohit K. Yadav*, Santanu Bandyopadhyay, Andrew Hoadley, and Roger Dargaville

IIT Bombay (India) & Monash University (Australia)

The full paper follows on the next page.

Research Article - Peer Reviewed Conference Proceeding
PSE ASIA 2026 - 12th Asian Symposium on Process System Engineering
Yonsei University, Seoul, Republic of Korea. 5-8 July 2026

Hybrid Auxiliary Heating Optimization for Solar Thermal Integration in Industrial Processes: A Screening Curve Approach

Rohit K. Yadav[a,c]*, Santanu Bandyopadhyay[a], Andrew Hoadley[b], and Roger Dargaville[c]

[a] Indian Institute of Technology Bombay, Department of Energy Science and Engineering, Mumbai, Maharashtra, India
[b] Monash University, Department of Chemical and Biological Engineering, Melbourne, Australia
[c] Monash University, Department of Civil and Environmental Engineering, Melbourne, Australia
* Corresponding Author: rohit.yadav@iitb.ac.in

ABSTRACT

Industrial process heating contributes significantly to greenhouse gas emissions, and solar thermal energy offers a renewable pathway to supply heat at temperatures matching industrial requirements. However, the intermittent nature of solar energy necessitates auxiliary heating to ensure continuous process operation. While resistive heating is commonly used due to its low capital cost, its high operating cost at a coefficient of performance of unity can dominate the system economics. This paper presents a methodology that combines Pinch Analysis with screening curve analysis from power systems economics to co-optimize solar thermal system sizing and hybrid auxiliary heating technology selection. The screening curve approach determines the economically optimal capacity split between a heat pump and a resistive heater by identifying the crossover operating hours beyond which the heat pump becomes more economical. This crossover is mapped onto the auxiliary load duration curve, unique to each candidate design, to size both devices optimally. The methodology is applied to a dairy processing plant using evacuated tube collectors with thermal storage. A two-stage grid search over collector area and storage volume minimizes the Total Annualized Cost over 8,760 hourly timesteps with cyclic steady-state convergence. Results show an optimal solar fraction of 51.2% with the heat pump handling 99% of auxiliary energy demand at an energy-weighted average COP of 2.26. The total annualized cost is $837,476/year with an LCOH of $57.04/MWh. Sensitivity analysis identifies electricity tariff, heat pump COP, and discount rate as the primary economic drivers, each capable of shifting the TAC by more than 14%.

Keywords: Energy Systems Modelling, Renewable Energy, Solar Thermal Energy, Pinch Analysis, Heat Exchanger Network, Screening Curves, Load Duration Curve

1. INTRODUTION

Industrial activities account for approximately one-third of global final energy consumption [1]. Under these activities industrial process heating is associated with a substantial amount of greenhouse gas emissions. The decarbonization of industrial process heat presents a challenge for achieving global climate targets. While the electrification and fuel switching address some of the industrial energy requirements, process heat applications often require dedicated thermal solutions. Solar thermal energy offers a pathway to supply heat directly at temperatures matching industrial requirements, which is renewable and unlimited in supply. In regions with good solar resources, solar thermal energy has the potential to reduce significantly the carbon footprint of industrial processes while also providing economic benefits such as lower energy operating costs. Pinch Analysis is a widely accepted method for analyzing industrial processes' heating and cooling requirements. It can help identify the optimal integration points for solar thermal energy [2]. Recent advances have demonstrated the feasibility of integrating solar thermal systems with industrial processes across diverse sectors including food processing, dairy and chemical manufacturing [3]. The primary technical challenge for solar thermal integration in industrial applications is the mismatch between intermittent availability of solar energy and the process heat demand. Thermal energy storage can provide short -term buffering, but during the extended periods of low radiation such as monsoons in tropical climates, auxiliary heating becomes important to satisfy the process heat duty in a continuous or semi-continuous operation. Previous studies have employed electrical resistive heating due to its simplicity and low-cost [4]. However, due to a Coefficient of Performance (COP) of 1, the electrical resistive heating leads to a high operating cost that dominates the Total Annualized Cost (TAC) and the Levelized Cost of Heat (LCOH).

A thermodynamically superior alternative to the electrical resistive heating is a heat pump, delivering more units of heat per unit of electricity consumed. However, a heat pump is costlier than an electrical resistive heater and its application can only be justified if it is used for a sufficient number of hours in a year. When the auxiliary heating is the combination of both the heat pump and electrical resistive heater, the question of the size of the equipment and number of hours they should run arises. This has not been sufficiently covered in literature. This study addresses this gap by utilising the concept of a screening curve and load duration curve (LDC) from power system economics [5]. The screening curve approach plots the total annualized cost per unit capacity as a function of annual operating hours of each of the auxiliary heating equipment. The intersection of these curves gives the crossover hours, which, when mapped to auxiliary LDC, gives the optimal capacity or the size of the equipment. This approach ensures that the heat pump covers the base-load demand of the auxiliary heating and the resistive heating covers the peak demands.

The methodology is applied to a dairy processing plant with the environmental conditions of Pune, India. Pinch Analysis is used to determine the minimum hot utility requirement, heat exchanger size and the optimal mass flow rate of the working fluid through the heat exchanger network. An exhaustive search over the collector area and storage volume minimizes the TAC, with the hybrid auxiliary heating sized optimally for each design point using the screening curve approach. The annual simulation models 8,760 hours with two-stage collector flow control and iterates to cyclic-steady state convergence between the start and end of the year.

2. SYSTEM DESCRIPTION

2.1 System Configuration

A schematic of the solar thermal system is developed to satisfy the industrial process heat demand and is represented by Figure 1. The system comprises four primary subsystems: (i) an evacuated tube collector (ETC) field, (ii) a well-mixed thermal energy storage tank, (iii) a counter-current heat exchanger network, and (iv) a hybrid auxiliary heating unit consisting of a heat pump and a resistive heater.

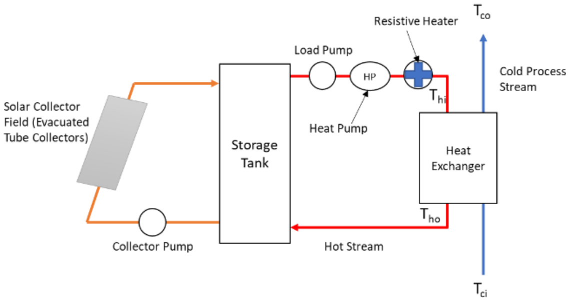

Figure 1. Schematic of the solar thermal system.

The collector field heats the working fluid, which is stored in the well-mixed tank. Hot water from the storage tank is circulated through the heat exchanger through a load pump, transferring heat to the cold process stream. The heat exchanger is sized based on the Grand Composite Curve (GCC) of the process, with its performance characterized by the overall heat transfer coefficient-area product (UA). If the heat delivered by the storage tank is insufficient to satisfy the process demand, the hybrid auxiliary unit comprising of a heat pump and resistive heating is activated to compensate for the deficit. This schematic ensures that the auxiliary heater does not interact with the storage tank energy balance; the tank exchanges energy only with the collector field, the process load, and the ambient environment through thermal losses.

The dairy processing plant is based on the case study of Atkins et al. (2010) [7]. The process comprises pasteurization, separation, evaporation, and cleaning-in-place (CIP) operations. The cold-water stream (15 to 45 °C, 118.5 kW/ °C) provides cooling water for the process. The skim milk stream (45 to 10 °C, 110.6 kW/ °C) is cooled after separation. Above the Pinch temperature of 42.5 °C, the process requires 1,676 kW of hot utility. Below the Pinch, 2,085 kW of cold utility is required. A detailed process flow diagram and stream data are provided in Atkins et al. (2010) [7].

2.2 Energy Balance

The temperature of the hot stream coming out of the storage tank is determined by the solution of energy balance around the storage tank [6]. Energy balance equation is:

$$\rho \times c_p \times V_{st} \cdot \frac{dT_{st}}{dt} = F' \times A_c \times [S \times \tau\alpha - U_L \times \ (T_m - T_a)]^{+} - q_{Ls} - U_{st} \times A_{st} \times (T_{st} - T_a) \qquad (1)$$

The solution of Eqn 1 gives the temperature of the the storage tank at the end of a time step:

$$T_{stf} = T_{sti} + \frac{t}{\rho \times c_p \times V_{st}} [F' \times A_c \times [\mathrm{S} \times \tau\alpha - U_L \times (T_m - T_a)]^+ - q_{Ls} - U_{st} \times (T_{sti} - T_a)] \quad (2)$$

The tank surface area is estimated from the storage volume using the correlation [6]:

$$A_{st} = 5.64 \times (V_{st})^{(2/3)} \quad (3)$$

2.3 Grand Composite Curve and Enthalpy-Interval Formation

The Grand Composite Curve (GCC) serves as a tool for visualising process-heat requirements and linking them with external utility systems. It is developed through a systematic analysis of all process streams to determine net heating and cooling demands. The GCC identifies the temperature and heat-duty range at which solar thermal integration is feasible. Integration above the Pinch ensures that the addition of solar heat does not violate the minimum energy requirements defined by Pinch Analysis principles. The GCC is divided into discrete enthalpy intervals to quantify heat requirements across different temperature levels. The heat duty within each interval is calculated by equation 4:

$$\Delta Q_i = Q_i - Q_{i+1} \quad (4)$$

2.4 Heat Exchanger Network Representation and UA Targeting

The heat exchanger network is treated as a single unit characterized by an overall heat-transfer coefficient-area product (UA value). For each enthalpy interval, the UA contribution is calculated using the log-mean temperature difference (LMTD). The total UA value is the sum across all enthalpy intervals and is given by equation 5:

$$UA_{Total} = \sum_{i=1}^{n-1} UA_i \quad (5)$$

Targeting a specific UA enables the determination of the optimal mass flow rate required to meet the process-heat requirements. The optimal hot-stream mass flow rate (m_{hex}) is obtained by solving for the flow rate that achieves the target UA value. The Secant Method is employed for its computational efficiency and reliable convergence for continuous functions.

2.5 Hot Stream Outlet Temperature Calculation

After solving for the optimal mass flow rate, the outlet temperature of the hot stream from the heat exchanger is calculated. For enthalpy interval i in the GCC, the hot stream outlet temperature (T_{ho}) at the end of the interval is given by equation 6:

$$T_{ho} = T_{hi} - Q_{interval}/(m_{hex} \times c_p) \quad (6)$$

This calculation is performed for every enthalpy interval. The outlet temperature of one interval becomes the inlet temperature for the next. The inlet temperature for the first interval is the temperature of the well-mixed storage tank. The final hot stream outlet temperature ($T_{ho,final}$) at the coldest end of the heat exchanger is an important parameter because it returns to the well-mixed storage tank and affects the overall energy balance. This approach captures the relationship between storage temperature and heat delivery: at higher storage temperatures, more heat can be transferred to the process, while at lower temperatures, the heat delivery degrades.

2.6 Hybrid Auxiliary Heating

When the solar-delivered heat (q_{Ls}) is less than the process heat demand, the deficit is supplied by the hybrid auxiliary system. At each hourly timestep, the auxiliary dispatch follows the rule:

If deficit ≤ $HP_{capacity}$: HP delivers full deficit; RH is idle

If deficit > $HP_{capacity}$: HP operates at full capacity; RH covers the remainder

The sizing of the heat pump and resistive heater capacities is determined by the screening curve analysis described in Section 3.3.

3. METHODOLOGY

3.1 Pinch Analysis

Pinch Analysis is employed to identify minimum hot utility requirement so that the process can be integrated with solar thermal heating. The case study uses a dairy processing plant based on process data from Atkins et al. [7], as presented in Table 1.

Table 1: Process streams running in the dairy plant.

Stream	Supply Temperature (°C)	Target Temperature (°C)	Heat Capacity Flow Rate (kW/°C)
Cold Water	45	15	118.5
Cream A	80	10	4.8
Cream	45	80	4.8
Raw Milk	10	43	115.8
Skim Milk	45	10	110.6

After doing Pinch Analysis on this data, the minimum hot utility requirement comes out to be 1,676 kW and is shown on the GCC in Figure 2. The GCC also provides the enthalpy-temperature intervals used to model the heat exchanger performance.

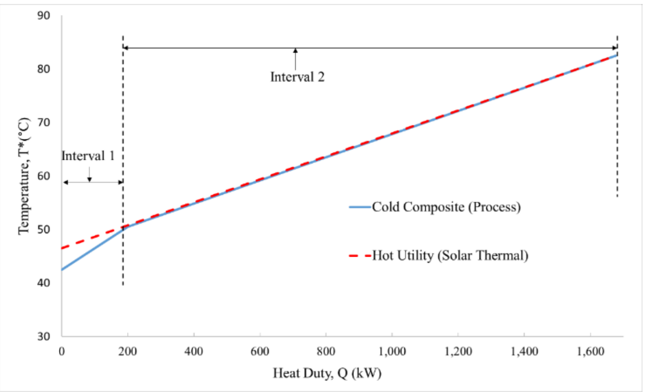

Figure 2. GCC and enthalpy intervals for the dairy process streams.

3.2 Annual Simulation Framework

The system is simulated over a complete year (8,760 hours) using hourly solar radiation and ambient temperature data for Pune, India. The simulation employs a two-stage collector flow control strategy:

Stage 1 - Natural flow: When sufficient solar radiation is available and the temperature difference between the collector outlet target and storage tank exceeds a minimum useful threshold (ΔT_{min} = 10°C), the collector mass flow rate adjusts naturally to achieve the target outlet temperature. This flow rate is determined by the available heat and the required temperature rise.

Stage 2 - Forced minimum flow: When the natural flow rate falls below 25% of the peak flow, the pump enforces a minimum flow rate. In this mode, the actual collector outlet temperature is lower than the target, determined by the available solar energy and the forced flow rate.

3.3 Screening Curve Analysis for Auxiliary Heating

The screening curve methodology determines the economically optimal split between heat pump and resistive heater capacities. For each technology, the total annualized cost per unit capacity ($/kW/year) is expressed as a linear function of annual operating hours (h):$Cost\ (h) = Fixed\ Cost + Variable\ Cost \times h$ (7)

where the fixed cost is the annualized capital plus the maintenance cost per kW and the variable cost is the operating cost per kWh of heat delivered.

Resistive Heater: The equipment cost is 66 $/kW (60 euros/kW, Guccione et al. [9]). The Lang factor of 1.96 for a solids-fluids processing plant (Peters et al. [8]) is applied, giving an installed cost of 129.4 $/kW. Annual O&M is 5% of equipment cost. The economic lifetime is 20 years at a 10% discount rate. The variable cost equals the electricity tariff ($0.1205/kWh, INR 10/kWh at INR 83 per USD).

Heat Pump: The installed cost is 462 $/kW (420 euros/kW$_{th}$, including system integration, Schlosser et al. [10]). No additional installation factor is applied as the reported cost includes integration. Annual O&M is 1.5% of equipment cost (maintenance factor $f_{m,C}$ = 1.5 from Schlosser et al. [10]). The variable cost is the electricity tariff divided by the energy-weighted average COP of 2.266. The COP is estimated hourly using the empirical correlation of Schlosser et al. [10]:

$$\mathrm{COP} = a \times (\Delta T_{lift} + 2b)^{c} \times (T_{h,out} + b)^{d} \qquad (8)$$

The condenser delivery temperature $T_{h,out}$ = 90 °C accounts for a 5 °C approach difference at the heat exchanger and a further 5 °C at the condenser. The process requires hot water at 85 °C (actual temperature). The resistive heater does not require any temperature driving force and heats the water directly to 85 °C.

Using these values, the screening curve parameters are presented in Table 2. where the fixed cost is the annualized capital plus the maintenance cost per kW and the variable cost is the operating cost per kWh of heat delivered.

Table 2: Screening curve parameters.

Parameter	Heat Pump	Resistive Heater
Equipment/installed cost ($/kW)	462	66
Installation factor ($/kW/year)	0 (included in installed cost)	0.96 (Lang 1.96)
Annual O&M (%)	1.5	5
Fixed cost ($/kW/y)	61.21	18.50
COP	2.26	1
Variable cost ($/kWh$_{heat}$)	0.0532	0.1205

The crossover hour is h* = 634 hours (Figure 3). For loads operating more than 634 hours per year, the heat pump is more economical. For loads operating fewer than 634 hours, the resistive heater is cheaper. The crossover hour determines a capacity threshold on the load duration curve, not a temporal threshold. At position h* = 634 on the sorted LDC, the deficit value gives the heat pump capacity. The load above this level occurs for fewer than 634 hours and is assigned to the resistive heater.

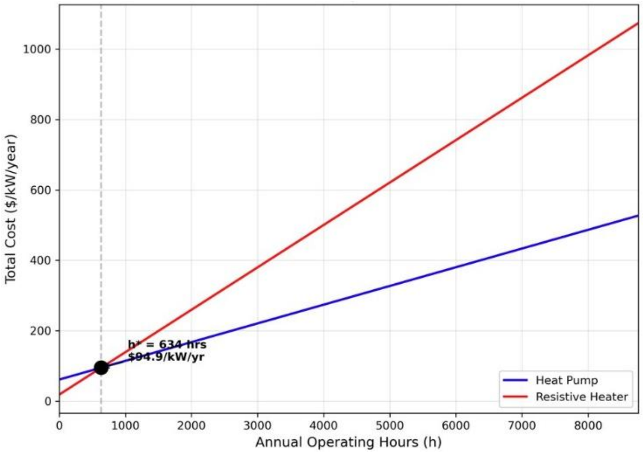

Figure 3. Screening curves for the heat pump and resistive heater. The crossover occurs at h* = 634 hours.

3.4 Load Duration Curve and Optimal Auxiliary Sizing

For each candidate design (A_c, V_{st}, UA), the annual simulation produces 8,760 hourly values of solar-delivered heat (q_{Ls}). Deficit of heat happens when the there is not enough energy in the storage tank and it is given by equation 8:

$$Deficit(t) = \max\left(0, 1676 - q_{Ls}(t)\right) \qquad (9)$$

The auxiliary Load Duration Curve (LDC) is constructed by sorting these 8,760 deficit values in descending order. The LDC represents the auxiliary load as a function of the number of hours that load level is exceeded.
The crossover hours (h* = 634) are mapped onto the LDC to determine the optimal capacities:

- **Heat pump capacity** = LDC value at h = 634 (base-load duty)
- **Resistive heater capacity** = Peak deficit – Heat pump capacity (peak-load duty)

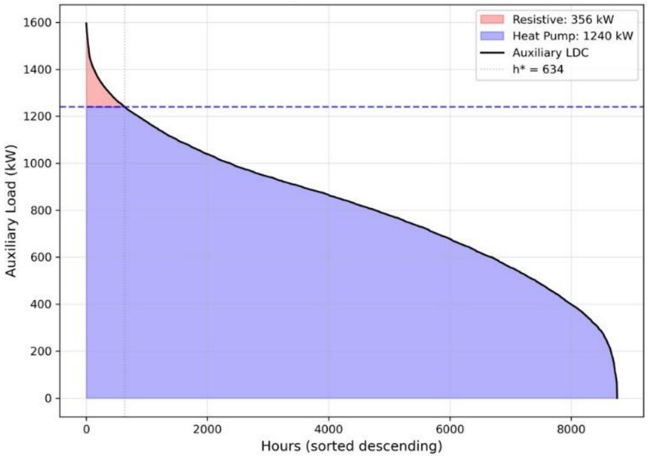

Figure 4. Auxiliary load duration curve with heat pump (base) and resistive heater (peak) regions.

This sizing is performed independently for each design point as different combinations of A_c and V_{st} produce different deficit profiles and hence different LDCs. The screening curve methodology ensures that the auxiliary heating is economically optimized for every design point in the search space.

3.5 Total Annualized Cost Formulation

The objective function for optimization is the Total Annualized Cost (TAC), defined as:

$$TAC = TAC_{solar} + TAC_{pumping} + TAC_{auxilairy} \qquad (10)$$

Solar system costs (TAC_{solar}) include annualized capital and O&M for the collector field, thermal storage tank, heat exchanger, circulation pumps, and electric motors. The collector cost is 350 $/m² with 2% annual O&M over 20 years. The storage tank cost follows a power-law correlation indexed to CEPCI 2025. The heat exchanger is sized from UA using an overall heat transfer coefficient of 1,000 W/(m²·K), with costs following published correlations for a plate and frame type heat exchanger [8].
Pumping costs ($TAC_{pumping}$) are calculated from the hourly electrical energy consumption of the collector and process-side pumps at the existing electricity tariff. Auxiliary heating costs ($TAC_{auxiliary}$) are calculated using the screening curve equations.

3.6 Optimization Approach

A two-stage grid search is employed to minimize TAC over the design space:

Stage 1 - Coarse grid: The collector area (A_c), storage volume (V_{st}) and heat exchanger UA are varied over a wide range at coarse resolution. Each combination undergoes a full annual simulation, followed by hybrid auxiliary sizing and TAC evaluation

Stage 2 - Local refinement: A fine grid is constructed around the Stage 1 optimum with ±5% variation and approximately 1% resolution. This refines the optimal UA, A_c and V_{st} to higher precision.
For each design point evaluated, the auxiliary heating is independently optimized using the screening curve + LDC methodology, ensuring that the TAC reflects the best possible auxiliary configuration for the particular solar thermal system size.

