

Systems & Control *Transactions*

Volume 5

Proceedings of the 36th

European Symposium on Computer Aided Process Engineering

ESCAPE 36



Solomon F. Brown
Maria Papathanasiou
David Bogle
Joan Cordiner
Michael Fairweather

Systems & Control Transactions

Vol 5

Proceedings of the 36th European Symposium
on Computer Aided Process Engineering
ESCAPE 36

June 21–24, 2026

Sheffield, United Kingdom



PSEcommunity.org

PSE Press • Hamilton • Notre Dame

Systems & Control Transactions, Volume 5
PSE Press
Hamilton, Ontario, Canada

Individual articles copyright © 2026 by the authors and licensed to PSEcommunity.org and PSE Press.
Remaining text © 2026 by the PSE Press. All rights reserved.
Cover photo credit: Photo 119650316 © Scanrail | Dreamstime.com

This book and all individual articles are released under the Creative Commons CC-BY-SA 4.0 License
Credit must be given to creator and adaptations must be shared under the same terms.
See <https://creativecommons.org/licenses/by-sa/4.0/> for license details.



Living Archive for Process Systems Engineering (LAPSE) Archive ID: LAPSE:2026.0200
Digital Object Identifier (DOI): 10.69997/sct.161019

Library and Archives Canada Catalogue

A catalogue record and copy of this book is available from Library and Archives Canada

Archival Permissions

This book, as well as the individual articles within, may be deposited in digital research archives, personal archives, or institutional archives.

Electronic Book

ISBN (Volume 5) 978-1-7779403-5-5

ISSN (Series): 2818-4734

10 9 8 7 6 5 4 3 2 1

The information presented in this book was provided by individual contributors in the form of new scientific research contributions, data, and findings that were believed to be reliable and provided in good faith. Some, but not all, content has undergone peer review as marked. Neither PSE Press, PSEcommunity.org, the University of Sheffield, the EFCE CAPE Working Party, the CACHE Foundation, Inc., the editors, nor authors guarantee the accuracy or completeness of any information provided, nor shall they be responsible for errors, omissions, incomplete information, or damages arising from its use. The information within does not consist of engineering or professional services.

Typeset in Inter

Suggested Citation for Individual Articles

Student MC, Supervisor QR. Title of the article. *Systems & Control Transactions 5*:startpage-endpage (2026). <https://doi.org/10.69997/sct.restofarticledoi>

Suggested Citation for Entire Proceedings

Brown SF (ed). Proceedings of the 36th European Symposium on Computer Aided Process Engineering, Sheffield, United Kingdom, June 21-24 (2026). ISBN: 978-1-7779403-5-5

Scientific Editors

Solomon F. Brown (University of Sheffield), Maria Papathanasiou (Imperial College London), David Bogle (University College London), Joan Cordiner (University of Sheffield), Michael Fairweather (University of Leeds)

PSE Press Production Team

Thomas A. Adams II (NTNU), Mina Naeini (Jacobs Consultancy), Noelia Gudiño, Daniel R. Lewin (Technion)

Table of Contents

PREFACE

Introduction	xxiii
Solomon F. Brown	
Peer Review Policy	xxiv
International Scientific Committee	xxvi