4. RESULTS

The two-stage optimization was performed for an evacuated tube collector system integrated with the dairy process described in Section 3.1, using hourly solar radiation and ambient temperature data for Pune, India. The simulations were re-run with corrected cost parameters and condenser delivery temperature ($T_{h,out}$ = 90 °C) as described in Section 3.3.

4.1 TAC vs Solar Fraction

Figure 5 presents the Total Annualized Cost as a function of solar fraction across all feasible designs evaluated in the coarse optimization. The curve exhibits a characteristic U-shape, with the minimum TAC occurring at a solar fraction of approximately 51%. At low solar fractions (SF < 30%), the TAC is high because the system relies heavily on auxiliary heating. At high solar fractions (SF > 70%), the TAC increases again due to the large collector area and storage volume required to achieve marginal gains in solar contribution. The optimal region lies between SF = 46% and 56%, where the trade-off between solar system capital costs and auxiliary operating costs is most favourable.

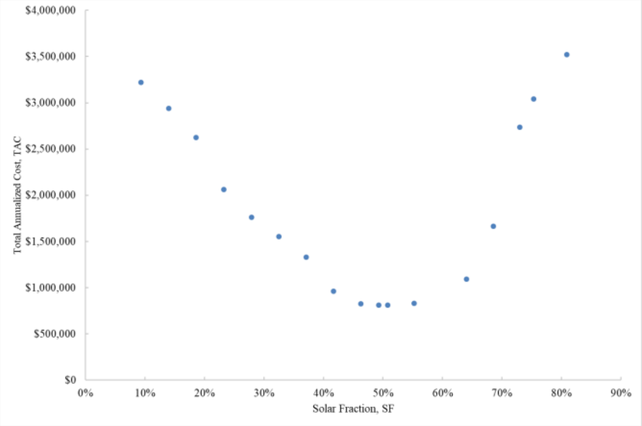

Figure 5. Total Annualized Cost vs Solar Fraction for all coarse grid designs.

4.2 Optimal Design Parameters

The optimal design identified by the optimization is summarized in Table 3.

Table 3: Optimal design parameters.

Parameter	Value
Collector Area (m²)	5,555
Storage Volume (m³)	975
Heat Exchanger UA (kW/K)	110
Solar Fraction (%)	51
Annual Solar Delivered (MWh)	7,518
Annual Process Demand (MWh)	14,682
Avg Storage Temperature (°C)	67.3

4.3 Screening Curve and Auxiliary Sizing Results

The screening curve analysis yields a crossover at h* = 634 hours. When mapped onto the auxiliary load duration curve for the optimal design, this produces a heat pump capacity of 1,240 kW and a resistive heater capacity of 356 kW, against a peak auxiliary deficit of 1,596 kW. The heat pump is therefore sized at 77.7% of the peak deficit, while the resistive heater covers the remaining 22.3%.

In terms of energy, the heat pump delivers 7,102 MWh/year while the resistive heater contributes only 62 MWh/year. The heat pump handles 99.1% of the total auxiliary energy (7,164 MWh/year), and the resistive heater serves purely as a peak-shaving device for hours when the deficit exceeds the heat pump capacity. The heat pump consumes 3,134 MWh of electricity to deliver 7,102 MWh of heat, corresponding to a system-level COP of 2.266.

The trade-off between oversizing the heat pump and using a hybrid configuration was evaluated. A heat-pump-only configuration (sized at the full peak deficit of 1,596 kW) incurs approximately $21,800/year in additional fixed costs compared to the hybrid, while saving only approximately $7,500/year in operating costs. The hybrid configuration achieves the lowest auxiliary cost.

4.4 TAC Breakdown

Table 4 presents the breakdown of the Total Annualized Cost for the optimal design. The total TAC is $837,476 per year.

Table 4: TAC breakdown for the optimal design.

Component	Cost ($/year)	Share (%)
Solar system (total)	369,948	44.2
Heat pump fixed cost	75,900	9.1
Heat pump operating cost	377,666	45.1
Resistive heater fixed cost	6,586	0.8
Resistive heater operating cost	7,471	0.9
Total	**837,476**	**100**

The heat pump operating cost (45.1%) and solar system cost (44.2%) together account for 89.3% of the TAC. The resistive heater contributes only 1.7% to the total cost. The LCOH is $57.04/MWh.

4.5 Sensitivity Analysis

A single-parameter sensitivity analysis was conducted at the optimal design point. The ranking from most to least sensitive is: (1) electricity tariff (plus or minus 18.6%), (2) heat pump COP (plus or minus 15.0%), (3) discount rate (plus or minus 14.5%), (4) collector cost (plus or minus 8.6%), (5) HP installation factor (plus or minus 3.1%), (6) RH Lang factor (plus or minus 0.5%). The system economics are governed by energy costs and financial parameters. Installation cost uncertainties have minimal impact.

5. DISCUSSION

The heat pump operating cost and solar system cost together dominate the TAC, each contributing approximately 44-45%. This near-equal balance has important implications for system design. First, reducing the electricity tariff or improving the heat pump COP would have a significant impact on system economics. Second, the screening curve confirms the value of the hybrid approach: although the heat pump handles 99.1% of the energy, the resistive heater eliminates the need to oversize the heat pump for the few peak hours, saving approximately \$14,300/year in net costs. The solar fraction of 51% at the optimum indicates that the system does not attempt to maximize solar contribution. Beyond this point, the marginal cost of additional collector area and storage volume exceeds the marginal savings in auxiliary heating cost. This is consistent with the heat pump COP advantage: the effective auxiliary cost is \$0.0532/kWh compared to \$0.1205/kWh for resistive heating, a 56% reduction. The economic penalty for low solar fraction is therefore lower with the hybrid system than with resistive-only auxiliary.

An alternative configuration that places the heat pump evaporator below the Pinch point at 25 to 30 °C, using process waste heat instead of ambient air, would stabilize the COP and improve performance during winter months. The heat extracted by the evaporator would also reduce the cooling utility requirement. This configuration requires modification of the below-Pinch heat exchanger network and is identified for further investigation.

The screening curve methodology provides a systematic framework for auxiliary technology selection that adapts automatically to each design point. As the solar fraction changes across the optimization space, the shape of the auxiliary load duration curve changes, and the optimal HP/RH capacity split adjusts accordingly. The effect of heat exchanger fouling on the UA value over the 20-year operating life is not modelled. A sensitivity study with reduced UA values is recommended for detailed design. In the present analysis, other parameters (electricity tariff, COP, discount rate) dominate the TAC variation, suggesting that moderate fouling is unlikely to change the qualitative conclusions.

6. CONCLUSION

This This study presents a methodology for co-optimizing solar thermal system sizing with hybrid auxiliary heating technology selection for industrial process heating. The screening curve approach from power systems economics was applied to determine the optimal capacity mix of heat pump and resistive heater, and the load duration curve was used to size each device for every design point in the optimization space. The key findings are as follows.

The screening curves for the heat pump and resistive heater intersect at h* = 634 hours, establishing the heat pump as the base-load auxiliary device and the resistive heater for peak duty. For the optimal design (A_c = 5,555 m^2, V_{st} = 975 m^3, UA = 110 kW/K), the heat pump is sized at 1,240 kW and the resistive heater at 356 kW.

The optimal solar fraction is 51%, with a Total Annualized Cost of \$837,476 per year (LCOH = \$57.04/MWh).

The heat pump operating cost (45.1%) and solar system cost (44.2%) together account for 89.3% of the TAC. Electricity tariff, heat pump COP, and discount rate are the three most sensitive parameters, each capable of shifting the TAC by more than 14%.

The screening curve methodology provides a systematic framework for auxiliary heating optimization in solar industrial process heating systems. Future work will investigate the below-Pinch placement of the heat pump evaporator for improved COP, the effect of heat exchanger fouling on system performance, and the extension of this methodology to alternative flow topologies including bypass schemes.

AUTHOR IDENTIFIERS

Author ORCIDs:
Yadav RK: 0009-0006-4102-6399

NOMENCLATURE

A_c — Collector area (m^2)
C — Equipment or installed cost per unit capacity (\$/kW)
COP — Coefficient of performance (-)
CRF — Capital recovery factor (-)
D(t) — Auxiliary heat deficit at hour t (kW)
F — Annualized fixed cost per unit capacity (\$/kW/year)
f_{inst} — Installation factor (-)
f_{OM} — Annual O&M fraction (-)
h — Annual operating hours (h)
h* — Crossover hour (h)
LCOH — Levelized cost of heat (\$/MWh)
q_{Ls} — Solar-delivered heat (kW)
Q_{HP} — Heat delivered by heat pump (kW)
$Q_{hu,min}$ — Minimum hot utility from Pinch Analysis (kW)
Q_{RH} — Heat delivered by resistive heater (kW)
SF — Solar fraction (-)
$T_{h,out}$ — Condenser outlet temperature (°C)
$T_{l,in}$ — Evaporator inlet temperature (°C)
TAC — Total annualized cost (\$/year)
UA — Overall heat transfer coefficient-area product (kW/K)
V — Variable cost per unit of heat delivered (\$/kWh)
V_{st} — Storage volume (m^3)
ΔT_{lift} — Temperature lift (K)

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OS-C4-01

SESSION

C4 · July 7 (Tue) 10:00~10:15

PRESENTER

Sungmin Lee

Techno-economic and environmental assessment of SMR-based methanol production: Comparative analysis of biomass and DAC pathways with Allam cycle integration

Sungmin Lee, Matthew J. Realff*, Junghwan Kim*

Yonsei University (Korea) & Georgia Institute of Technology (USA)

The full paper follows on the next page.

Techno-economic and environmental assessment of SMR-based methanol production: Comparative analysis of biomass and DAC pathways with Allam cycle integration

Sungmin Lee[a], Matthew J. Realff[b]*, Junghwan Kim[a]*

[a] Department of Chemical and Biomolecular Engineering, Yonsei University, 50 Yonsei-ro, Seoul 03722, Republic of Korea

[b] School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA 30332, United States

* Corresponding Authors: kjh24@yonsei.ac.kr (J. Kim), matthew.realff@chbe.gatech.edu (M. J. Realff)

Abstract

This study presents a comparative assessment of four nuclear small modular reactor (SMR)-driven methanol production routes at the ~100 kt MeOH/yr scale, combining two carbon sources (biomass gasification and Direct Air Capture, DAC) with two cycle configurations (with or without Allam oxy-fuel integration). A validated Co-SOEC/SOEC electrochemical model was embedded in the Aspen Plus flowsheet to resolve stack-level performance consistently across all four designs. The Levelized Cost of Methanol (LCOM) falls in the range of approximately 762–1,167 $/ton, with biomass-based pathways consistently delivering the lower cost. Under a well-to-gate boundary, gross carbon footprints are reduced by 65–96% relative to the fossil reference of 0.630 tCO_2/tMeOH. Three of the four configurations become carbon-negative when DAC capture is credited, with the DAC route integrating the Allam cycle reaching the deepest mitigation (Case 3). These results highlight the trade-off between cost competitiveness and decarbonization depth, and illustrate how carbon-source selection and cycle integration jointly shape the techno-economic and environmental profile of nuclear-driven methanol production.

Keywords: Small modular reactor, Direct air capture, Carbon-negative methanol, Techno-economic analysis

1. INTRODUCTION

Methanol (CH_3OH) is a central feedstock for producing formaldehyde, MTBE, and downstream olefins; it is also gaining traction as a marine bunker fuel and as a carrier for energy storage [1]. World production is already close to 100 Mt/yr and is projected to climb further as international shipping rules and regional renewable-fuel mandates tighten. Even so, roughly two-thirds of today's supply comes from natural gas reforming and the balance from coal [1], which places gas-derived methanol at a cradle-to-gate footprint of about 2.0 tCO_2/tMeOH and coal-derived routes even higher [2]. Cutting these emissions is therefore a pressing priority.

Three candidate routes dominate the alternatives space: gasification of biomass, carbon supply from DAC, and synthesis driven by renewable-powered electrolysis. Each confronts its own balance between the depth of emissions cuts it can deliver and the price it imposes on the final product. Biomass-based gasification typically achieves the lowest LCOM, but its climate performance hinges on how the boundary is drawn and what the upstream supply chain looks like. DAC allows deeper reductions while suffering from steep thermal and investment costs [3,4]; e-methanol, meanwhile, remains sensitive to both power pricing and electrolyzer capital outlay. Credits like the US 45Q are often framed as correctives, though whether they adequately compensate for the underlying structural differences between these routes is still an open debate [5,6,7].

Closing the gap requires decarbonizing the energy inputs themselves. Small modular reactors (SMRs) offer dispatchable zero-carbon power and steam with industrial-scale flexibility, and they pair well with solid oxide electrolysis cells (SOECs) and with DAC contactors that need moderate-temperature regeneration heat [3,8]. Here the SMR supplies electricity to every case and desorption steam to the DAC cases, lowering indirect emissions across the board, at the cost of nontrivial lifecycle cooling water [9].

A second lever is integrating SOEC with the Allam cycle. Co-electrolysis (Co-SOEC) co-reduces steam and CO2 to syngas matched to methanol stoichiometry, while standard SOEC delivers hydrogen for DAC-based routes. The byproduct O2 in either mode feeds the Allam combustor, eliminating a dedicated air separation unit. The cycle itself is a supercritical-CO2 oxy-fuel power cycle with inherent high-purity capture, producing a CO2 stream eligible for 45Q sequestration credits [5,6].

Despite progress on each individual building block [10,11], several issues remain open. First, systematic comparisons isolating the effect of carbon source while holding the nuclear supply fixed are scarce. Second, how the SOEC–Allam integration reshapes cost and emissions for each carbon source has not been mapped. Third, the carbon price required for parity with fossil methanol, and the degree to which existing incentives close that gap, have not been placed inside a single consistent assessment.

This study addresses these gaps by evaluating four SMR-driven methanol plants (biomass or DAC, with or without the Allam cycle) under common hardware assumptions. The key contribution is a validated Co-SOEC/SOEC electrochemical cell model embedded directly in the process flowsheet, which links cell-level losses to system-level cost and carbon outcomes across all four configurations.

2. PROCESS DESCRIPTION

Four cases couple biomass or DAC-based carbon sources with SMR-driven high-temperature electrolysis, with the Allam cycle included or omitted and Co-SOEC or SOEC selected accordingly.

2.1. System overview

The design matrix has two axes: carbon source and Allam integration. Cases 1 and 2 use corn stover with Co-SOEC (800 °C); Cases 3 and 4 use DAC-captured CO2 with SOEC (750 °C). Cases 1 and 3 add the Allam cycle for extra power and CO2 storage. A single NuScale module (77 MWe; 370,080 kg/h steam at 343 °C / 33 bar) serves Cases 1–3; Case 4 requires two modules (154 MWe) because DAC desorption plus electrolysis exceeds one module. All cases target ≈100 kt MeOH/yr at 8,000 h/yr.

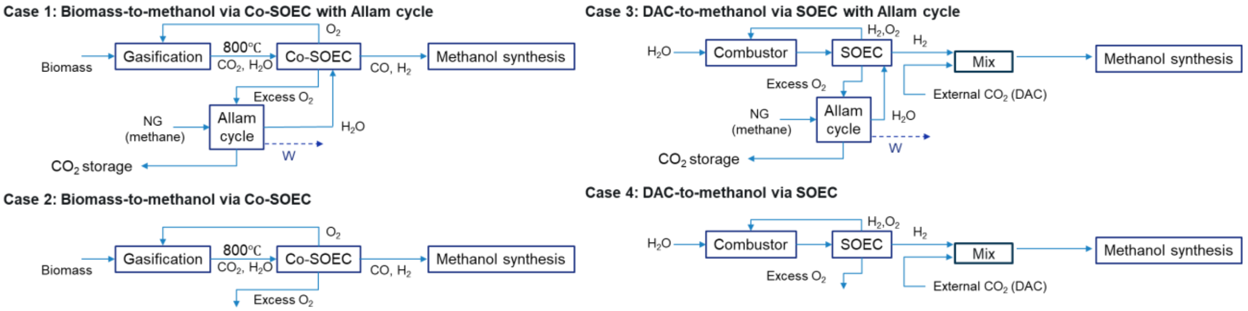


Figure 1. Block-level overview of the four SMR-coupled methanol pathways. Cases 1/2 use biomass gasification coupled with Co-SOEC; Cases 3/4 use a small oxy-combustor, SOEC hydrogen, and externally captured DAC CO2. Cases 1 and 3 further integrate an Allam cycle that consumes SOEC-byproduct O2 and produces a pressurized CO2 stream for geological storage.

2.2. Carbon and oxygen flows

Biomass routes gasify 11,277 kg/h of corn stover (Phyllis2 #1241). DAC routes draw atmospheric CO2 via temperature-swing sorbent contactors regenerated with nuclear steam. The Allam cases combust a small NG stream with SOEC oxygen, yielding a pressurized CO2 stream for geological storage without a dedicated ASU.

2.3. Methanol synthesis and purification

Syngas or H2+CO2 is compressed into a $Cu/ZnO/Al_2O_3$ fixed-bed reactor at ~80 bar and 230–260 °C. Unconverted gas is recycled after flash separation, and the crude product is purified by a heat-integrated high-pressure distillation train.

Table 1. Common flowsheet assumptions adopted for every case.

Parameter	Value
Thermodynamic model	PR-BM
Isentropic efficiency of compressor	0.85
Isentropic efficiency of turbine	0.85
Isentropic efficiency of pump	0.95
Operating hours per year	8,000 h/yr
Target MeOH capacity	~100 kt MeOH/yr

3. METHODOLOGY

3.1. Process simulation framework

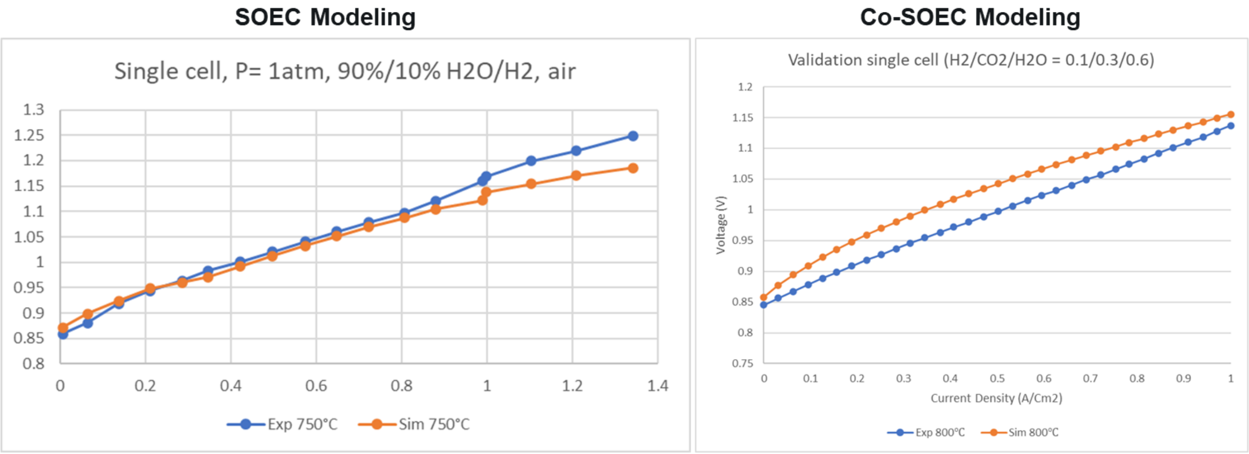
Each flowsheet was constructed in Aspen Plus V14 with the Peng–Robinson–Boston–Mathias (PR-BM) property method. The Co-SOEC and SOEC stacks were implemented as custom unit operations in Aspen Custom Modeler and coupled to the main flowsheet through vapor-phase interfaces. Gasification of corn stover is represented by a four-zone reactor model (pyrolysis, decomposition, oxidation, and reduction) fitted to the chemical composition of the Phyllis2 #1241 feedstock. Methanol synthesis on Cu/ZnO/Al2O3 uses the steady-state kinetic expressions of Vanden Bussche and Froment, including both CO2 hydrogenation and reverse water-gas-shift pathways. The Allam power block is modeled as a supercritical-CO2 oxy-fuel cycle with a regenerator, pump, and turbine set sized to balance the heat released during oxy-combustion. All four cases were converged to a tight mass and energy balance under the common hardware assumptions of Table 1 so that the comparison between them is controlled by carbon source and cycle integration only.

3.2. Electrochemical cell model

Because stack-level losses propagate into both system efficiency and LCOM, each electrolyzer was represented by a physically resolved, zero-dimensional lumped-cell formulation rather than a constant-efficiency surrogate. Co-SOEC employs a dual-channel co-electrolysis treatment for the H2 and CO reduction pathways, while SOEC uses a cathode-supported single-channel water-electrolysis formulation. In both cases the operating voltage is written as the open-circuit potential plus activation, ohmic, and concentration overpotentials:

$$V_{\text{cell}} = E_{\text{Nernst}} + \eta_{\text{act}} + \eta_{\text{ohm}} + \eta_{\text{conc}} \tag{1}$$

Rate expressions, kinetic parameters, and microstructural calibrations follow the approaches of Geng et al. [12] for Co-SOEC and Wehrle et al. [13] for SOEC. Both stacks were calibrated against published single-cell polarization data at their respective operating temperatures, with mean voltage errors of roughly 2% (SOEC, 750 °C) and 3–5% (Co-SOEC, 800 °C). Figure 2 shows the resulting fit, and Table 2 lists the operating points adopted in the process flowsheet. At the design current density, both stacks operate close to the thermoneutral voltage, so the small residual heat imbalance is absorbed by the upstream oxy-combustor that pre-heats the cathode feed with SOEC by-product O2; this avoids the need for a resistive heater and is the main reason each case can still export net electricity to the grid.



SOEC Modeling

Co-SOEC Modeling

Error: 1.80%

Error: 3.52%

Figure 2. Model fit to published single-cell polarization data: (a) SOEC at 750 °C (90/10 H2O/H2 feed, air sweep); (b) Co-SOEC at 800 °C (H2/CO2/H2O = 0.1/0.3/0.6). Markers, measured values; lines, simulated response.

Table 2. Operating points adopted for the Co-SOEC and SOEC stacks.

Parameter	Co-SOEC	SOEC
Operating temperature (°C)	800	750
Operating pressure (bar)	1.01	1.01
Design current density (A/cm²)	1.0	1.0
Single cell area (cm²)	96	128

3.3. Efficiency and economic metrics

Energy efficiency is the ratio of methanol LHV output to feedstock LHV inputs plus net nuclear electricity W_{net} (process demand minus Allam export):

$$\eta_{\text{energy}} = (m_{\text{MeOH}} \cdot LHV_{\text{MeOH}}) / (m_{\text{bio}} \cdot LHV_{\text{bio}} + m_{\text{NG}} \cdot LHV_{\text{NG}} + W_{\text{net}}) \tag{5}$$

Because every case exports surplus power, a system-level metric credits grid export:

$$\eta_{\text{sys}} = (m_{\text{MeOH}} \cdot LHV_{\text{MeOH}} + W_{\text{surplus}}) / (m_{\text{bio}} \cdot LHV_{\text{bio}} + m_{\text{NG}} \cdot LHV_{\text{NG}} + W_{\text{SMR}}) \tag{6}$$

Exergy efficiency uses methanol exergy of 716.0 kJ/mol, CH4 exergy of 831.65 kJ/mol, and a biomass exergy-to-LHV ratio $\beta = 1.137$. LCOM is:

$$LCOM = (CRF \cdot C_{\text{CAPEX}} + C_{\text{OPEX}} - \text{Revenue}) / m_{\text{MeOH,annual}} \tag{7}$$

with CRF = $i(1+i)^n/[(1+i)^n-1]$, $i = 7\%$, $n = 25$ yr. Bare-module costs use the Turton technique, indexed to CEPCI2023 = 797.9 [14]. SMR capex is linearized from the twelve-module NuScale reference [15] to \$294.9 M per module (2023). Revenue includes surplus power at \$50/MWh and, for Cases 2 and 4, O2 at \$50/t. Prices are in Table 3.

Table 3. Prices assumed for feedstocks, utilities, and co-products in the economic model.

Item	Unit price
Electricity (sold to grid)	\$50/MWh
By product O2	\$50/ton
DAC sorbent [4]	\$1.80/tCO2
Corn stover (dry)	\$5.27/GJ
Natural gas (LHV)	\$4.3/MMBtu
MeOH catalyst	\$21,360/ton (4-yr life)
Process water	\$1.0/ton
Cooling water	\$0.354/GJ

3.4. Carbon, water, and carbon-price accounting

A well-to-gate boundary covers feedstock extraction and transport, on-site emissions, and nuclear lifecycle emissions; downstream distribution and end-use are excluded because their treatment depends on chemical-vs-fuel use. Surplus grid electricity is treated as a zero-burden co-product.

Gross carbon footprint sums direct and indirect emissions; two net metrics are then applied depending on end-use:

$$CF_{\text{A}} = CF_{\text{Direct}} + CF_{\text{Indirect}} \tag{8}$$

$$CF_{\text{B,fuel}} = CF_{\text{A}} - CF_{\text{Allam CCS}} \tag{9}$$

$$CF_{\text{B,chem}} = CF_{\text{A}} - CF_{\text{Allam CCS}} - CF_{\text{DAC}} \tag{10}$$

Vent emissions are climate-neutral under the boundary: Cases 1–2 carry biogenic carbon, Cases 3–4 carry DAC-captured carbon. Indirect factors follow R&D GREET 2025 [16]: 0.00992 kgCO2e/MJ (NG), 0.00265 kgCO2e/kWh (nuclear), 32.18 kgCO2e/t (corn stover). The water footprint combines electrolyzer feed and DAC makeup, cooling-tower evaporation at 5 cycles of concentration, and GREET 2025 indirect lifecycle water.

The required carbon price (C_P^*) is the tax level at which a renewable pathway matches fossil methanol:

$$C_P^* = (LCOM - P_{\text{fossil}}) / (CF_{\text{fossil}} - CF_{\text{B}}) \tag{11}$$

with P_{fossil} = \$400/t [17] and CF_{fossil} = 0.630 tCO2/tMeOH [2,16]. C_P^* is reported for both fuel-use and chemical-use net footprints. 45Q credits [5,6] (\$85/tCO2 for Allam storage and \$130/tCO2 for DAC utilization) enter LCOM additively and are independent of end-use because eligibility is fixed at capture.

4. RESULTS AND DISCUSSION

Key performance indicators of the four routes are compared in Table 4, focusing on the headline cost, efficiency, and carbon metrics that allow the four configurations to be directly contrasted against the fossil benchmark.

Table 4. Headline performance indicators for the four SMR-coupled methanol routes benchmarked against fossil reference values.

Metric	Fossil	Case 1	Case 2	Case 3	Case 4
LCOM ($/t)	400	802	762	1,167	1,068
η_energy (%)	—	57.4	63.6	46.9	61.0
Gross CF (tCO2/tMeOH)	0.630	0.104	0.041	0.222	0.024
Net CF, chemical-use	0.630	−0.260	0.041	−2.429	−1.492
Net CF, fuel-use	0.630	−0.260	0.041	−0.913	0.024

Two qualitative patterns stand out from the table. On the cost side, biomass pathways (Cases 1 and 2) remain closer to the fossil benchmark than DAC pathways (Cases 3 and 4), because DAC-captured CO2 is chemically inert and forces the SOEC to supply all reducing equivalents, which roughly doubles the nuclear electricity duty relative to the biomass pair. Adding the Allam oxy-combustion cycle increases LCOM by a modest percentage on the biomass side and by a larger percentage on the DAC side, reflecting the scaling of the combustor with electrolyzer size and the loss of O2 co-product revenue when all of the oxygen is consumed internally.

On the carbon side, every SMR-driven route delivers a large reduction in gross footprint relative to fossil methanol, and three of the four configurations become carbon-negative under the chemical-use accounting, with Case 3 achieving the deepest negative value. Under the fuel-use accounting, re-emission of DAC-captured CO2 during combustion narrows the advantage of the DAC routes but does not erase it relative to the fossil baseline. These results illustrate a clear cost-versus-emissions trade-off at the system level: biomass favors LCOM, DAC favors carbon depth, and the Allam-integrated variants position themselves between the two groups.

5. CONCLUSION

Four nuclear SMR-driven methanol routes were assessed by coupling a validated electrochemical cell model (Co-SOEC for biomass-based syngas, SOEC for DAC-based hydrogen) to an Aspen Plus flowsheet, with and without integration of the Allam oxy-fuel power cycle. Biomass-based routes are the most cost-competitive at this capacity, while DAC-based routes can reach carbon-negative performance once capture is properly credited. The Allam cycle acts as a secondary lever that trades a modest cost increase for a cleaner carbon balance, with its net benefit depending on the prevailing capture-incentive regime. Stack longevity and cell-level losses, captured in the electrochemical model presented here, emerge as a shared technological bottleneck across all four configurations and set a clear direction for further improvement of both LCOM and decarbonization depth.

ACKNOWLEDGEMENTS

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P-13

SESSION

P1 · July 6 (Mon) 13:30~14:30

PRESENTER

Chonghyo Joo

Learning Temperature-Aware Molecular Representations for Organic Solubility Prediction

Chonghyo Joo and Lauren Ye Seol Lee*

University College London, United Kingdom

The full paper follows on the next page.

Research Article - Peer Reviewed Conference Proceeding
PSE ASIA 2026 - 12th Asian Symposium on Process System Engineering
Yonsei University, Seoul, Republic of Korea. 5-8 July 2026

Learning Temperature-Aware Molecular Representations for Organic Solubility Prediction

Chonghyo Joo[a] and Lauren Ye Seol Lee [a,*]

[a] Department of Chemical Engineering, University College London, Torrington Place, London, WC1E 7JE, United Kingdom
* Corresponding Author: lauren.lee@ucl.ac.uk

ABSTRACT

Accurate prediction of organic solubility across temperature is essential for solvent selection and process design. Although many machine learning models have been developed for solubility prediction, most focus on fixed-temperature setting or treated temperature as a simple scalar input, limiting their ability to capture nonlinear temperature-dependent effects in solute-solvent behavior. To address these challenges, we introduce a temperature-aware molecular representation (TAMR) that embeds temperature directly into latent features through feature-wise linear modulation (FiLM). The proposed method is evaluated using two representative architectures: Chemprop, which learns graph-based molecular representations, and Fastprop, which uses fixed molecular descriptors. Models are trained on BigSolDB dataset and evaluated under both interpolation conditions and extrapolation to unseen solutes using different datasets. The results show that the TAMR improves predictive performance and temperature sensitivity, with particularly strong gains observed for the graph-based Chemprop model. These findings suggest that representation-level temperature conditioning is an effective strategy for capturing temperature-dependent molecular interactions in solubility prediction.

Keywords: Molecular representation, Solubility, Organic solvents, Machine learning

INTRODUCTION

Solubility is a fundamental property that plays a critical role across various industrial applications, particularly in crystallization processes and pharmaceutical development. It influences not only the performance of the final product but also the overall efficiency of manufacturing processes[1,2]. Consequently, understanding solubility behavior in different organic solvents is essential for selecting optimal solvent systems tailored to specific objectives[3].

However, experimentally measuring solubility over a wide range of solvents and temperatures is both time-intensive and costly. To address this challenge, machine learning approaches have been increasingly adopted to predict solubility and related properties without relying on extensive experimental efforts.

Recent studies have demonstrated the effectiveness of deep learning models for molecular property prediction. For instance, Kevin J. Heid and colleagues employed directed message-passing neural networks (D-MPNNs) to predict various chemical properties[4,5], showing that these models can capture complex molecular interactions and reaction patterns[6]. Their work also highlighted that learned molecular representations can be transferred across different tasks, improving model flexibility. Similarly, Michael J. Vermeire et al. incorporated thermodynamic principles into D-MPNNs to enable solubility prediction across varying temperatures[7].

In parallel, descriptor-based approaches have also been explored. Burns and Green proposed a deep learning architecture based on predefined molecular descriptors, achieving high computational efficiency[8]. Building on this idea, Attia et al. further developed a framework that incorporates predictive uncertainty into solubility modeling[9].

Despite these advances, most existing methods treat temperature either implicitly or as a simple scalar input, which limits their ability to fully capture temperature-dependent molecular interactions. This highlights the need for more explicit temperature-aware modeling strategies.

In this work, we propose a temperature-aware molecular representation (TAMR) that explicitly incorporates thermal effects into solubility prediction using feature-wise linear modulation (FiLM)[10–12]. First, following the benchmarking protocol of Attia et al., we curated the dataset and designed data splits to evaluate both interpolation (seen solutes) and extrapolation (unseen solutes) performance. Second, temperature is transformed into a temperature-aware parameters through kernel-based expansion and FiLM. Finally, we evaluate the proposed approach using two state-of-the-art (SOTA) architectures, Chemprop[6] and Fastprop[8], to investigate the impact of TAMR across different molecular representation frameworks.

METHODOLOGY

Data collection

To build and evaluate data-driven models for solubility prediction, recently compiled datasets of organic solubility were utilized. The BigSolDB dataset[13] was used as the main source for model training and validation, while the Leeds dataset[14] was employed to assess extrapolation performance.

BigSolDB contains a large collection of solubility measurements spanning a broad temperature range (248.2–403.15 K). From the original dataset of 54,273 entries, a refined subset of 41,724 data points was obtained after excluding water as a solvent and removing duplicate solute entries.

The Leeds dataset includes solubility data for 1,007 organic solutes in three solvents—acetone, ethanol, and benzene—mostly measured near room temperature. Although the range of solvents is relatively limited, the diversity of solute molecules makes this dataset well-suited for evaluating the model's ability to generalize to unseen compounds.

Molecular representation

Two complementary molecular representation strategies were explored, as illustrated in Figure 1: a) learned graph-based representations and b) fixed descriptor-based representations. These two approaches were selected to examine how different types of structural encoding interact with temperature information in solubility prediction tasks.

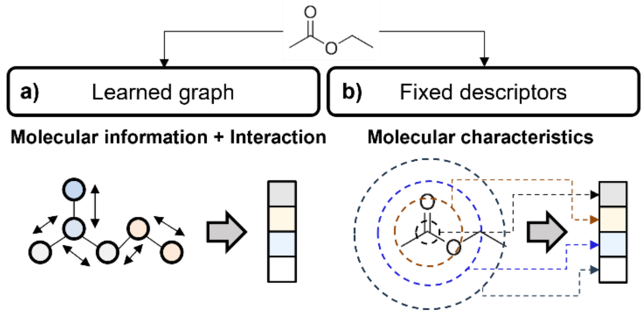

Figure 1. Two types of molecular representations for machine learning-based solubility prediction (e.g. ethyl acetate): **a)** learned graph and **b)** fixed descriptors-based representations

In the graph-based approach, each molecule is represented as a graph, where atoms and bonds correspond to nodes and edges, respectively. Message passing neural networks (MPNNs) are employed to iteratively aggregate and update information from neighboring atoms and bonds, enabling the construction of latent molecular embeddings that capture both local atomic environments and bond-dependent interactions. Formally, a molecular graph G consists of atom features x_v and bond features e_{vw}. During message passing, node-level messages m_v^{t+1} and hidden states h_v^{t+1} are updated at each step t using learnable message and update functions. Through multiple iterations, the model progressively incorporates higher-order structural information, and the resulting node embeddings are finally pooled to produce a molecule-level representation suitable for downstream property prediction. The message passing mechanism is described as follows:

$$m_v^{t+1} = \sum M_t(h_v^t, h_w^t, e_{vw}) \tag{1}$$

$$h_v^{t+1} = U_t(h_v^t, m_v^{t+1}) \tag{2}$$

where h_v^t indicates the hidden state of v at t step, M_t and U_t are message and update functions. After T iterations, the final embeddings are pooled to obtain a molecular representation suitable for downstream property prediction[5,6,15].

In contrast, the descriptor-based representation relies on a fixed vector of many predefined physicochemical descriptors[16]. These descriptors encompass a wide range of molecular characteristics, including constitutional, topological, and connectivity-based features, and have demonstrated strong performance in various property prediction benchmarks. However, a key limitation of this approach is its inability to explicitly capture complex molecular interactions. In particular, many descriptors are inherently invariant to temperature—such as counts of functional groups or atom connectivity indices—making it difficult for descriptor-based models to reflect temperature-dependent behavior in molecular systems.

Feature-wise linear modulation

In this study, feature-wise linear modulation (FiLM) was adopted to incorporate temperature information into molecular representations[10]. Since temperature is originally provided as a scalar in the dataset, it was first expanded into a higher-dimensional space using a radial basis function (RBF) kernel[17]. This transformation enables a smoother and more stable parameterization[18] of temperature prior to applying FiLM.

As illustrated in Figure 2, the expanded temperature embedding is then used to condition molecular features through the FiLM layer. This process allows each feature dimension of the molecular representation to be adaptively scaled and shifted according to temperature. The resulting modulated representation is referred to as a temperature-aware molecular representation (TAMR). Further details of the underlying mechanism can be found in the original FiLM framework[10,12].

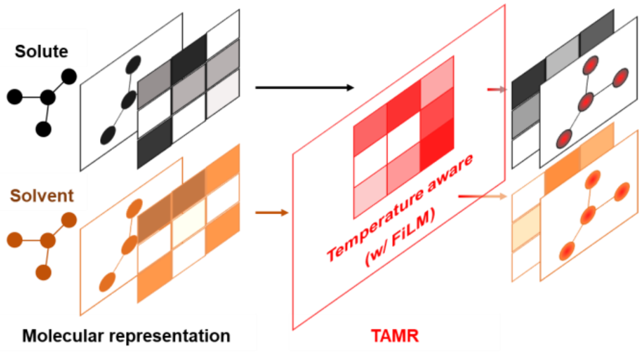

Figure 2. Overview of temperature-aware molecular representations

RESULTS AND DISCUSSION

Training behavior of data-driven models

Figure 3 presents the training and validation loss curves for Chemprop and Fastprop models, with and without FiLM-based TAMR. Overall, incorporating FiLM modifies the optimization behavior in both architectures.

For Chemprop, the introduction of TAMR results in faster convergence and consistently lower loss values across both training and validation sets (Figure 3 **a)** and **b)**). In addition, the variance in loss across training runs is significantly reduced after approximately 50 epochs, suggesting improved training stability.

In contrast, Fastprop shows only minor changes in its training dynamics when FiLM is applied (**Figure 3 c)** and **d)**). Although there is a slight decrease in both loss magnitude and variance, the overall convergence pattern remains largely similar to the baseline model. This limited impact of TAMR can be attributed to the nature of descriptor-based representation. Since the descriptor-based molecular representation relies on predefined, static descriptors rather than learned graph-based features, its ability to dynamically adapt representations during training is constrained. As a result, the optimizer exhibits lower sensitivity to temperature-dependent modulation in both stability and convergence speed.

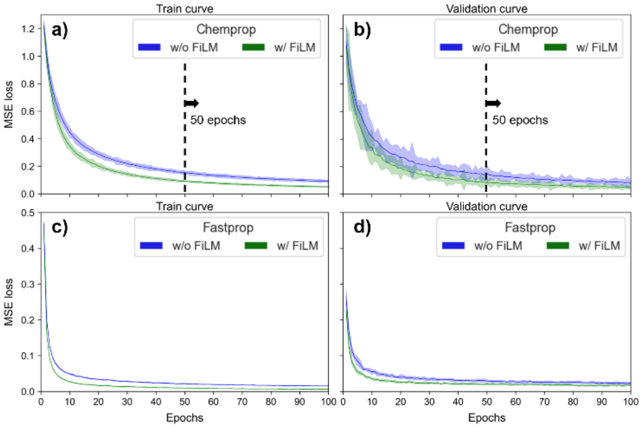

Figure 3. Training and validation curve for data-driven models with and without FiLM

Model evaluation

TAMR was introduced to explicitly capture the influence of temperature on solubility by modulating temperature-sensitive molecular features. To evaluate its effectiveness, root mean squared errors (RMSEs) were analyzed across different temperature ranges for solutes that were already observed during training (**Figure 4**). The figure reports the mean and standard deviation of RMSE values obtained from ten validated models at each temperature.

As shown in **Figure 4 a)**, Chemprop combined with FiLM demonstrates enhanced sensitivity to temperature variations. In particular, at higher temperatures (above 330 K), where thermodynamic properties such as enthalpy and solvation energy become increasingly temperature-dependent[7,19], the prediction error is significantly reduced, with improvements ranging from 13% to 51%.

In contrast, Fastprop shows only marginal improvements when TAMR is applied (**Figure 4 b)**). While slight error reductions are observed in the interpolation regime, the prediction error increases at temperatures above 350 K. This behavior suggests that TAMR is less effective for fixed descriptor-based representations, particularly at elevated temperatures. Since many descriptors used in Fastprop are inherently temperature-invariant[20,21], applying FiLM may distort the latent representation.

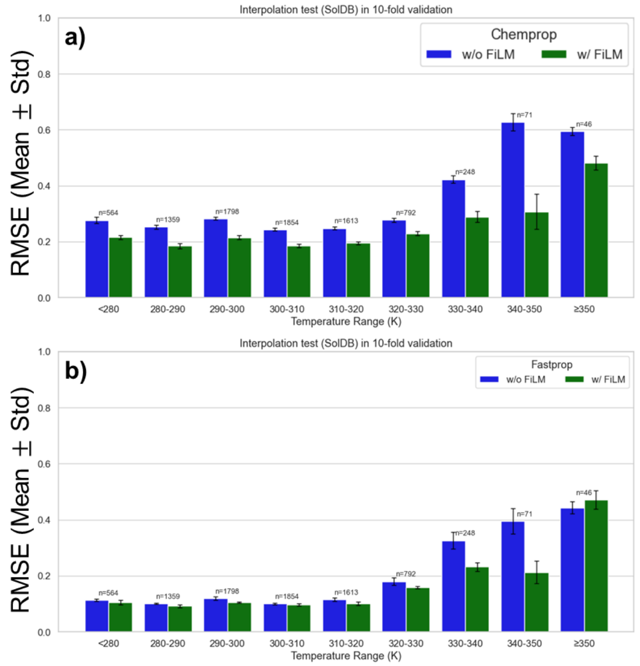

Figure 4. RMSE of the developed models on the BigSolDB validation set across different temperature ranges. Blue bars indicate baseline state-of-the-art (SOTA) models, while green bars represent SOTA models enhanced with TAMR: **a)** Chemprop vs. Chemprop with FiLM, and **b)** Fastprop vs. Fastprop with FiLM.