PEER REVIEWED CONFERENCE PROCEEDINGS

Section 1: CAPE in Circular Economy

Circular Zero Liquid Discharge Systems with Renewable Energy Integration: A Technoeconomic Assessment	2
Fatima Mansour, Sabla Y. Alnouri, Sabah Solim, Ali Al-Sharshani, and Dhabia Al-Mohannadi	
Development of a Novel Microwave-assisted Process that Converts Mixed Plastic Waste to Olefins and Aromatics	11
Aseel Al-Sakkaf, Chunlin Luo, Yuxin Wang, and Srinivas Palanki	
Process-Informed Design of Electrochemical Cells for Urea Production: A Techno-Economic and Systems Engineering Approach	18
Zhimian Hao, Shilong Fu, Chengtian Cui, Ruud Kortlever, Ruud van Ommen, and Ana Somoza-Tornos	
Computed-Aided Design of an Intensified Process for the Sustainable Production of Biodiesel from Waste Cooking	25
Tania G. Salgado-Rodríguez, Fernando I. Gómez-Castro, and Nelly Ramírez-Corona	
Integrated Multiproduct Facility for the Green Production of Chemicals and Food from Apples	31
Vanessa Villazón-León, Carlos Sanz, Adrián Bonilla-Petriciolet, and Mariano Martín	
Hybrid Modeling of a Sewage-Sludge Gasifier using Flowsheet Simulation and Machine Learning	37
Malte Lutz, William Würpel, Fabian E. Habicht, Burcu Aker, and Jan C. Schöneberger	
Lifetime-Adjusted LCA of Biochemical and Thermochemical Circular Plastic Pathways	45
Alexandra Krestnikova and Gonzalo Guillén-Gosálbez	
Optimization of Circular Supply Chains for Electric Vehicle Batteries	52
Kaapo Kopra and Iiro Harjunkoski	
Integration of carbon dioxide capture in a wine effluent biorefinery through the use of deep eutectic solvents .	59
Carlos E. Guzmán Martínez, Valeria Caltzontzin Rabell, Sergio I. Martínez Guido, Salvador Hernández, and Claudia Gutiérrez Antonio	
Techno-economic feasibility of gallium recovery from semiconductor wastewater	68
Kilian Kozerke, Thomas Eberius, and Nathaniel J. Cooper	
Integrated solvent and process design with technoeconomic and lifecycle assessment for solvent-based recycling of end-of-life vehicle plastics	77
Riccardo Standish, Jian Yin, Jakob Burger, Mirjana Minceva, Hannah Mangold, Christian Holtze, Markus Schoerner, Bernhard von Vacano, Amparo Galindo, George Jackson, and Claire S. Adjiman	

(article retracted)	87
Advancing Circularity in Biopharma: Leveraging Industrial Symbiosis for Resource Efficiency	94
Miriam Sarkis, Andrea Bernardi, Cleo Kontoravdi, and Maria M. Papathanasiou	
Beyond Decarbonization: Quantifying Circularity in Energy System Planning	100
Javiera Vergara-Zambrano and Styliani Avraamidou	
Hybrid Modelling of Segmented Flow Extraction Process for Digital Twin Development in Critical Metals Recovery	108
Arun Pankajakshan, Konstantinos Katsoulas, Malik Olasinde, Cong Chao, Eric S. Fraga, Panagiota Angeli, and Federico Galvanin	
Life Cycle Modeling towards Regional Symbiosis for Valorizing Mixed-Lignocellulosic Biomass from Agriculture and Forestry	117
Yasunori Kikuchi, Nobuhide Takahashi, and Satoshi Ohara	
Design and Assessment of Regional Symbiosis: A Case Study of Plant-oil Production in Japan	125
Yukito Watanabe, Yuichiro Kanematsu, Hiro Tabata, Heng Yi Teah, Kousuke Hiromori, and Yasunori Kikuchi	
OpenAD-lib: Open-Source Framework for Uncertainty-Aware Anaerobic Digestion Digital Twins	131
Benaissa Dekhici, Rohit Murali, and Michael Short	
Achieving Net-Zero Emissions in Industrial Parks Through Optimized Symbiotic Exchanges and Carbon Capture Utilization	143
Ricardo N. Dias, Fátima N. Serralha, Carla I.C. Pinheiro	
(article retracted)	152
Techno-Economic Assessment and Optimisation of Self-Sufficient Biomethane Systems for Regional Decarbonisation	161
Meshkat Dolat, Benaissa Dekhici, and Michael Short	
Dynamic material flow analysis of iridium circularity in proton exchange membrane water electrolyzers in Japan	169
Shu Yamaki, Ayumi Yamaki, Heng Yi Teah, Yuichiro Kanematsu, and Yasunori Kikuchi	
Value-Based Assessment for Strategic Selection and Optimization of POME Valorization Pathways	175
Yiwei Gao, Heng Yi Teah, Yuichiro Kanematsu, and Yasunori Kikuchi	
Chemical Additives in Plastics: Understanding the Reactions, Fate, and Releases during Pyrolysis	183
Ronald Borja-Roman, Andres Castellar-Freile, John D. Chea, Monica Rodriguez Morris, Gerardo J. Ruiz-Mercado, and Kirti M. Yenkie	
Banana peel as a Source of Polyphenols: Perspectives of Sustainability	192
Kajal Chaudhary and Soumyajit SEN GUPTA	
A Whole Systems Thinking Model Towards Optimal Decarbonization Strategies for China's Cement Sector	198
Yushu Wang, Wenli Du, Minglei Yang, and Vassilis M. Charitopoulos	
A Decision-Support Framework for Process Design of Sustainable Aviation Fuel Production via Integrated Biorefineries	205
Vibhu Baibhav, Daniel Florez-Orrego, and Francois Maréchal	
Modeling standardized industrial profiles for the optimization of eco-industrial parks	215
Dilafuz Mavlanova, Marianne Boix, Rachid Oualet, and Stephane Negny	
Understanding Environmental Impacts of Lithium-Ion Battery Recycling	222