Application study for unseen solutes

This section evaluates the model performance on the Leeds dataset, which was not used during training. Although TAMR improves predictive performance for both molecular representation approaches, the effect is more pronounced in Chemprop, which utilizes learned graph-based representations. **Figure 5** provides a detailed comparison of this trend across different temperature ranges. As shown in **Figure 5 a)**, Chemprop with FiLM demonstrates notable performance gains near room temperature, particularly in the range of 290–310 K. This suggests that the benefit of TAMR stems from its ability to modulate molecular representations in response to subtle yet physically meaningful temperature-dependent variations under ambient conditions.

In contrast, **Figure 5 b)** indicates that TAMR has minimal impact on the performance of Fastprop. This observation is consistent with the interpolation (BigSolDB) results and further emphasizes the limitation of TAMR for fixed descriptor-based approaches.

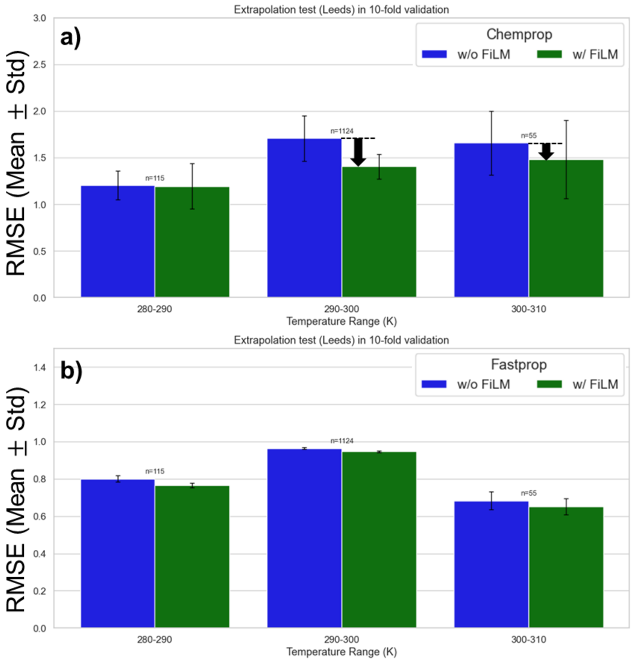

Figure 5. RMSE of the developed models on the Leeds test set across different temperature ranges. Blue bars indicate baseline SOTA models, while green bars represent SOTA models enhanced with TAMR: **a)** Chemprop vs. Chemprop with FiLM, and **b)** Fastprop vs. Fastprop with FiLM.

CONCLUSION

This study introduces a temperature-aware molecular representation (TAMR) to explicitly incorporate temperature effects into molecular representations for improved solubility prediction in organic solvents. Two state-of-the-art architectures, Chemprop and Fastprop, were systematically evaluated using carefully curated datasets, considering both interpolation and extrapolation scenarios.

In the interpolation setting, TAMR led to more stable training behavior and improved predictive accuracy, with a more pronounced effect observed in Chemprop. Even though interpolation involves solutes seen during training, enhanced temperature sensitivity was clearly evident, especially at higher temperature ranges. In extrapolation tasks involving unseen solutes, TAMR further improved model robustness, again with a significantly stronger impact on Chemprop compared to Fastprop. Overall, these findings highlight that TAMR is particularly effective when applied to learned graph-based representations, as it enables the model to capture temperature-dependent molecular behavior.

Moreover, this framework provides a flexible foundation for incorporating other environmental factors, such as pressure, suggesting its broader applicability to diverse property prediction problems.

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P-15

SESSION

P1 · July 6 (Mon) 13:30~14:30

PRESENTER

Cuimei Bo

Dynamic Multi-Objective Operational Optimization of the Green Hydrogen Ammonia Synthesis Process under Uncertainty Disturbance

Zijun Wang, Shida Gao, Kangkang Feng, Xiangjian Shi, Cuimei Bo*

Nanjing Tech University & affiliates, China

The full paper follows on the next page.

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Dynamic Multi-Objective Operational Optimization of the Green Hydrogen Ammonia Synthesis Process under Uncertainty Disturbance

Zijun Wang[a], Shida Gao[b], Kangkang Feng[c], Xiangjian Shi[c], and Cuimei Bo[a]*

[a] College of Electrical Engineering and Control Science, Nanjing Tech University, Nanjing, 211816, Jiangsu, China
[b] Ningbo Artificial Intelligence Institute, Shanghai Jiao Tong University, Ningbo, 315012, Zhejiang, China
[c] Nanjing Nanrui Jibao Engineering Technology Co., Ltd, Nanjing, 211102, Jiangsu, China
* Corresponding Author: Cuimei Bo. lj_bcm@163.com

ABSTRACT

Green hydrogen-coupled ammonia synthesis is a promising pathway for the low-carbon transition of the fertilizer industry. However, the fluctuation of renewable energy output conflicts with the strict requirements of ammonia synthesis for safe and stable operation, posing major challenges to online optimization. To address this issue, this paper proposes a dynamic multi-objective operational optimization method for ammonia synthesis under fluctuating green hydrogen loads. A flexible power-hydrogen-ammonia process and a mechanistic model are first developed. Then, a dynamic multi-objective optimization model is established to maximize hydrogen conversion and minimize total energy consumption under constraints on product purity and critical operating variables. Furthermore, a DAPB-NSGAII algorithm is proposed by integrating an online Gaussian process surrogate, environmental change detection, Pareto-based dual-metric infill sampling, and centroid-prediction-based population reconstruction, enabling efficient tracking of the Pareto front in time-varying environments. The results show that the complete algorithm achieves superior HV and IGD statistics on FDA1-FDA3, verifying the contribution of each core mechanism to dynamic front tracking. In a continuous one-week online optimization case, the proposed method also exhibits faster responses to load switching and better operational decision-making capability.

Keywords: Energy Conversion , Process Design, green ammonia synthesis, load fluctuation, dynamic multi-objective optimization, Gaussian process surrogate model.

1. INTRODUCTION

Ammonia is not only a core basic chemical for the nitrogen fertilizer industry, but also a potential hydrogen storage carrier and carbon-free fuel with a high hydrogen content. Its low-carbon production is therefore of great significance for emission reduction in energy and chemical systems [1-2]. The conventional Haber-Bosch process mainly relies on gray hydrogen produced from fossil fuels, resulting in substantial carbon emissions during both hydrogen production and ammonia synthesis [3-5]. Driven jointly by carbon neutrality targets and the need for large-scale renewable energy accommodation, green hydrogen production through water electrolysis powered by renewable electricity, such as wind and photovoltaic power, and its further coupling with ammonia synthesis units to produce green ammonia have become important technical routes for the deep decarbonization of the ammonia industry [6-8]. Meanwhile, regions such as Northwest and North China possess abundant wind and solar resources as well as a relatively mature chemical industrial base, providing practical conditions for the large-scale deployment of green ammonia systems [9]. However, green hydrogen-based ammonia synthesis is not a single energy-efficiency optimization problem; rather, it involves the coupling of multiple factors, including hydrogen conversion, energy consumption, product purity, load adaptability, and safe operating constraints, and thus requires systematic investigation from the perspective of multi-objective operational optimization [10-11]. In particular, when wind and solar power fluctuations are transmitted to the synthesis section even after electrolysis, battery storage, and hydrogen storage buffering, the recycle-gas composition, reactor heat load, cooling demand, and compression power consumption vary accordingly, further affecting the H2/N2 ratio, net ammonia production, and reactor-temperature safety margin [12-13]. If fixed operating parameters tuned for steady-state conditions are still adopted, the unit may suffer from reduced conversion, increased specific energy consumption, and operation close to temperature constraint boundaries under low-load or rapid load-switching conditions [14]. Therefore, operational optimization of ammonia synthesis under green hydrogen fluctuations must dynamically update operating decisions while simultaneously considering multi-objective trade-off performance and safety-constraint feasibility.

Flexible operation and dynamic optimization of green ammonia systems have been investigated from the perspectives of transition strategies, mechanistic modeling, capacity planning, and multi-state scheduling. For example, Wen [15] reduced energy costs and raw-material losses by improving load-regulation transition strategies; Deng [16] combined machine learning with intelligent optimization algorithms for the modeling and operational optimization of green ammonia synthesis; Zhou [17] proposed a multi-stable flexible operation strategy to accommodate renewable energy fluctuations; and Wu [18] further investigated capacity-operation matching for flexible green ammonia systems under multi-frequency scheduling. These studies demonstrate the necessity of flexible optimization for improving the adaptability of green ammonia systems. Nevertheless, two limitations remain. First, many methods rely on frequent calls to complex process models, leading to high computational overhead for hour-level online decision-making. Second, existing studies mostly focus on single-objective or quasi-static scenarios and insufficiently characterize the drift of the Pareto front with load variations in dynamic environments, making it difficult to systematically evaluate front-tracking capability and long-term operational benefits under continuous disturbances.

To address the high computational cost of mechanistic ammonia synthesis models, the difficulty of online decision-making, and the challenge of coordinated multi-objective optimization under green hydrogen fluctuations, this paper proposes an integrated solution framework that combines surrogate-assisted optimization with dynamic multi-objective optimization. First, a flexible power-hydrogen-ammonia conversion process and its process parameters are designed, and a mechanistic model of the ammonia synthesis process is developed to represent the transmission and smoothing effects of wind/solar output, battery storage, and hydrogen storage buffering on green hydrogen fluctuations. Second, a dynamic multi-objective optimization model is established with hydrogen conversion maximization and total energy consumption minimization as the objectives and ammonia product purity and key operating-variable ranges as constraints, thereby describing the coordinated multi-objective optimization problem of the ammonia synthesis process under fluctuating green hydrogen supply. Finally, a DAPB-NSGAII dynamic multi-objective optimization algorithm is proposed, and its front-tracking capability, disturbance-response capability, and engineering applicability under a limited computational budget are verified through ablation experiments on dynamic benchmark functions and continuous online optimization experiments.

The remainder of this paper is organized as follows. Section 2 presents the analytical modeling of the green hydrogen-based ammonia synthesis process. Section 3 formulates the dynamic multi-objective optimization problem under green hydrogen fluctuations and describes the proposed method. Section 4 reports the results and discussion. The final section summarizes the main conclusions and industrial application value.

2. PROCESS ANALYSIS AND MODELING OF GREEN HYDROGEN-BASED AMMONIA SYNTHESIS

To characterize the influence of green hydrogen load fluctuations on the operational performance of an ammonia synthesis plant, this paper constructs an integrated system consisting of wind-solar power generation, PEM electrolysis for hydrogen production, hydrogen storage buffering, and an ammonia synthesis unit. Renewable electricity is first used to drive the PEM electrolyzer to produce hydrogen. The produced hydrogen and nitrogen from the air separation unit enter the synthesis section at the stoichiometric ratio. A two-level buffering structure comprising a battery and a hydrogen storage tank is configured in the system. The battery mainly attenuates power fluctuations on the minute-to-hour scale, whereas the hydrogen storage tank smooths fluctuations on the hydrogen-production side and improves the continuity of hydrogen supply to the synthesis unit.

The system capacity configuration is based on the wind-solar complementary hydrogen production study by Shi [19], in which the installed wind and photovoltaic capacities are set to 225 MW and 233 MW, respectively, to form a complementary energy supply structure. In terms of operating logic, surplus renewable electricity is preferentially used for water electrolysis and battery charging. When wind-solar output is insufficient, the battery compensates for short-term power deficits, and the hydrogen storage tank maintains a relatively stable feed load to the synthesis section. The overall system structure is shown in Fig. 1.

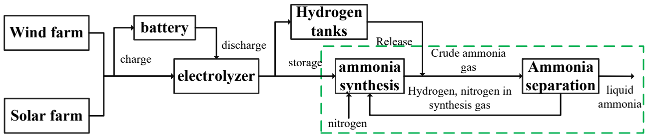

Fig. 1. Structure of the ammonia synthesis system under green hydrogen fluctuation

The ammonia synthesis section adopts a typical reaction-cooling-separation-recycle process. The hydrogen-nitrogen mixture undergoes a reversible synthesis reaction under high temperature, high pressure, and catalyst conditions. The main reaction equation is as follows:

$$N_2 + 3H_2 \rightleftharpoons 2\mathrm{NH}_3 \tag{1}$$

Because ammonia synthesis is jointly governed by chemical equilibrium, adsorption processes, and catalytic kinetics, this paper uses the LHHW kinetic equation to describe the reaction rate, accounting for the effects of reactant partial pressures, product inhibition, and temperature variations on the reaction rate. The kinetic expressions are shown in Eqs. (2) and (3).

$$r = ke^{-\left(\frac{E}{RT}\right)} \times \left(k_1 \prod_{i=1}^{N} P_i^{\alpha_i} - k_2 \prod_{j=1}^{N} P_j^{\beta_j} \right) \tag{2}$$

$$ln(k_1, k_2) = A + \frac{B}{T} + C \times lnT + D \times T \tag{3}$$

As shown in Fig. 2, fresh hydrogen and nitrogen gases are mixed, compressed, and preheated before entering three adiabatic reactors connected in series. The outlet streams from each reactor are cooled and subjected to gas-liquid separation to obtain liquid ammonia product. Most unreacted hydrogen and nitrogen are returned to the recycle loop, while a small fraction is discharged as purge gas to suppress inert accumulation and maintain a stable recycle-gas composition.

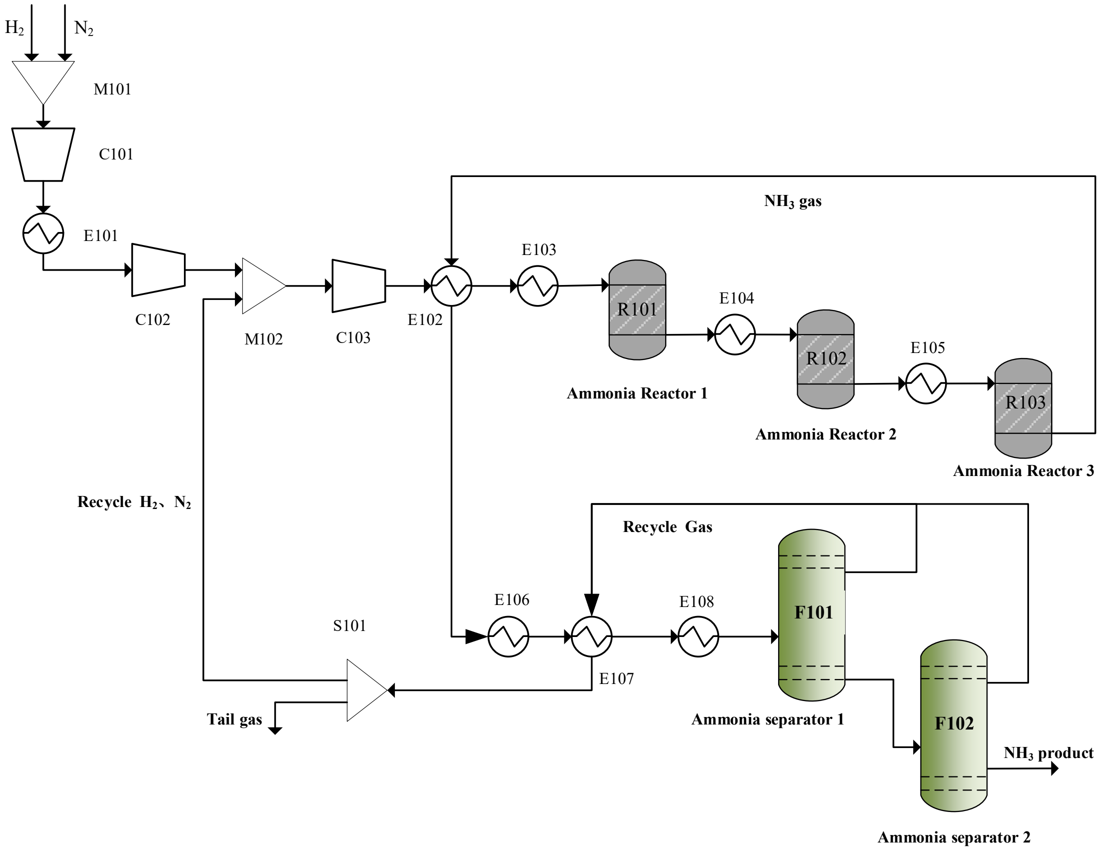

Fig. 2. Process flow diagram of the green-hydrogen-to-ammonia process

In the process simulation, the RKS-BM property method and the RPLUG reactor model are used to establish a steady-state mechanistic model incorporating LHHW kinetics. Typical values of the main fixed process and operating parameters are listed in Table 1.

The steady-state validation results show that the model can reproduce the industrial reference condition satisfactorily. Taking the ammonia mole fraction at the R103 outlet as an example, the simulated value is 18.19%, and the relative error compared with the reference value of 18.25% is 0.33%, which meets the requirements for subsequent dynamic optimization evaluation.

Table 1. Main fixed process parameters and operating parameters

No.	Process parameters	Value	Unit
1	Reactor R101 inlet temperature	310	°C
2	Reactor R102 inlet temperature	340	°C
3	Reactor R103 inlet temperature	360	°C
4	Reactor R101 inlet pressure	118	Bar
5	Reactor pressure drop	2	Bar
6	First-stage ammonia refrigeration outlet temperature	20	°C
7	Second-stage ammonia refrigeration outlet temperature	-10	°C
8	Separator F101 inlet pressure	107.5	Bar
9	Separator F102 set temperature	15	°C
10	Separator F102 set pressure	160	Bar
11	Reactor length	3	m
12	Reactor diameter	3	m
13	Hydrogen molar flow rate at 100% load	1165.43	Kmol/h
14	Nitrogen molar flow rate at 100% load	388.48	Kmol/h

3. DYNAMIC MULTI-OBJECTIVE OPTIMIZATION UNDER GREEN HYDROGEN FLUCTUATION

3. 1 Dynamic Multi-Objective Optimization Problem

For the ammonia synthesis operation problem under fluctuating green hydrogen supply, this paper establishes a dynamic multi-objective optimization model to coordinate hydrogen conversion, energy consumption, and safety constraints at each operating time. The model uses nine key operating variables to form the decision vector and treats green hydrogen feed load as a time-varying external disturbance. Under constraints on product ammonia purity and operating-variable bounds, the dynamic Pareto-optimal solution set is sought. The mathematical formulation is as follows:

$$minF(x,t) = \left(-X_{H2}(x,t), E_{elec}(x,t)\right)^T \tag{4}$$

$$\text{subject to } \begin{cases} \omega_{NH3} \geq 99\% \\ x_{\text{i,lowerbound}} \leq x_i \leq x_{\text{i, upperbound}}, i = 1,2,\cdots,9 \end{cases} \tag{5}$$

where $\boldsymbol{x}$ denotes the vector of operating variables, t denotes the time-dependent disturbances such as green hydrogen supply, ω_{NH3} denotes the ammonia product purity. The dynamic nature of this model is mainly reflected in the fact that load disturbances change the input conditions of the process model and the mapping relationships of the objective functions, thereby causing the Pareto front to drift over time.

The objective function for hydrogen conversion is defined as follows:

$$X_{H2}(x,t) = \frac{F_{H2,in}(x,t) - F_{H2,out}(x,t)}{F_{H2,in}(x,t)} \times 100\% \tag{6}$$

Where $F_{H2,in}(x,t)$ is the molar flow rate of hydrogen in the mixed gas entering the reactor 1; $F_{H2,out}(x,t)$ is the molar flow rate of hydrogen in the mixed gas leaving the reactor 3. Hydrogen conversion directly reflects the utilization efficiency of feed hydrogen in the reaction system and is one of the core indicators for evaluating the operational performance of green hydrogen-based ammonia synthesis.

The objective function for energy consumption is defined as follows:

$$\begin{cases} E_{elec}(x,t) = E_{N2}(x,t) + \dfrac{E_{COM}(x,t)}{\eta_{COM}} + \dfrac{E_{COOL}(x,t)}{\eta_{COOL}} \\ E_{N2}(x,t) = F_{wN2}(x,t) \times P_{N2} \\ E_{COM}(x,t) = E_{C101}(x,t) + E_{C102}(x,t) + E_{C103}(x,t) \\ E_{COOL}(x,t) = \sum E_{CW}(x,t) \times \eta_{CW} + \sum E_{CA}(x,t) \times \eta_{CA} \end{cases} \tag{7}$$

In the above formula, the total production power consumption mainly comes from three parts: the power consumption $E_{N2}(x,t)$ for nitrogen production by air separation, which is estimated by the product of the nitrogen raw material mass flow $F_{wN2}(x,t)$ and its unit separation energy consumption P_{N2}; The total power consumption of the compressor $E_{COM}(x,t)$ (the sum of the power consumption of the compressors C101, C102 and C103) needs to be divided by the comprehensive efficiency η_{COM} to be converted into the input power of the grid side; The total power consumption $E_{COOL}(x,t)$ of the cooling system is calculated from the water cooling load $E_{CW}(x,t)$, the ammonia cooling load $E_{CA}(x,t)$ and their respective energy efficiency coefficients, and then divided by the total system efficiency η_{COOL}.

Based on process constraints and sensitivity analysis, this paper selects nine key operating variables as decision variables, including the inlet temperatures of the three reactors, the outlet temperature of the water cooler, the outlet temperatures of the two ammonia refrigeration stages, and the pressures of three compressors. Their default values and ranges are listed in Table 2. The green hydrogen feed load is taken as an external disturbance input and is not involved in the optimization search, but it determines the operating environment of the process model at each time.

Table 2. Default values and ranges of the nine operating variables and the disturbance variable

	Operation parameters	Variable type	Unit	default value	range
1	Reactor R101 inlet temperature	Operational	°C	310	300-340
2	Reactor R102 inlet temperature	Operational	°C	340	330-355
3	Reactor R103 inlet temperature	Operational	°C	360	340-400

4	Cooling-water outlet temperature	Operational	°C	26	10-40
5	First-stage ammonia cooling temperature	Operational	°C	20	10-30
6	Second-stage ammonia cooling temperature	Operational	°C	0	-12-10
7	Compressor C101 pressure	Operational	Bar	40	10-50
8	Compressor C102 pressure	Operational	Bar	75	60-90
9	Compressor C103 pressure	Operational	Bar	120	108-130
10	Green hydrogen feed load	Disturbance	Kmol/h	1165	300-1900

3. 2 Optimization Method

To solve the above dynamic multi-objective optimization problem, this paper proposes the DAPB-NSGAII algorithm. The algorithm uses NSGA-II as the basic search framework and introduces an online Gaussian Process (GP) surrogate model with adaptive parameters to reduce calls to the expensive process model. It also combines environmental change detection, Pareto-based bi-indicator (PB) sample screening, and a centroid-drift-based environmental response mechanism to improve the ability to track the dynamic Pareto front under limited computational budgets. The algorithmic workflow is shown in Fig. 3.

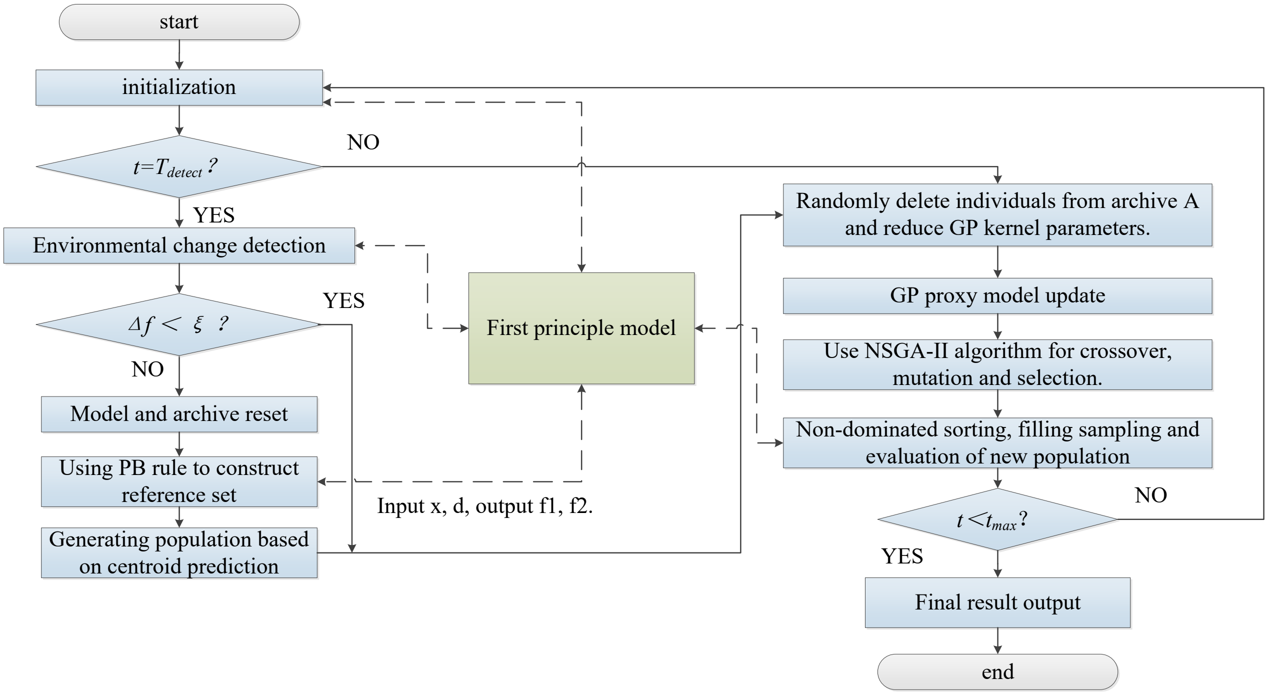

Fig. 3. Flowchart of the DAPB-NSGAII algorithm

The main steps of the algorithm are as follows:

(1) An initial population of size P is generated using Latin hypercube sampling, and the first-principles model (FPM) is called for real function evaluations. The archive A, the ideal point $z^{\min}$, and the Gaussian process (GP) surrogate model are initialized accordingly.

(2) During the optimization process, environmental change detection is performed according to the predefined monitoring period T_{detect}. If the monitoring period has not been reached, the algorithm directly proceeds to the regular surrogate-assisted optimization stage. Otherwise, the top 10% dominant individuals are selected from the current population using the PB criterion as detection samples, and their objective-value variations Δf are calculated through FPM re-evaluation.

(3) The environmental variation Δf is compared with the threshold ξ. If $\Delta f < \xi$, the current environment is considered to have no significant change, and the algorithm continues to use the existing population and archive information. If $\Delta f \geq \xi$, an environmental drift is identified, and the environmental response mechanism is triggered.

(4) When a significant environmental change occurs, the relevant hyperparameters of the GP surrogate model are reset, and historical archive information that is no

longer applicable to the new environment is removed. While retaining the detection samples, an additional 40% of dominant individuals are selected from the original population according to the PB criterion and re-evaluated by the FPM under the new operating condition to form an environmental response solution set.

(5) The centroid of the environmental response solution set C_R and the centroid of the historical archive C_A are calculated. The centroid drift vector between them is then used to estimate the migration direction of the Pareto-optimal region. Subsequently, predicted individuals are generated by superimposing the migration vector and random perturbations onto historical individuals. These predicted individuals, together with the response solution set, form the initial population under the new environment, and the archive A is updated.

(6) Capacity maintenance is performed on archive A. If the number of archive samples S_n exceeds the maximum capacity S_a, individuals with weaker representativeness are gradually removed according to non-dominated ranks and crowding distances. Meanwhile, the initial scale parameter θ_{k0} of the GP kernel function is adjusted appropriately to balance sample quality and surrogate-model training efficiency.

(7) The maintained archive A is used to train or update the GP surrogate model corresponding to each objective function. The surrogate model is then employed to replace the expensive FPM and drive NSGA-II for N generations of rapid evolutionary search. After surrogate-assisted optimization, candidate solutions are selected from the current non-dominated solution set using the PB criterion for real FPM evaluation, and the evaluation results are added to archive A.

(8) The algorithm checks whether the system operating time has reached the predefined upper limit $t_{\max}$. If not, the procedure returns to the environmental monitoring and surrogate-assisted optimization process. If $t_{\max}$ has been reached, non-dominated sorting is performed on the final archive A, and the optimal operating parameter set for ammonia synthesis under the current green hydrogen condition is output after inverse normalization.

Considering the high computational cost associated with frequent FPM calls in a dynamic environment, GP is adopted as the online surrogate model in this study, and separate predictive models are established for the two optimization objectives. The Gaussian process surrogate model [20] is defined as follows:

$$y(x) = \mu + \epsilon(x), \qquad (x) \sim N(0, \sigma^2) \tag{8}$$

Where $y(x)$ represents the observed value at the input point x, μ represents the global mean of the Gaussian process; $\epsilon(x)$ is an error term, which obeys a normal distribution with a mean of 0 and a variance of σ^2. By training the GP model with historical true-evaluation samples, the algorithm can rapidly approximate candidate operating points without frequently calling the process simulation.

In surrogate-assisted optimization, the selection of truly evaluated samples directly determines the quality of subsequent model correction. To avoid excessive concentration of candidate samples in local regions, the PB criterion [21] is adopted in environmental detection, response-sample expansion, and final infill evaluation. This criterion incorporates both convergence and diversity into the auxiliary optimization objectives, enabling newly added true samples to approach the potential Pareto front while improving the coverage of the objective space. Its mathematical expression is as follows:

$$\begin{cases} minG(X^*) = \left(CI(X^*), -DI(X^*)\right) \\ CI(X^*) = \|F(X^*) - Z^*\| \\ DI(X^*) = min_{p=1:N}\left(\|X^* - X_p\|^2\right) \end{cases} \tag{9}$$

$$\text{subject to } X^* \in \text{Trial Solutions}$$

When a significant environmental change occurs, high-quality individuals under the old environment are not necessarily still located in the effective search region of the new environment. To shorten the recovery time after environmental switching, this paper draws on the centroid-prediction idea of the SGEA algorithm [22] and estimates the migration direction of the Pareto-optimal region based on the geometric displacement between the response solution set and the historical archive. First, the center CR of the current population and the center CA of the archive are calculated:

$$C_R = \frac{1}{|P|}\sum_{x \in P} x, \qquad C_A = \frac{1}{|A|}\sum_{x \in A} x \tag{10}$$

Then, the centroid offset is used as an approximation of the migration trend in the decision space, and predicted individuals are generated by superimposing this offset and random perturbations on historical individuals:

$$x_{new} = x_{old} + (C_A - C_R) + \delta \tag{11}$$

where x_{old} denotes an individual selected from the original population or archive, δ denotes a Gaussian random perturbation vector, and $C_A - C_R$ denotes the migration vector estimated from centroid changes. This strategy exploits historical search information to improve response speed while maintaining a certain degree of exploration through random perturbations.

In Step 7, the NSGA-II algorithm proposed by Deb [23] in 2002 is adopted. NSGA-II determines the Pareto rank of individuals through fast nondominated sorting and maintains distribution diversity within the same rank using crowding distance. This mechanism balances convergence pressure and solution-set dispersion in medium-scale multi-objective optimization problems, making it suitable as the basic search framework for the surrogate-assisted dynamic optimization in this paper. The crowding-distance calculation is as follows:

$$I_d(i) = \sum_{m=1}^{M} \frac{f_m(i_{next}) - f_m\left(i_{prev}\right)}{f_m^{max} - f_m^{min}} \tag{12}$$

4. RESULTS AND DISCUSSION

4.1 Experimental Setup

The experiments in this study are carried out on a co-simulation platform integrating MATLAB 2022b and Aspen Plus V12.1. Aspen Plus is used for mechanistic calculations of the ammonia synthesis process, whereas MATLAB is responsible for dynamic multi-objective optimization, surrogate-model updating, and calls to comparison algorithms. Hourly data interaction between the two platforms is implemented through the MAP interface. The hardware used in the experiments consists of an Intel i5-12500 processor and 32 GB RAM.

The experiments include two parts: ablation analysis on dynamic benchmark functions and continuous online operation verification for the ammonia synthesis process. For the dynamic benchmark part, FDA1, FDA2, and FDA3 are selected as three typical dynamic multi-objective test problems to examine the front-tracking capability of the algorithm under different patterns of front position, shape, and distribution changes. Five algorithmic variants are configured around the key mechanisms of DAPB-NSGAII: FULL denotes the complete algorithm; NO_ED removes the environmental change detection module; NO_RESP retains environmental detection but removes the centroid-prediction-based environmental response mechanism; NO_SUR removes the online surrogate-assisted search module; and NO_DUAL removes the PB bi-indicator infill-sampling mechanism. Except for the ablated module, all algorithms use a population size of 30 and a unified surrogate-assisted evolution length of 10 generations per round, ensuring that performance differences mainly originate from the corresponding modules.

For the online ammonia synthesis operation experiment, a continuous 168 h historical sequence with pronounced green hydrogen supply fluctuations in October 2024 is selected to construct a one-week dynamic disturbance scenario, and 1 h is used as the single optimization decision window. To evaluate the engineering applicability of the proposed method, three comparative strategies are considered: fixed operating parameters, SGEA, and DAPB-NSGAII. The fixed strategy always uses the benchmark operating point and does not adjust with load changes; SGEA serves as the comparison method based on a dynamic multi-objective evolutionary algorithm; and DAPB-NSGAII performs online optimization under the same load sequence and constraint conditions. At each decision time, a comprehensive trade-off operating point is selected from the current Pareto solution set, and the average hydrogen conversion and cumulative energy consumption over the continuous 168 h period are calculated.

4.2 Comparative Analysis of Algorithm Performance

Table 3 summarizes the HV and IGD statistics of the five algorithmic variants on FDA1, FDA2, and FDA3. Overall, the complete algorithm achieves the highest HV and the lowest IGD on all three dynamic test problems, indicating that the advantage of the proposed algorithm arises from the synergy among environmental identification, response migration, surrogate search, and sample updating, rather than from an isolated improvement of a single operator.

Table 3. Performance statistics of the five ablation algorithms on dynamic benchmark functions

	FULL	NO_ED	NO_RESP	NO_SUR	NO_DUAL
HV（FDA1）	**6.8371e-1**	6.5808e-1	5.6843e-1	5.3510e-1	6.5693e-1
IGD（FDA1）	**3.7360e-2**	8.0475e-2	2.4279e-1	2.8997e-1	8.5570e-2
HV（FDA2）	**4.9925e-01**	4.3404e-1	4.3344e-1	3.6598e-1	3.9310e-1
IGD（FDA2）	**1.9658e-02**	1.7458e-1	1.4426e-1	2.9068e-1	2.0660e-1
HV（FDA3）	**6.1714e-1**	6.1127e-1	6.1140e-1	6.0932e-1	5.9266e-1
IGD（FDA3）	**2.1137e-2**	2.6697e-2	2.6906e-2	2.9461e-2	6.0562e-2

As shown in Table 3, FULL achieves the highest HV and the lowest IGD on FDA1-FDA3, demonstrating the synergistic effect of environmental detection, response migration, surrogate search, and PB sample updating. Among the variants, NO_SUR shows the most severe degradation, with IGD increasing to 0.2900 and 0.2907 on FDA1 and FDA2, respectively, indicating that the online surrogate model is crucial for approximating the dynamic front under a limited evaluation budget. The IGD of NO_RESP increases to 0.2428 on FDA1, showing that centroid-prediction-based population reconstruction helps shorten the recovery process after environmental switching. The IGD of NO_ED rises to 0.1746 on FDA2, reflecting that explicit environmental detection can reduce the interference of old-environment search information with the localization of the new front. On FDA3, the HV differences among the algorithms are relatively small, but the IGD of NO_DUAL reaches 0.0606, approximately 2.87 times that of FULL, indicating the importance of PB bi-indicator sampling for maintaining front coverage. Overall, the performance advantage of DAPB-NSGAII is jointly supported by environmental identification, response reconstruction, surrogate acceleration, and representative sampling.

4.3 Analysis of Online Operation Results

After verifying the roles of the key modules using dynamic benchmark functions, hour-level online optimization experiments are further conducted for the ammonia synthesis process based on one week of green hydrogen load data. Fig. 4 presents the online optimization process under continuous 168 h green hydrogen fluctuations, where Fig. 4(a) shows the green hydrogen feed flow rate, Fig. 4(b) shows the continuous hydrogen conversion results relative to the fixed operating-parameter baseline, and Fig. 4(c) compares cumulative energy savings relative to the fixed operating-parameter baseline. Table 4 summarizes the average hydrogen conversion and cumulative energy consumption of the fixed operating-parameter, SGEA, and DAPB-NSGAII strategies.

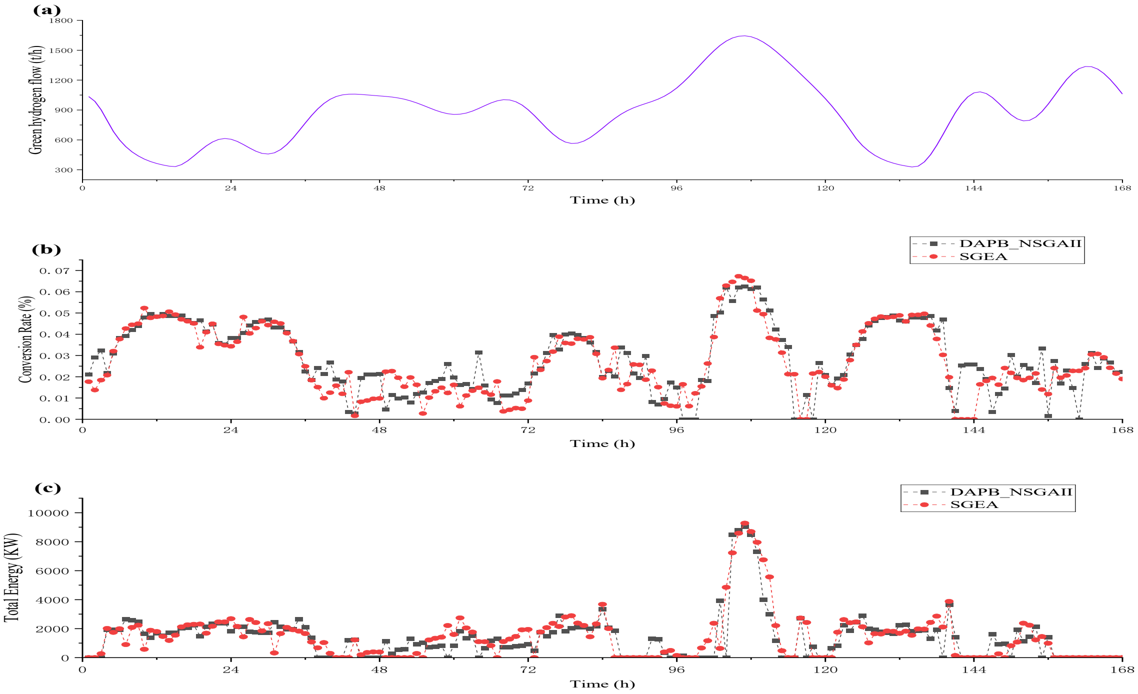

Fig. 4. Continuous 168 h green hydrogen input disturbance and long-term optimization performance comparison

As shown in Fig. 4(a), the green hydrogen feed exhibits continuous fluctuations and staged load switching within one week, indicating that the ammonia synthesis unit does not operate near a single steady state. Changes in feed flow rate simultaneously affect reactor residence time, recycle-gas composition, compressor load, and cooling load. Therefore, fixed operating parameters are unable to maintain both high conversion and low energy consumption over all time periods. Fig. 4(b) further shows that the dynamic optimization strategies can update reactor inlet temperatures, cooling temperatures, and compression pressures with load variations, thereby improving hydrogen conversion relative to the fixed-parameter baseline. Fig. 4(c) reflects, from the perspective of cumulative energy consumption, whether such hour-level operating improvements can be translated into long-term energy-saving benefits.

Table 4. Online operation performance comparison of different operating strategies over 168 h

Operating strategy	Fixed operating parameters	SGEA	DAPB-NSGAII
Average hydrogen conversion (%)	33.037%	35.728%	**35.819%**
Total energy consumption (kWh)	5031532.937	4913797.727	**4891483.434**

Table 4 summarizes the statistical results over the 168 h operating period. The fixed operating-parameter strategy achieves an average hydrogen conversion of 33.037% and a cumulative equivalent electricity consumption of 5,031,532.937 kWh. SGEA increases the average hydrogen conversion to 35.728% and reduces the cumulative equivalent electricity consumption to 4,913,797.727 kWh. DAPB-NSGAII further achieves an average hydrogen conversion of 35.819% and a cumulative equivalent electricity consumption of 4,891,483.434 kWh. Compared with the fixed operating-parameter strategy, DAPB-NSGAII improves the average hydrogen conversion by 2.782% and reduces the cumulative equivalent electricity consumption by 140,049.503 kWh, corresponding to a reduction of approximately 2.78%.

It is worth noting that, compared with SGEA, DAPB-NSGAII only further improves the average hydrogen conversion by 0.091%, but additionally reduces the cumulative equivalent electricity consumption by 22,314.293 kWh. This result indicates that the main advantage of the proposed method does not lie solely in substantially increasing hydrogen conversion. Instead, it can further identify Pareto-compromise solutions with lower energy consumption while maintaining a comparable and relatively high conversion level. For the ammonia synthesis process, further increasing hydrogen conversion often requires additional compression or cooling costs. Therefore, reducing long-term cumulative energy consumption while maintaining a nearly stable conversion level is more meaningful from an engineering application perspective.