Marco Vaccari, Leonardo Tognotti, and Monica Puccini

Accelerating Design of Chemical Recycling of Plastic Waste through Digitalization: A Bubbling Fluidized Bed Reactor Case Study 229

Stefano Iannello, Vassilis M. Charitopoulos, and Massimiliano Materazzi

Principal Component Analysis (PCA) for Evaluation of Fatty Acid Monoalkyl Ester (FAME) Quality towards Sustainable Biodiesel Production from Indonesian Microalgae Strains 236

Dea Nilam Mustika and Dimitrios I. Gerogiorgis

Section 2: CAPE in Clean Energy Systems

A MIBLP model for a Northern European negative-emission hydrogen supply chain with CCS in the North Sea 244

Matthias Maier, Sungho Shin, Simon Roussanaly, and Thomas A. Adams II

Integration of exergy and economic optimization for green hydrogen and power co-generation based on sorbent-enhanced biogas reforming with CO₂ capture 252

Arthur-Maximilian Báthori and Calin-Cristian Cormos

Green Hydrogen Supply Chain Design Towards Social Sustainability: A Case Study in Brazil..... 259

Leonardo Santana, Fernando Pessoa, and Ana Barbosa-Póvoa

Sustainable Design of an Integrated Seawater-Based Green Hydrogen Production Process267

Antonio Torres-Ayala, Eduardo Sánchez-Ramírez, Marcelino Carrera-Rodríguez, and Juan Gabriel Segovia-Hernández

Net Carbon Balance (NCB): a Better Way to Evaluate and Optimize Carbon Capture Technologies 274

André F. Young, Aline R. Eckstein, Leonardo D. Ferreira, Vítor M. Sermoud, and Ingrid A. de Oliveira

Multi-Scale Design for Clean Energy Systems: Industrial Electrification and Flexible Operation of Ammonia Synthesis 282

Nicholas N. Kalamaris and Christos T. Maravelias

Optimizing Renewable Energy Storage Systems to Accelerate Sustainable Data Center Deployment 289

Matthew J. Palys and Prodromos Daoutidis

Temporal aggregation bias in model-based Direct Air Capture performance under weather variability297

Eleni Chalasti, Gbemi Oluleye, Maria M. Papathanasiou, and Ronny Pini

Dynamic Optimization of an Adsorption Heat Storage to satisfy the Heat Demand of a House 306

Alix Untrau, Lorenz T. Biegler, and Sabine Sochard

Direct iron reduction system analysis with mixture of hydrogen feed.....314

Marwa Mortadi, Carl Haikarainen, Guanwei Zhou, and Henrik Saxén

Optimization of Site-wide Heat-Integrated Utility Systems with Heat Pumps using MILP..... 320

Thorben Hochhaus, Marcus Grünewald, and Julia Riese

Investigating the Effects of Heat Ingress and Tank Motion on the Ullage Space of a Partially Filled Liquid Hydrogen Tank Using CFD 328

Anna Pakarinen and Anders Brink

Development of a methodology for heat pump-based heat integration in batch processes 334

Johannes Wloch, Marcus Grünewald, and Julia Riese

Pareto-Optimal Pathways for Refinery Decarbonization: Retrofit of Small Modular Nuclear Reactors..... 342