5. CONCLUSIONS

This paper addresses the online operational optimization problem of ammonia synthesis under green hydrogen load fluctuations. A dynamic multi-objective optimization model is constructed with hydrogen conversion maximization and total energy consumption minimization as the objectives and product purity and key operating variables as constraints. A DAPB-NSGAII algorithm integrating environmental detection, an online GP surrogate, PB infill sampling, and centroid-prediction-based reconstruction is proposed. The ablation experiments on dynamic benchmarks show that the complete algorithm achieves the highest HV and the lowest IGD on FDA1-FDA3. The continuous 168 h online operation results show that, compared with the fixed operating-parameter strategy, the proposed method improves the average hydrogen conversion by 2.782 percentage points and reduces the cumulative equivalent electricity consumption by approximately 2.78%. Compared with SGEA, DAPB-NSGAII further reduces the cumulative energy consumption by approximately 0.45% while maintaining a slightly higher hydrogen conversion. The results demonstrate that the proposed method can realize multi-objective online operational optimization under continuous green hydrogen load fluctuations while satisfying product purity and operating safety constraints, thereby providing a feasible methodological support for flexible, safe, and low-energy operation of green ammonia units.

ACKNOWLEDGEMENTS

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SESSION

P2 · July 7 (Tue) 13:30~14:30

PRESENTER

Kyojin Jang

Process-Aware Shapley Flow Analysis for Interpretable Fault Diagnosis

Kyojin Jang*, Jeongdong Kim

Samsung Electronics Co., Korea; Massachusetts Institute of Technology, USA

The full paper follows on the next page.

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Process-Aware Shapley Flow Analysis for Interpretable Fault Diagnosis in Chemical Processes

Kyojin Jang[a,] *, and Jeongdong Kim[b]

[a] Samsung Electronics Co., Suwon, Republic of Korea
[b] Massachusetts Institute of Technology, Department of Chemical Engineering, MA, United States of America
* Corresponding Author: kj1230.jang@samsung.com

ABSTRACT

Interpreting industrial fault diagnosis requires more than accurate classification, since operators also need to understand which process variables and temporal patterns drive a model's decision. This paper presents a fault-specific Shapley Flow framework for the Tennessee Eastman Process. We first select a compact fault-specific feature set using process relevance, model relevance, and temporal utility, and then build two explanation models on the same base variables: a process-guided static directed acyclic graph (DAG) and a lagged temporal DAG. Shapley Flow is applied to both graphs using residual-augmented structural equations so that observed baseline and target samples are faithfully reproduced during explanation. Experiments on Fault 14 show that both graph variants identify reactor temperature and reactor cooling water outlet temperature as the dominant contributors to predicted fault probability, consistent with the physical fault mechanism. The lagged DAG achieves classification performance comparable to the static DAG while providing additional interpretability by revealing short-term temporal propagation. At the same time, residual-related edges retain non-negligible explanatory credit, indicating that the proposed graphs capture the dominant process-consistent fault signature but do not fully reconstruct the underlying causal mechanism. These results suggest that fault-specific graph construction combined with Shapley Flow provides a practical way to obtain more process-aware and temporally informed explanations for industrial fault diagnosis.

Keywords: Shapley Flow, Process Interpretability, Fault Diagnosis, Graph-based Analysis

1. INTRODUCTION

Industrial process fault diagnosis is not limited to detecting whether a process is abnormal; it also requires identifying which variables are responsible for the abnormal behavior and how their effects propagate through the process. Data-driven process monitoring has been widely studied for fault detection, identification, reconstruction, and diagnosis using multivariate process measurements [1]. However, as machine learning models become more accurate and more complex, their predictions often provide insufficient diagnostic insight for operators, especially when the process involves strongly coupled variables, feedback control, and delayed responses. Recent work on explainable artificial intelligence for industrial fault diagnosis also emphasizes that black-box models require human-understandable explanations to support trust, auditability, and decision making [2].

The Tennessee Eastman (TE) process is a representative benchmark for evaluating process monitoring and fault diagnosis methods. The original TE process describes a plant-wide chemical process with reactor, separator, recycle, and product-quality related units [3]. Because of its nonlinear dynamics, variable interactions, and diverse fault scenarios, the TE process has been repeatedly used as a reference problem for statistical process monitoring and machine learning based fault detection studies [3,4].

Machine learning classifiers such as XGBoost can provide strong predictive performance for tabular process data by modeling nonlinear feature interactions through gradient-boosted decision trees [5]. Nevertheless, high classification accuracy alone does not explain why a sample is classified as a fault. Feature attribution methods such as SHAP address this issue by assigning an importance value to each input feature for an individual prediction [6]. Although these methods are useful for identifying influential variables, conventional feature-level explanations are essentially flat: they do not explicitly represent how contributions are transmitted along process pathways. This is a key limitation in process fault diagnosis, where the interpretation of a variable often depends on its location in the process structure.

Graph-based attribution methods provide a natural way to address this limitation. Shapley Flow extends Shapley-value-based explanation to directed acyclic graphs (DAGs) and assigns credit to edges rather than only to individual nodes, enabling the explanation of how importance flows through a structured system [7]. For chemical process data, however, a useful explanatory graph should also reflect temporal behavior. Dynamic process monitoring methods have long used time-lagged variables to capture process dynamics, as in dynamic principal component analysis [8]. These observations motivate the use of a process-guided and temporally extended DAG for explaining fault classification decisions.

Motivated by these limitations, this paper addresses the problem of explaining the fault in the TE process beyond conventional feature-level attribution. Instead of treating the classifier output as a flat function of input variables, we organize fault-relevant variables into a process-guided and temporally extended DAG and use Shapley Flow to attribute changes in fault across structured edges. The proposed framework combines fault-specific variable selection, process-flow-based DAG construction, first-order temporal extension, and residual-credit analysis. Through this design, the study aims to provide not only accurate fault classification, but also an interpretable description of how diagnostic evidence propagates through process structure and time, and where the current graph fails to fully explain the observed prediction change.

2. BACKGROUND

2.1 Feature Attribution for Fault Diagnosis

Data-driven process monitoring and fault diagnosis methods use multivariate process measurements to detect, identify, and diagnose abnormal operating conditions [1]. As machine learning models have been increasingly adopted for industrial fault diagnosis, explainability has become important because high predictive performance alone does not provide sufficient information for operators to understand why a fault decision was made [2]. Feature attribution methods are widely used for this purpose because they assign relevance scores to input variables for a given model prediction. In particular, SHAP provides a unified additive feature attribution framework and assigns each feature an importance value for an individual prediction [6]. In fault diagnosis, such attributions can indicate which process variables contribute to a fault probability. However, conventional feature-level explanations are typically flat and do not explicitly represent how diagnostic evidence propagates through process structure, such as from feed-related variables to reactor, separator, and quality-related variables. This limitation motivates a structured explanation approach that goes beyond independent feature scores.

2.2 Causal Graph and Shapley Flow

Graph-based explanation methods provide a way to include relationships among variables in model interpretation. In process systems, these relationships can be represented by a directed graph based on process flow, engineering knowledge, or causal assumptions. In this study, the graph is used as a process-guided explanatory DAG, rather than as a fully validated causal model. Shapley Flow extends Shapley-value-based attribution from node-level feature importance to edge-level credit assignment on a directed acyclic graph [7]. This allows the prediction difference to be interpreted in terms of pathways rather than isolated variables. Such a graph-based view is useful for fault diagnosis because an abnormal signal may not only be associated with one variable, but may also propagate through upstream and downstream process units. However, chemical process data are also dynamic, and static graphs alone may miss delayed effects. Dynamic principal component analysis has shown that incorporating time-lagged variables can improve disturbance detection and isolation in dynamic process systems [8]. Therefore, a lagged DAG structure is appropriate for explaining not only which variables matter, but also how previous states contribute to the current fault prediction.

2.3 Tennessee Eastman Fault Diagnosis

The Tennessee Eastman (TE) process is a widely used benchmark for process control, monitoring, and fault diagnosis. The original TE process was introduced as a plant-wide industrial process control problem involving reactor, separator, recycle, and product-quality related operations [3]. Because the process contains nonlinear dynamics, interacting variables, and multiple fault scenarios, it has been extensively used to compare statistical and data-driven monitoring methods. For example, basic process monitoring and fault diagnosis methods such as PCA, DPCA, PLS, FDA, ICA, and related approaches have been evaluated on the TE benchmark [9]. More recent work has also emphasized the need for standardized TE datasets to support fair comparison of fault detection and decision-support methods [4].

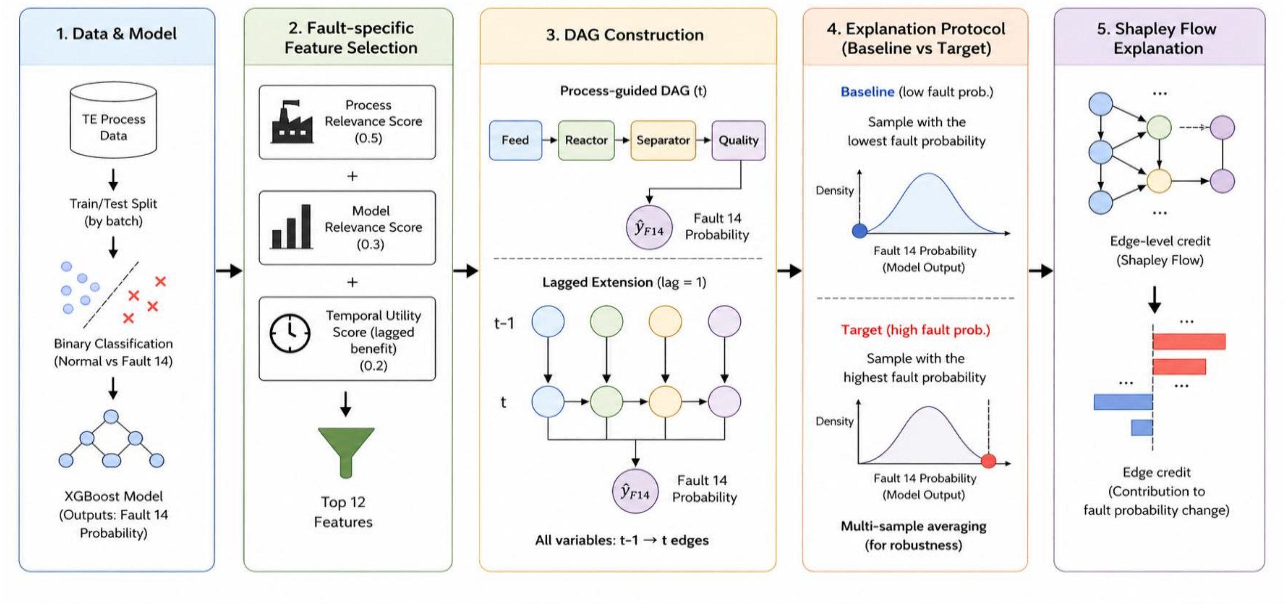

Figure 1. Overall framework of the proposed fault-specific lagged DAG explanation method.

3. METHOD

The overall workflow in shown in Figure 1.

3.1 Fault-Specific Feature Selection

We first construct a fault-specific core feature set that can be shared by both the static and temporal explanation models. Instead of using all measured variables, we restrict the explanation space to variables that are simultaneously meaningful from a process perspective and useful for prediction. To this end, we define a candidate set for each fault based on process knowledge and group the candidates into functional layers, such as upstream load variables, internal process-state variables, downstream response variables, and quality-related variables.

Each candidate variable is then scored using three criteria. First, process relevance reflects how directly the variable is related to the physical mechanism of the target fault. Variables near the source of the fault receive higher scores, while downstream symptom variables receive lower but non-zero scores. Second, model relevance measures how informative the variable is for fault discrimination in a current-time classifier. We estimate this score from feature importance obtained from an XGBoost model trained on the current-time candidate variables. Third, temporal utility quantifies whether explicitly modeling short-term history improves discrimination for that variable. For each candidate, we compare a current-time model using only the present value with a lagged model using values at multiple recent time steps, and compute the performance gain in terms of validation ROC-AUC and F1.

The final score is computed as a weighted sum of these three components,

$$s_i = \alpha s_i^{proc} + \beta s_i^{model} + \gamma s_i^{temp} \qquad (1)$$

where s_i^{proc}, s_i^{model}, s_i^{temp} denote the normalized process relevance, model relevance, and temporal utility scores, respectively. In our implementation, process knowledge is emphasized by assigning the largest weight to s_i^{proc}, while model relevance and temporal utility are used to refine the ranking. To prevent the selected set from collapsing into a single functional layer, we additionally impose a layer-wise minimum quota and then fill the remaining slots according to the global ranking. The resulting core feature set is used consistently in both the static DAG and the lagged temporal DAG.

3.2 Fault-Specific DAG Construction

Given the selected core feature set, we construct two graph variants: a static process-guided DAG and a lagged temporal DAG. Both graphs use the same base variables so that differences in explanation can be attributed to temporal modeling rather than to changes in the feature set.

In the static setting, each selected variable is assigned to a process layer according to its physical role. Directed edges are then added between layers following the process flow, for example from upstream operating conditions to internal state variables and from internal states to downstream response or quality variables. In addition, a target node representing the fault probability is connected to the subset of variables designated as its

Table 1. Selected feature set for Fault 14 obtained from the proposed three-stage scoring scheme. Each feature is scored by process relevance, current-time model relevance, and temporal utility, and the final 12-feature set is chosen under layer-wise quota constraints.

rank	feature	layer	description	s_i^{proc}	s_i^{model}	s_i^{temp}	final_score
1	xmv-25	feed	Component C in Reactor Feed Analysis	0.3667	0.4737	0.3396	0.3934
2	xmv-6	feed	Reactor Feed Rate	0.5000	0.2105	0.2246	0.3581
3	xmv-21	reactor	Reactor Cooling Water Outlet Temperature	1.0000	0.9474	1.0000	0.9842
4	xmv-9	reactor	Reactor Temperature	1.0000	1.0000	0.7352	0.9470
5	xmv-7	reactor	Reactor Pressure	0.8333	0.6842	0.5293	0.7278
6	xmv-18	separator	Stripper Temperature	0.6667	0.8947	0.1819	0.6381
7	xmv-10	separator	Purge Rate	0.6000	0.3684	0.1551	0.4415
8	xmv-13	separator	Product Separator Pressure	0.5333	0.4211	0.2259	0.4382
9	xmv-37	product	Component D in Product Analysis	0.3333	0.7895	0.2972	0.4630
10	xmv-41	product	Component H in Product Analysis	0.3333	0.8421	0.0969	0.4387
11	xmv-39	product	Component F in Product Analysis	0.3333	0.7368	0.1717	0.4221
12	xmv-40	product	Component G in Product Analysis	0.3333	0.6316	0.2498	0.4061

direct parents. These parent variables are the inputs to the trained fault classifier. This construction yields a compact graph that preserves causal ordering at the level of process stages while remaining tractable for Shapley Flow analysis.

To capture short-horizon temporal propagation, we extend the same base variables into a lagged representation with nodes at $t-1$ and t.

The lagged graph contains two types of edges. First, temporal self-links connect each variable across adjacent time steps, e.g., $x_i^{t-1} \rightarrow x_i^t$. Second, the current-time variables x_i^t are linked to the fault-probability node using the same direct-parent logic as in the static graph. This design allows the lagged model to represent both the instantaneous contribution of current process variables and the propagation of influence through short-term temporal history.

The static and lagged graphs therefore share the same physical interpretation but differ in representational granularity. The former emphasizes process-stage structure, whereas the latter additionally models local temporal evolution.

3.3 Shapley Flow Explanation

For a given trained classifier and graph structure, we explain the change in predicted fault probability between a baseline normal sample and a target fault sample using Shapley Flow. The baseline samples are selected from low-probability normal instances, and the target samples are selected from high-probability fault instances. To reduce dependence on any single pair, we allow multiple baseline and target samples and aggregate the resulting edge credits over all baseline-target pairs.

A key issue is that many internal graph nodes are observed variables rather than latent quantities generated exactly by the fitted parent functions. To ensure that the graph reproduces the actual observed values for both the baseline and the target instance, we augment every non-source observed node with an explicit residual source node. Concretely, for each observed intermediate variable x_i, we write

$$x_i = \hat{f}_i(\mathrm{pa}_i) + r_i \qquad (2)$$

Where $\hat{f}_i(\mathrm{pa}_i)$ is the learned structural function from its parent nodes and r_i is a residual term. The residual is instantiated separately for the baseline and target samples so that the graph-level forward pass matches the observed values exactly. This residual augmentation is important because it avoids forcing all observed deviations to be explained only through imperfect learned parent models.

We then run Shapley Flow on the residual-augmented graph and compute edge-level contribution scores. From these scores, we derive three complementary summaries. First, we analyze target-edge credits, i.e., edges that directly enter the fault-probability node, to identify the variables most responsible for increasing or decreasing the predicted fault probability. Second, we compute graph-wide summary edge credits by averaging edge attributions over multiple baseline-target pairs. Third, for the lagged graph, we aggregate credits by time step to quantify the relative contributions of t and $t-1$. In addition, we report the fraction of absolute credit carried by residual-related edges to assess the extent to which the explanation is dominated by unexplained observed variation rather than by the modeled process pathways.

4. EXPERIMENTAL SETUP

4.1 Dataset and Graph Construction

We evaluate the proposed framework on the Tennessee Eastman Process (TEP) benchmark under a binary fault-diagnosis setting, where the goal is to distinguish a target fault from normal operation. In this study, we focus on Fault 14, which is associated with the reactor cooling water valve, and perform binary classification between Fault 14 samples and normal-operation samples. Normal samples are taken from the standard normal-operation dataset, and fault samples are collected from multiple batches corresponding to Fault 14. To reduce leakage across repeated temporal patterns, training and test data are separated by batch. In our implementation, several Fault 14 batches are used for training and validation, while disjoint batches are reserved for testing.

For the target fault, we first construct a fault-specific candidate variable pool and then select a compact core feature set using the procedure described in Section 3.1. The same selected base feature set is used in both graph variants. In the static setting, the features are organized into process-guided layers and connected according to process flow. In the temporal setting, the same variables are expanded into lagged nodes over $t-1$ and t yielding a lagged DAG that preserves comparability with the static graph while adding short-term temporal structure.

4.2 Classifier and Explanation Configuration

We use XGBoost as the fault classifier for both the static and lagged settings. In the static DAG, the classifier is trained on the current-time direct parent variables of the target node. In the lagged DAG, the classifier is trained on the current-time nodes of the selected base variables, while the historical nodes are used to model temporal propagation in the graph. A validation split is created from the training pool for model selection and threshold determination.

Shapley Flow is then applied to the residual-augmented graph described in Section 3.3. For explanation, baseline instances are selected from low-probability normal samples and target instances from high-probability fault samples. We consider both single-pair explanations and multi-sample explanations obtained by averaging over multiple baseline-target pairs. In the robustness analysis, we vary the decision threshold, the numbers of baseline and target samples, and the random seed while keeping the lag horizon fixed.

5. RESULT

5.1 Classification and Explanation Overview

Table 1 summarizes the selected core feature set for the target fault. The final set contains 12 variables spanning four functional layers: feed and load conditions, reactor thermal state, separator/stripper response, and product quality. This layer-balanced selection is important because it prevents the explanation model from collapsing into only the most predictive local variables while still preserving process context. Among the selected variables, the reactor-related measurements receive the highest overall scores, particularly xmv-21 (reactor cooling water outlet temperature) and xmv-9 (reactor temperature), indicating that they are both physically relevant to the fault mechanism and highly informative for classification. Additional variables such as xmv-7, xmv-18, xmv-10, and xmv-13 were retained to represent downstream process response, while feed and product-quality variables were also included to preserve upstream and downstream context in the graph.

Table 2. Test-set F1 scores of the static and lagged DAG-based classifiers for Fault 14. Results are reported for a fixed threshold of 0.5 and, for the lagged model, an additional validation-optimized threshold.

Model	Threshold	Test F1
Static DAG	0.5	0.8871
Lagged DAG	0.5	0.8871
Lagged DAG	val-optimal (0.2350)	0.8732

Using this selected feature set, we trained both a static DAG-based classifier and a lagged DAG-based classifier for Fault 14. Table 2 reports the test-set F1 scores. At a fixed threshold of 0.5, the two models show nearly identical performance: the static DAG achieves an F1 score of 0.8872, while the lagged DAG achieves 0.8871. When the lagged model uses the validation-optimized threshold, the test F1 decreases slightly to 0.8732. These results indicate that the lagged formulation does not substantially improve classification accuracy under the current setting, but it preserves essentially the same predictive performance as the static model.

This observation is important for interpreting the later explanation results. Because the static and lagged models operate on the same selected base feature set and exhibit comparable classification performance, differences in their Shapley Flow attributions can be interpreted primarily as differences in explanatory structure rather than as artifacts of unequal predictive quality. In other words, the lagged DAG is introduced not to maximize classification performance, but to expose whether short-term temporal dependencies provide additional explanatory insight beyond the process-guided static graph.

5.2 **Process and Temporal Credit Attribution**

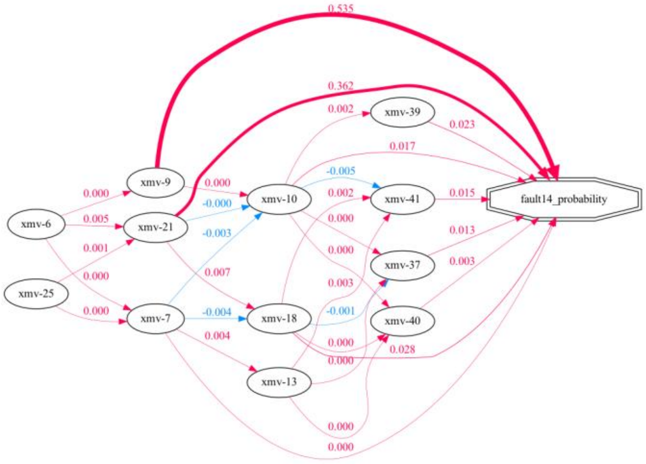

Figure 2. Summary Shapley Flow edge-credit graph for the static process-guided DAG in Fault 14. Edge color indicates the sign of the contribution and edge thickness reflects the magnitude of the credit.

Figures 2 and 3 show the Shapley Flow explanation results obtained from the static process-guided DAG and the lagged temporal DAG, respectively. In both graphs, the dominant contributors to the predicted Fault 14 probability are the reactor-related variables, especially reactor temperature (xmv-9) and reactor cooling water outlet temperature (xmv-21). In the static DAG, the direct credits of these two variables are 0.5353 and 0.3624, respectively, accounting for about 90% of the total probability increase. Smaller positive contributions are assigned to stripper temperature (xmv-18, 0.0279), component F in product analysis (xmv-39, 0.0234), purge rate (xmv-10, 0.0165), and component H in product analysis (xmv-41, 0.0152). This ranking is physically consistent with the fault scenario, since a reactor cooling-water-related fault is expected to be reflected most strongly in the reactor thermal state and only secondarily in downstream separation and product-quality variables.

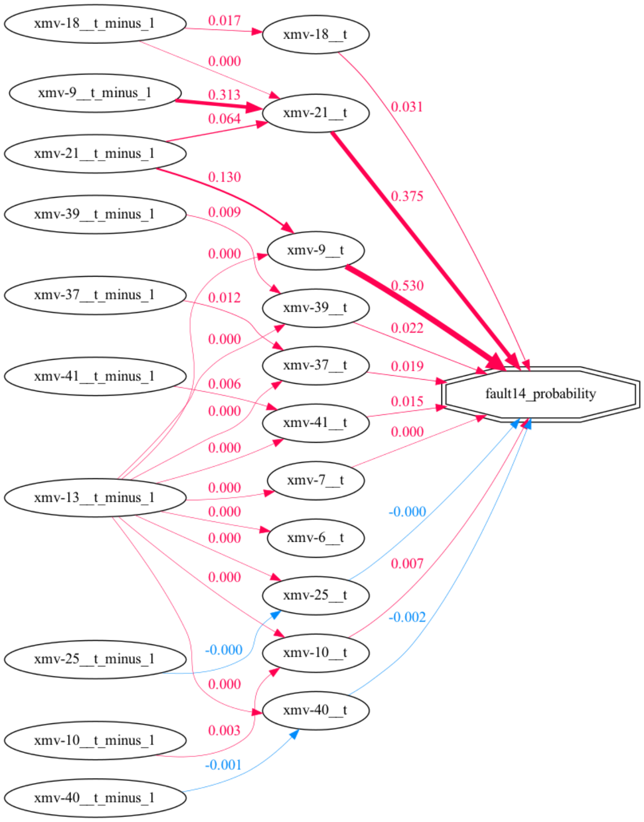

Figure 3. Summary Shapley Flow edge-credit graph for the lagged temporal DAG in Fault 14. The graph preserves the dominant current-time contributors while additionally revealing short-term temporal propagation across adjacent time steps.

The lagged DAG preserves this same high-level explanation pattern at the current time. The two dominant direct target-edge credits are again assigned to xmv-9__t and xmv-21__t, with contributions of 0.5303 and 0.3746, respectively, indicating that the final fault decision is still governed primarily by the present reactor thermal state. At the same time, the lagged graph reveals how this current-time evidence is supported by short-term temporal propagation. In the graph-wide aggregation, edges from $t-1$ to t contribute a total absolute credit of 0.5543, showing that a substantial portion of the explanation is carried through one-step temporal transitions before reaching the current-time nodes. Among these temporal links, the flow from xmv-9__t_minus_1 to xmv-21__t is qualitatively consistent with the process interpretation that reactor thermal changes can be reflected in the subsequent cooling-water-related response. Thus, while the classification decision itself is made at time t, the lagged DAG provides additional interpretability by exposing how recent temporal evolution helps shape the present-time fault signature.

At the same time, the lagged explanation is not fully captured by modeled temporal propagation alone. Residual-related edges contribute 0.4510 in total absolute credit, indicating that a non-negligible portion of the explanation is still carried by observed variation not completely reconstructed by the learned parent functions. In this sense, the lagged DAG succeeds in recovering the dominant thermal pathway associated with the fault, but it does not eliminate the need for residual terms. This result is still meaningful: it suggests that the graph captures the main process-consistent propagation pattern, while the remaining residual contribution reflects either modeling error or fault-related variation that is not explicitly represented in the current graph structure.

6. CONCLUSION

This study presented a fault-specific Shapley Flow framework for explaining fault diagnosis in the Tennessee Eastman Process. A compact fault-specific feature set was first selected using process relevance, model relevance, and temporal utility, and both a process-guided static DAG and a lagged temporal DAG were constructed on the same base variables. This design enabled a consistent comparison between static and temporal explanations.

In the Fault 14 case, both graph variants identified reactor temperature and reactor cooling water outlet temperature as the dominant contributors to the predicted fault probability, which is physically consistent with the fault mechanism. While the lagged DAG did not substantially improve classification performance over the static DAG, it provided additional interpretability by revealing short-term temporal propagation before the final present-time decision.

A remaining limitation is that part of the explanation is still carried by residual-related edges, indicating that not all observed variation is fully reconstructed by the modeled graph structure. This suggests that the proposed approach captures the dominant process-consistent fault signature, but does not yet fully recover the underlying causal mechanism. Overall, the results show that combining fault-specific graph construction with Shapley Flow can provide more process-aware explanations than a purely static attribution view. Future work can extend this framework by incorporating richer actuator-level variables and broader evaluations across additional fault types.

ACKNOWLEDGEMENTS

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P-100

SESSION

P2 · July 7 (Tue) 13:30~14:30

PRESENTER

Sangdeok Kim

Effects of Photoacid Generator Composition on Proton Transport, Deprotection Kinetics, and Line Edge Roughness in Chemically Amplified Resists: A Reactive Molecular Dynamics Study

Sangdeok Kim, Jaehyun Ryu, Seungtae Kim, Sangwoo Kwon, Claire S. Adjiman, and Won Bo Lee*

Seoul National University (Korea) & Imperial College London (UK)

The full paper follows on the next page.

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Effects of Photoacid Generator Composition on Proton Transport, Deprotection Kinetics, and Line Edge Roughness in Chemically Amplified Resists: A Reactive Molecular Dynamics Study

Sangdeok Kim[a], Jaehyun Ryu[a], Seungtae Kim[a], Sangwoo Kwon[a], Claire S. Adjiman[b], and Won Bo Lee[a]*

[a] School of Chemical and Biological Engineering, Seoul National University, Seoul 08826, Republic of Korea
[b] Department of Chemical Engineering, Imperial College London, South Kensington Campus, London SW7 2AZ, United Kingdom
* Corresponding Author: wblee@snu.ac.kr.

ABSTRACT

Line edge roughness (LER) is a primary limitation of extreme ultraviolet (EUV) lithography for sub-7 nm patterning. It depends on how the photoacid produced by the photoacid generator (PAG) diffuses through the resist during post-exposure bake (PEB). Classical molecular dynamics (MD) cannot represent the proton directly, so we substitute Li^+ as a proxy, following Bottoms et al. [19,20] who validated an inert ionic surrogate for acid diffusion. We compare three PAG combinations: triphenylsulfonium triflate (TPS–TFO), diphenyliodonium triflate (DPI–TFO), and triphenylsulfonium perfluorobutanesulfonate (TPS–PFBS). Reactive MD with a 0.5-nm Li^+–carbonyl distance criterion is used to model deprotection. For TPS–TFO, three activation levels (50%, 75%, 100%) are simulated in both homogeneous (bulk) and heterogeneous (bilayer) configurations. In the bulk, Li^+ diffusivity is similar across PAGs, but TPS–PFBS yields a notably larger simulation box at all conversions because PFBS interacts more strongly with the polymer. The expanded matrix lowers the effective acid concentration and slows the reaction. In the bilayer, LER decreases monotonically with deprotection. DPI–TFO gives the lowest LER (about 5 nm at 65% deprotection), TPS–TFO is intermediate, and TPS–PFBS is highest. Higher PAG activation in TPS–TFO also lowers LER at fixed deprotection. The molecular factor that distinguishes the three systems is the ion–polymer interaction, which controls matrix volume and reaction rate. Smaller PAG ions, particularly smaller cations, favor lower LER.

Keywords: extreme ultraviolet lithography, chemically amplified resist, photoacid generator, reactive molecular dynamics, line edge roughness, ion transport

1. Introduction

Extreme ultraviolet (EUV) lithography at 13.5 nm is the leading technology for sub-7 nm semiconductor patterning [1]. The high photon energy of EUV (≈92 eV) means fewer photons are delivered per unit dose than at conventional UV wavelengths, which raises photon shot noise and contributes to line edge roughness (LER) [2,3]. Reducing LER without sacrificing sensitivity is a central concern in modern photoresist design.

Chemically amplified resists (CARs) dominate EUV photoresist platforms [4,5]. The PAG decomposes during exposure and releases an acid–anion catalyst pair [6,7]. The acid then diffuses through the polymer matrix during post-exposure bake (PEB) and cleaves acid-labile protecting groups [8,9]. The spatial distribution of this reaction sets the resolution and LER of the developed pattern [4,10], so understanding acid transport at the molecular level is essential.

Atomistic modeling of acid transport in CARs has been hampered by a basic constraint: classical MD cannot represent a proton within standard force fields, since its small mass and quantum behavior fall outside the model. Reaction–diffusion approaches have therefore been calibrated against indirect measurements [10–18]. Bottoms et al. recently showed that an inert ion pair (Na^+TFL^-) reproduces H^+TFL^- diffusion in a model CAR terpolymer to within experimental uncertainty as measured by TOF-SIMS [19]. A follow-up study used a geometric reaction criterion in reactive MD to capture the catalyst diffusion accelerated by reaction-induced free volume [20]. We adopt the same approach but use Li^+ rather than Na^+, since Li^+ is the smallest classical cation and provides the closest proxy to a proton-bearing acid species without resorting to quantum methods.

A typical PAG consists of an onium cation (TPS, DPI) and a weakly coordinating anion (TFO, PFBS). The acid is liberated from the cation during exposure, but the anion remains in the matrix and accompanies the acid throughout PEB. Both ions interact with the polymer, and these ion–polymer interactions affect proton transport and the resulting LER. On the experimental side, Higgins et al. [31] have shown that iodonium PAGs outperform sulfonium PAGs in EUV resolution-LER-sensitivity (RLS) at matched anion, attributing the advantage to a higher EUV absorption cross-section of the iodonium cation. Sub-10 nm CAR patterning has also been studied with atomistic simulation [21–23], but the contributions of the anion and the cation to deprotection kinetics during PEB itself have not been systematically separated.

We address this gap by comparing three PAG combinations (TPS–TFO, DPI–TFO, TPS–PFBS) using reactive MD in two complementary setups. Homogeneous simulations characterize bulk dynamics under uniform exposure. Heterogeneous bilayer simulations model the EUV exposure pattern and yield LER directly as a function of deprotection level and PEB time. Together, the two setups link PAG identity, ion–polymer interactions, deprotection kinetics, and macroscopic LER.

2. Simulation Methodology

2.1 Polymer and PAG models

The polymer is modeled as a fully protected pentamer (1528 g/mol per chain) with tert-butyl ester protecting groups. After acid-catalyzed cleavage, the pentamer becomes the fully deprotected form (1047 g/mol per chain). Each system contains 400 polymer chains and 370 PAG molecules, giving a PAG loading of about 15 wt%. The polymer matrix and Li^+ are described by OPLS-AA [24]. The PAG ions (TFO, PFBS, TPS, DPI) use GAFF [25] with RESP-fitted partial charges [26].

2.2 Reactive Deprotection Criterion

We use the geometric reaction criterion of Bottoms et al. [20]. When Li^+ is within 0.5 nm of a carbonyl oxygen on a protected unit, that protecting group is irreversibly removed and the unit is converted to its deprotected form. Reaction checks are performed periodically, and reaction byproducts are removed instantaneously, in line with the rapid escape of volatile fragments observed experimentally.

2.3 Two Simulation Setups

Two complementary simulation setups are used to disentangle bulk dynamics from spatial pattern formation:

(i) Homogeneous simulations apply uniform exposure throughout the box. For TPS–TFO, three activation levels (50%, 75%, 100%) are simulated at six conversion levels (0, 20, 40, 60, 80, 100%) in the NPT ensemble. For the PAG comparison (TPS–TFO, DPI–TFO, TPS–PFBS), activation is fixed at 50%.

(ii) Heterogeneous simulations expose only the central region of the box. For TPS–TFO, three activation levels (50%, 75%, 100%) are studied. For the PAG comparison, activation is fixed at 50%. After PEB, the high-deprotection region is removed to mimic development.

2.4 Simulation Parameters and LER Measurement

All simulations use GROMACS 2021.6 [27] in the NPT ensemble at 550 K (above the polymer Tg) and 1 bar. Initial polymer melts are obtained by annealing from 1000 K to 550 K. The integration time step is 0.2 fs in the early reactive period and 0.5 fs afterward. Thermostat and barostat coupling times are set to $1000\times\Delta t$ and $10000\times\Delta t$. We compute the radial distribution function (RDF), coordination number (CN), and diffusivity from MSD slopes, and we track box volume.

After development in the heterogeneous setup, two rough polymer surfaces remain, one above and one below the developed (washed-away) region. For each surface, the local interface height $z(x, y)$ is sampled on a 2D grid across the lateral plane of the simulation box. The mean position $\langle z\rangle$ is subtracted, and LER is taken as the root-mean-square deviation about this mean: LER = $[\langle(z-\langle z\rangle)^2\rangle]^{1/2}$. The reported value for each system is the average of the standard deviations at the upper and lower interfaces, which typically agree to within a few percent. Self-diffusion coefficients are obtained from the long-time slope of the mean square displacement using the Einstein relation, and coordination numbers are obtained by integrating the corresponding radial distribution functions up to the first minimum. Atomistic snapshots used for visualization are rendered with OVITO [28] at t = 150 ns post-exposure.

3. Results and Discussion

3.1 Bulk System: Box Volume and Conversion

The box volume in TPS–TFO decreases as PAG activation increases (Figure 1a), with the strongest effect at high conversion: 192 nm^3 at 50% activation drops to 171 nm^3 at 100% activation when fully converted. Two factors contribute. Li$^+$ has a smaller volume than the displaced TPS cation, and the matrix becomes more polar as conversion proceeds, which strengthens the electrostatic interaction between each Li$^+$ and its surroundings.

Comparing the three PAGs at 50% activation (Figure 1b), the cation has little effect on box volume, in line with the small TPS–DPI size difference. Replacing TFO with PFBS, on the other hand, swells the matrix substantially: 305 vs 287 nm^3 at 0% conversion, and 206 vs 191 nm^3 at full conversion. The expansion reflects stronger PFBS–polymer interaction; the larger and more hydrophobic anion drives more volume into the matrix. The result is a lower effective acid concentration, which we revisit in Section 3.4.

The two trends in Figure 1 (activation dependence and PAG dependence) compound multiplicatively when both are varied at once. The relative volume change with conversion is roughly 30–40% across all systems, while the inter-PAG difference at any fixed conversion is 7–8%. Box volume therefore provides a sensitive readout of how the chosen ion pair perturbs the polymer matrix density, and we use it as a thermodynamic baseline against which the dynamic and structural results of Sections 3.2–3.3 should be interpreted. The magnitude of the activation effect (about 10% volume reduction at 100% conversion) is comparable to the size difference between Li$^+$ and the displaced TPS cation, supporting a simple substitution picture in which the volume change tracks ion-size at low conversion and gains an additional polarity-driven contribution at high conversion.

It is also useful to compare the order of magnitude of these volume changes against the size of the ions involved. The molar volume of TPS$^+$ is roughly 230 cm^3/mol, that of DPI$^+$ roughly 200 cm^3/mol, and the bare ionic volume of Li$^+$ is below 5 cm^3/mol; the difference between the displaced cation and the inserted Li$^+$ is therefore similar to the molar volume of a small organic fragment. With 370 PAG molecules per simulation cell, full activation removes ≈85 nm^3 of cation volume, in good agreement with the ≈20 nm^3 reduction observed at full conversion (50% to 100% activation), once one accounts for the simultaneous shrinkage of pendant groups during deprotection. This consistency indicates that no large-scale matrix reorganization, such as a glass transition or phase change, is needed to explain the box-volume trends; ordinary cation–replacement and pendant-group cleavage are sufficient.

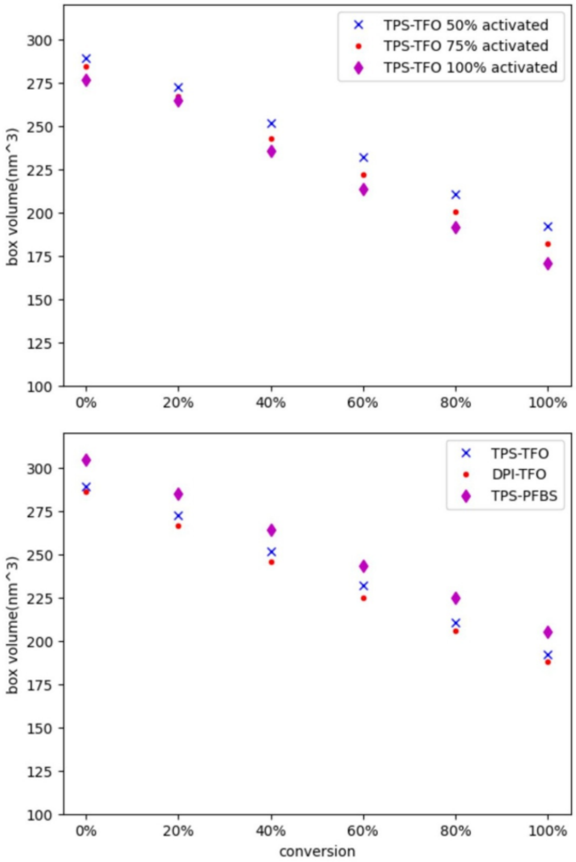

Figure 1. Simulation box volume vs. conversion. (a) TPS–TFO at three PAG activation levels. (b) Three PAG systems at 50% activation. PFBS exhibits consistently larger volumes due to stronger PFBS–polymer interactions.

3.2 Bulk System: Li$^+$–Anion Structure and Coordination

The first peak in the Li$^+$–anion RDF appears at $r/\sigma \approx$ 0.30–0.35 in all three systems at both 0% and 60% conversion (Figure 2). This sharp contact-pair peak indicates a tightly bound configuration in every case. The RDFs for TPS–TFO and DPI–TFO overlap almost exactly, so cation identity barely affects the local Li$^+$–anion structure. Switching from TFO to PFBS shifts the peak slightly outward and changes its height, which we attribute to the larger spatial footprint of PFBS. Quantitatively, the first peak height at 0% conversion is about 53 for TPS–TFO and 52 for DPI–TFO, but rises to 76 for TPS–PFBS, indicating a more rigid local arrangement of Li$^+$ around the larger anion in the unreacted matrix. By 60% conversion the corresponding values fall to 36, 35, and 45, reflecting weaker ion-pair correlation as the matrix becomes more polar and competes with the anion for Li$^+$ coordination.

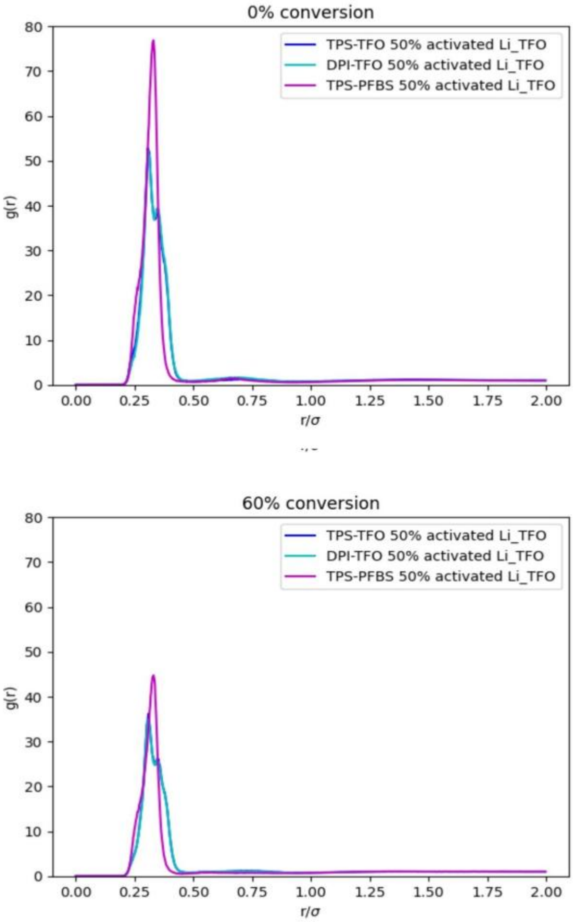

Figure 2. Li$^+$–anion RDF for the three PAG systems at 50% activation. (a) 0% conversion. (b) 60% conversion.

The Li$^+$–anion coordination number (CN) at 100% conversion (Figure 3) is similar between the TPS-based systems but lower for TPS–PFBS, again reflecting dilution by the swollen matrix. Note an apparent tension: the RDF peak height drops by about 80% from 0% to 100% conversion in TPS–TFO, while the corresponding CN change is only about 20%. The reason is that bulk density rises by about 33% as conversion proceeds, which partially compensates the lower g(r). The integrated CN reaches a first plateau at roughly 2 anions per Li$^+$ in all three systems, consistent with a tight contact-ion arrangement. The absolute difference between TPS–PFBS and the other two systems (about 0.2 ions) is small compared with the box-volume difference, so volume effects dominate the kinetic behavior examined next. The first-shell CN value of about 2 places each Li$^+$ in a tight cage formed by one or two oxygen-bearing groups. The narrowness of the first peak in g(r) (Figure 2) further indicates that this contact arrangement persists on simulation timescales, with the cation rarely visiting more dilute coordination shells. This rigid first-shell environment matters for the deprotection reaction: a Li$^+$ coordinated by two anions has only a small angular window in which a polymer carbonyl oxygen can approach within the reactive distance of 0.5 nm, which sets a baseline kinetic barrier independent of bulk diffusion.

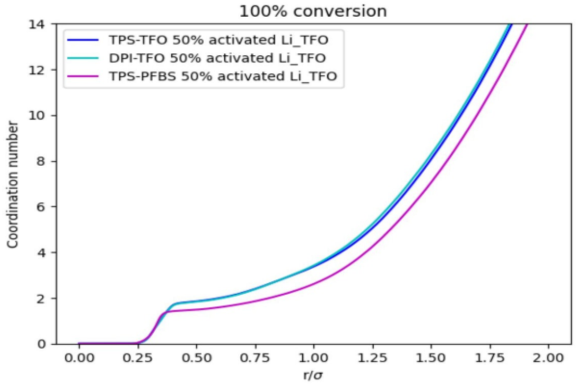

Figure 3. Li$^+$–anion coordination number at 100% conversion (50% activation) for the three PAG systems.

3.3 Bulk System: Li$^+$ Diffusivity

Li$^+$ diffusivity in TPS–TFO rises monotonically with conversion as the bulky tert-butyl groups are removed and free volume opens up [20] (Figure 4a). It also decreases with PAG activation: at 100% conversion, D_Li goes from about 6.7×10^{-12} nm^2/s at 50% activation down to 2.2×10^{-12} nm^2/s at 100%. Higher activation produces more Li$^+$ and more freed TFO, and the resulting Li$^+$–anion correlation slows transport.

The PAG comparison at 50% activation (Figure 4b) is more subtle. Apart from DPI–TFO at 100% conversion, where the small DPI cation enables faster matrix relaxation, the three systems give very similar Li$^+$ diffusivities across the conversion range. This is an important null result: bulk Li$^+$ transport is largely insensitive to PAG choice. The macroscopic differences (conversion rate, LER) must therefore come from elsewhere, namely the matrix volume effect identified in Section 3.1. The fact that bulk Li$^+$ diffusivity is roughly conserved across PAGs is consistent with preferential ion–polymer coordination: regardless of which anion is present, Li$^+$ spends most of its time interacting with the polar groups in the polymer matrix rather than with the anion itself, so its short-range mobility is set primarily by polymer dynamics. The anion identity instead modulates the global density and free volume distribution, which determines how often Li$^+$ encounters a reactive carbonyl over long times.

A useful way to read Figures 4a and 4b together is to think of them as decoupling two distinct contributions to Li$^+$ transport. Figure 4a isolates the effect of the local ion environment around each Li$^+$: more activated PAG means more Li$^+$–anion partners and more electrostatic friction along the diffusion path, hence the observed reduction in diffusivity with activation. Figure 4b isolates the effect of the surrounding polymer matrix: the bulk diffusivity becomes a property of the polymer environment, which is largely insensitive to PAG identity. Taken together, these two figures support the picture developed in Section 3.5: the macroscopic LER differences between PAG systems are not caused by intrinsic differences in Li⁺ mobility, but by the matrix-volume effect that determines how often a given Li⁺ meets a protected carbonyl.

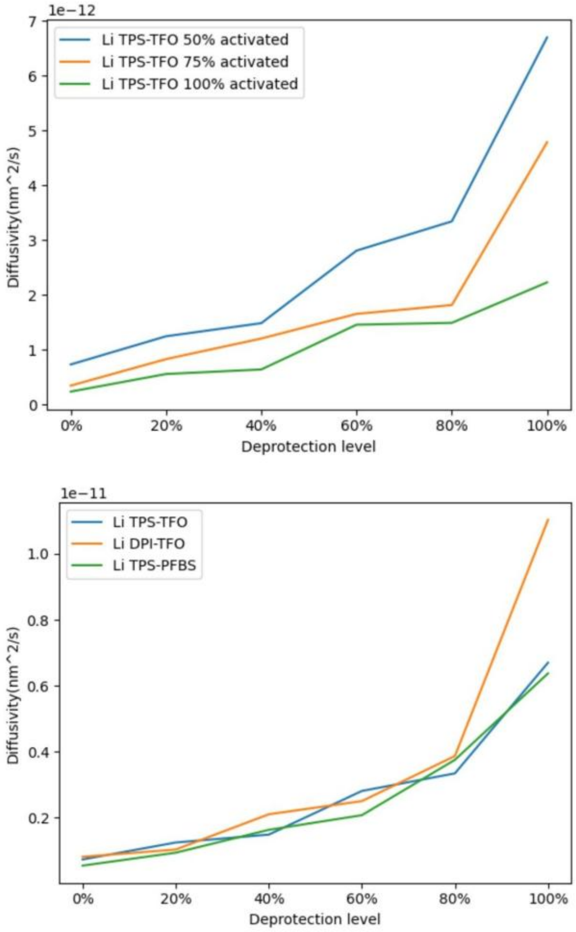

Figure 4. Li⁺ diffusivity vs. conversion. (a) Three PAG activation levels in TPS–TFO. (b) Comparison across PAG systems at 50% activation.

3.4 Heterogeneous System: Deprotection Kinetics

In the heterogeneous bilayer simulations (Figure 5), TPS–TFO at higher activation deprotects faster early on, with the curves converging at long times as the reaction nears completion (Figure 5a). At 50% activation, TPS–TFO reaches about 60% deprotection slightly ahead of DPI–TFO and TPS–PFBS (Figure 5b). TPS–PFBS is the slowest, particularly in the early stage, in line with its larger box volume reducing the local probability of a Li⁺–carbonyl encounter. Quantitatively, all three systems approach a final deprotection level of 0.85–0.95 within 600 ns of PEB, but the time required to reach 60% deprotection differs by roughly 25% between the fastest system (TPS–TFO) and the slowest (TPS–PFBS) at 50% activation. The relative kinetics in the heterogeneous setup mirror the ordering of the homogeneous conversion profiles, confirming that the matrix-volume effect identified in Section 3.1 propagates from the local diffusion environment to the global reaction rate.

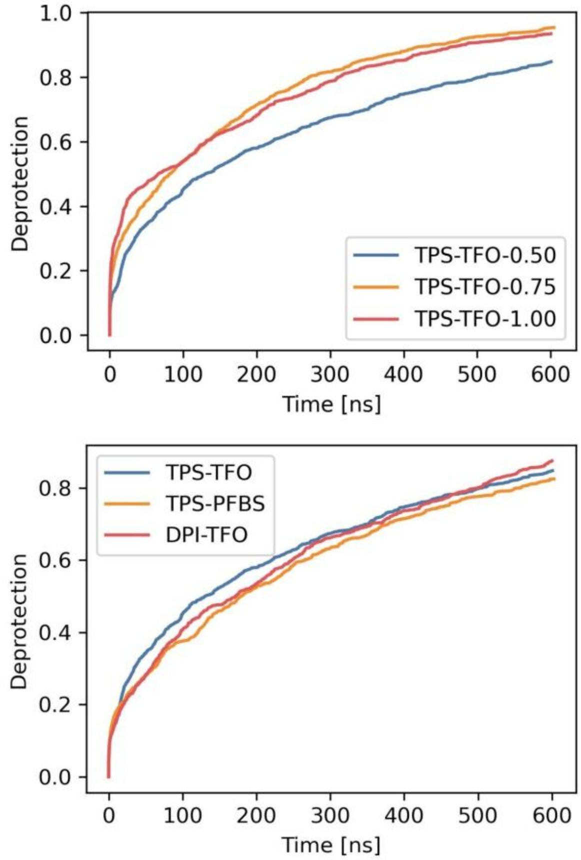

Figure 5. Deprotection level vs. time in heterogeneous simulations. (a) Three PAG activation levels for TPS–TFO. (b) PAG comparison at 50% activation.

3.5 Heterogeneous System: Line Edge Roughness

LER decreases sharply with deprotection level in every system (Figure 6). At 50% deprotection the boundary is diffuse (LER about 9–10 nm), but by 65–70% deprotection a well-defined boundary emerges (LER about 5–7 nm). The interpretation is straightforward: cluster separation between the unexposed polymer and the developed region emerges only once enough of the exposed polymer is converted to the hydrophilic, washable state.

For TPS–TFO (Figure 6a), higher PAG activation gives lower LER at every deprotection level, since a higher catalyst density yields a more uniform deprotection front. The PAG comparison at 50% activation (Figure

6b) gives the central practical result: across all deprotection levels, DPI–TFO has the lowest LER, then TPS–TFO, then TPS–PFBS. At 65% deprotection DPI–TFO is at LER ≈ 5 nm, while TPS–PFBS is still at ≈ 8 nm at 60% deprotection, a 60% increase.

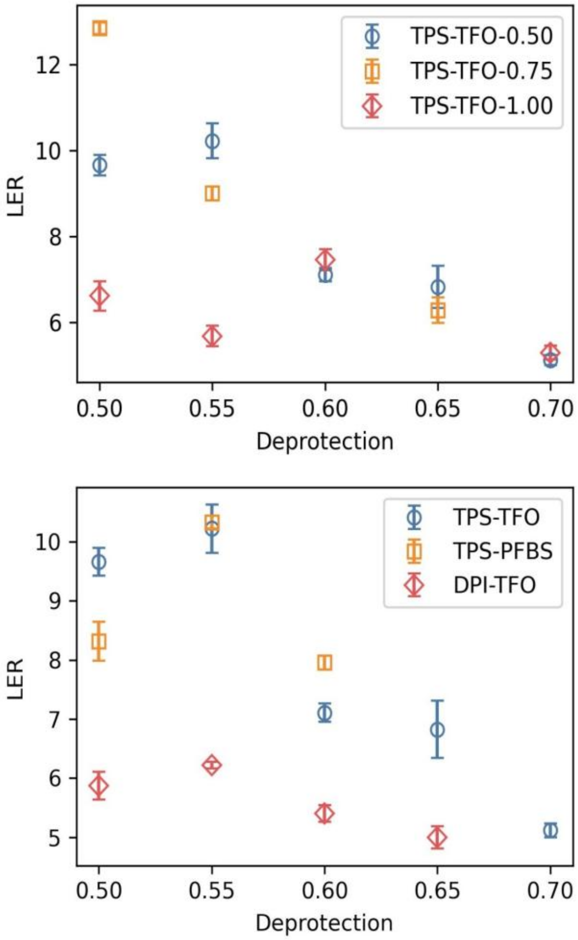

Figure 6. LER vs. deprotection level. (a) Three PAG activation levels for TPS–TFO. (b) PAG comparison at 50% activation. DPI–TFO consistently produces the lowest LER.

The relative ranking of the three PAG systems is preserved across the entire deprotection range we examined, which suggests that the underlying mechanism is robust rather than the result of an artifact at any particular deprotection level. Two further points are worth noting. First, in real EUV CARs, the developer dissolves polymer above a threshold deprotection level, and the LER reported in lithographic experiments is measured after development. Our LER values at 65–70% deprotection therefore correspond approximately to the regime probed by experimental LER measurements, and the magnitudes we obtain (5–7 nm) are within the range typically reported for thin-film CAR systems at sub-50 nm half-pitch. Second, the LER values shown here include only the contribution from the post-exposure-bake reaction–diffusion process, and ignore upstream contributions from photon shot noise, mask edge roughness, and aerial-image contrast. The differences between PAG systems that we report here can therefore be regarded as a lower bound on the LER differences that would appear in a full lithographic process. In particular, since the shot-noise and reaction-diffusion contributions arise from largely independent processes, they combine in quadrature rather than in simple addition, so the relative PAG ordering should be preserved once shot noise is included. Iodonium PAGs additionally have a higher EUV absorption cross-section than sulfonium PAGs [31], which reduces their shot-noise contribution and reinforces the DPI–TFO advantage observed here.

LER vs PEB time (Figure 7) tells the same story. TPS–TFO at 100% activation reaches LER ≈ 5 nm in about 200 ns, while at 50% activation roughly 350 ns is needed to reach LER < 6 nm. DPI–TFO again converges fastest, followed by TPS–TFO, then TPS–PFBS, in line with the deprotection kinetics of Figure 5. Two distinct mechanisms appear to reduce LER. The activation effect (Figures 6a and 7a) reflects a higher catalyst density producing a more uniform reaction probability across the exposed region. The cation-size effect (Figures 6b and 7b, DPI vs TPS) reflects faster local matrix relaxation around each acid site. Both push the deprotection boundary toward sharper definition, and they act largely independently of one another, so PAG redesign and increased catalyst density can both contribute to LER reduction with combined gains exceeding either alone. Quantitatively, raising activation from 50% to 100% in TPS–TFO reduces LER by roughly 30% at 65% deprotection, and switching the cation from TPS to DPI at the same activation reduces it by a comparable amount, so the activation effect and the cation-size effect are of comparable magnitude. The time-domain picture also makes clear that the cation-size advantage persists across the full bake window we examined: additional PEB does not close the gap between DPI–TFO and TPS–PFBS, indicating that the matrix-relaxation timescale that distinguishes them is not a transient feature of the early reaction.

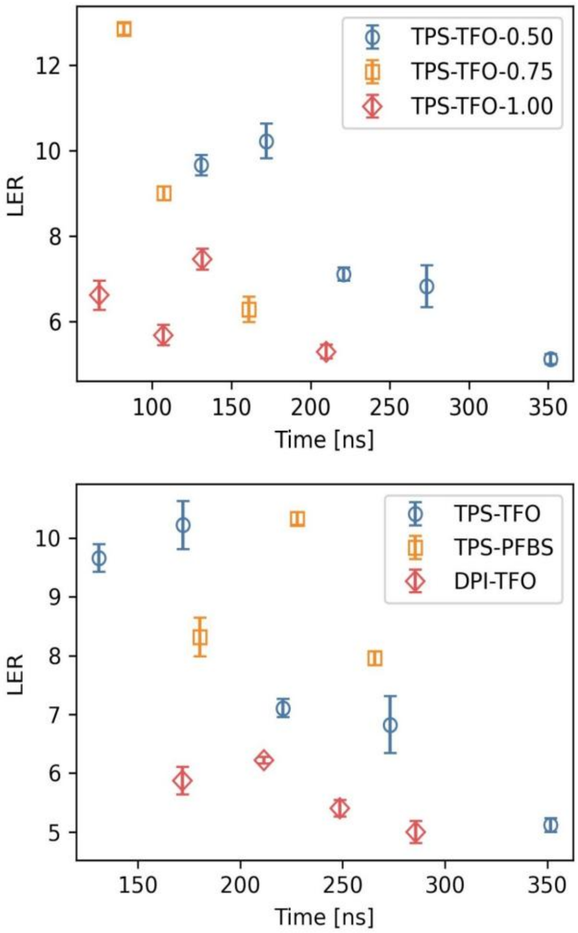

Figure 7. LER vs. PEB time. (a) Three PAG activation levels for TPS–TFO. (b) PAG comparison at 50% activation.

Atomistic snapshots after 150 ns of PEB (rendered with OVITO [28]) are shown in Figure 8 for TPS–TFO and DPI–TFO. Both show clear top/bottom polymer cluster separation, with the rough z-interfaces making the LER metric of Section 2.4 directly visible. The DPI–TFO interface (b) is visibly smoother than the TPS–TFO interface (a), in line with the measured LER values of 5.0 and 6.25 nm at 65% deprotection. The visual contrast between the two panels makes the central practical conclusion of this work directly accessible: at fixed deprotection level and fixed activation, the smaller cation produces a markedly sharper boundary, and this difference is achieved without changing PAG concentration or PEB time. The same comparison also illustrates how the LER metric defined in Section 2.4 maps onto the visible roughness of the polymer–air interface in the simulation: the standard deviation of the local interface position z(x, y) translates directly into the height variations seen in the snapshot, and the smoother top/bottom boundaries of DPI–TFO are visually consistent with its smaller numerical LER.

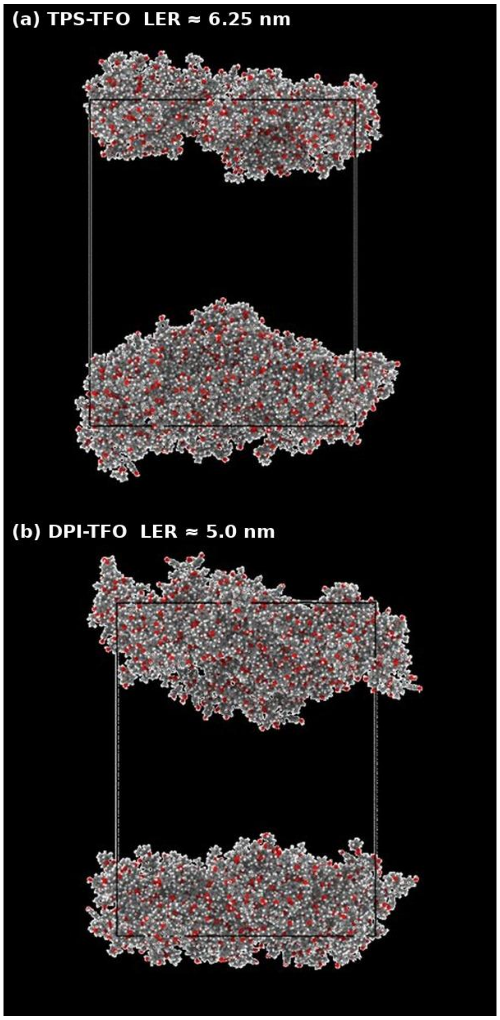

Figure 8. OVITO-rendered snapshots of polymer matrix after 150 ns PEB at 65% deprotection. (a) TPS–TFO (LER ≈ 6.25 nm) and (b) DPI–TFO (LER ≈ 5.0 nm). C: gray, O: red, H: white. The roughness of the upper and lower interfaces directly reflects the measured LER.

4. Conclusions

We have used reactive molecular dynamics to compare three PAG–polymer systems (TPS–TFO, DPI–TFO, TPS–PFBS) in homogeneous and heterogeneous setups, with Li^+ as a classical proton proxy following Bottoms et al. [19,20]. The combined results give a coherent picture:

(i) Bulk Li^+ diffusivity is essentially independent of PAG identity at fixed activation and conversion. Small DPI cations are an exception: they speed up matrix reorganization at high conversion.

(ii) The molecular feature that separates the three PAG systems is the ion–polymer interaction. PFBS, being larger than TFO, swells the matrix by 7–8% across all conversions. The expanded matrix lowers the effective Li^+

concentration, slows Li^+–carbonyl encounters, and produces a more diffuse interface, hence higher LER.

(iii) LER drops monotonically with deprotection level. The ordering DPI–TFO < TPS–TFO < TPS–PFBS holds at every deprotection level we examined. DPI–TFO reaches LER ≈ 5 nm at 65% deprotection; TPS–PFBS is still at ≈ 8 nm at 60%.

(iv) In TPS–TFO, higher PAG activation reduces LER at any given deprotection level. Catalyst density is therefore an additional design lever beyond ion identity.

(v) Cation size affects LER through molecular mobility: the smaller DPI cation enables faster matrix relaxation and a sharper deprotection boundary. The same DPI-over-TPS ordering has been reported experimentally by Higgins et al. [31] and attributed to a higher EUV absorption cross-section of iodonium PAGs; our results identify a complementary mechanism operating during PEB itself. Combining (ii) and (v), smaller PAG ions favor lower LER, and cation size effects are particularly pronounced.

Future work will extend the comparison to other PAG chemistries and use the atomistic results to inform mesoscopic reaction–diffusion models.

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