Aditya S Khatu, Sampri Chattohadhyay, and Ana I Torres

Exploring the Thermal Coupling of Solid Oxide Electrolysis and Ammonia Synthesis: A Plantwide Energy Integration Assessment	352
Alessandra Macchi, Federica Longobardi, Régis Anghilante, Andrea Isella, and Davide Manca	
Techno-Economic Assessment of Decarbonization Pathways for Methanol and Formaldehyde Production: A Superstructure Optimization Approach	360
Rafailia Mitraki, Muhammad Salman, and Grégoire Léonard	
Integrated Operating Strategies and Parameter Optimization for PEM Electrolyzers in Power-to-X Energy Systems.....	369
Luka Bornemann, Yifan Wang, and Martin Kaltschmitt	
Evaluating the Potential of Sustainable Aviation Fuel for Decarbonization of the Aviation Sector: An Agent-based Model.....	378
Geeta Joshi, Tejeswi Ramprasad, Harmandeep Singh, Narayanan Rajaraman, Vikrant Urade, Arnoud Higler, and Rajagopalan Srinivasan	
A Data-Driven Optimization Framework for the Design and Operation of Adaptive and Resilient Energy Supply Chain Networks under Uncertainty	386
Halil Iseri, Funda Iseri, Mahmoud El-Halwagi, Eleftherios Iakovou, and Efstratios Pistikopoulos	
Powering AI Beyond the Grid: Optimal allocation and Behind the Meter Investment Portfolios for Data Centers	396
Mohamed Abdelhady, Eleftherios Iakovou, and Efstratios N. Pistikopoulos	
Evaluating the potential of e-fuels for decarbonizing European truck transport: A techno-economic and life cycle approach	404
Marion Andritz, Severin Sendlhofer, Rafailia Mitraki, Grégoire Léonard, and Christoph Markowitsch	
Integration of computer aided design and emerging technology development based on a series of scale-up demonstration tests; Case study of thermal energy storage	413
Shoma Fujii and Yasunori Kikuchi	
Optimizing Heat Storage Integration for Solar Thermal Systems in Industrial Process Heat Networks.....	419
Håvard Falch, Henri Tande Espen, and Rahul Anantharaman	
Energy planning towards absolute environmental sustainability: identifying key demand-side sufficiency levers to stay within planetary boundaries using sensitivity analysis tool	424
Nicolas Ghuys, Diederik Coppitters, Anne van den oeveer, Mahdi Kchaou, Hervé Jeanmart, and Francesco Contino	
Assessing the potential of vehicle-to-grid (V2G) systems using dynamic simulation and life cycle assessment.....	432
Ayumi Yamaki and Yasunori Kikuchi	
Techno-economic assessment of green ammonia plants with multi-scale capacity	440
Ruitao Sun and Jie Li	
Terawatts for Petabytes: Exploring the impact of AI data centres on Europe's net zero goals	446
Mohammad Hemmati and Vassilis M. Charitopoulos	
Simulation of Methanol Production from Biogas: Impact of Feedstock Composition and Stoichiometric Number Adjustment	454
Muhammad Zulkefal, Magne Hillestad, Truls Gundersen, and Bjørn Austbø	
Strategic Design of CO₂-Reuse Pathways for Sustainable Aviation Fuel: A Game-Theoretic Techno-Economic Analysis.....	462
Andrés I. Cárdenas, Víctor A. Soria, and Ana I. Torres	

Feasibility of Integrating Sugarcane-Derived Biogas into the Allam–Fetvedt Cycle for BECCS Power Generation	470
João Pedro B. Vasconcelos, Miguel D. Carvalho, and Jean F. Leal Silva	
Optimising Waste-to-Energy Power Generation in Trinidad and Tobago.....	477
Sherard Sadeek, Thomas Hart, Arun Mangra, Daniel Chernick, Andrew Ross, Dhurjati Prasad Chakrabarti, Maria M. Papathanasiou, and Keeran Ward	
Harnessing waste heat in the optimal operation of power-to-X energy systems using detailed process models.....	483
Yifan Wang, Luka Bornemann, and Niklas von der Assen	
Comparative Life Cycle Assessment of Electrochemical and Conventional Regeneration Pathways in KOH-Based Direct Air Capture Systems.....	492
Georgia Ioanna Prokopou, Zoi Drakopoulou, Dominik Bongartz, and Alexander Mitsos	
Comparative Techno-economic and Environmental Evaluation of Single-Step vs. Dual-Step CO₂-to-Methanol Processes using Multiobjective Optimization	500
Biswarup Mondal, Johannes Leipold, and Achim Kienle	
A Multi-Objective Optimization and Superstructure-Based Decision-Support Tool for Regional Low-Carbon Hydrogen Roadmaps: Methodology and Application to a region of Spain	507
Silvia Moreno, Alejandro Aragón-García, Ángel L. Villanueva-Perales, Bernabé Alonso-Fariñas, and Pedro Haro	
Electrified refineries in the Power Flow Network.....	514
Sampriti Chattopadhyay, Ana I. Torres, Ignacio E. Grossmann, and Saif R Kazi	
Techno-economic Analysis of Alternatives for Carbon Capture and Utilization and Green Ammonia Production from a Cement Plant Flue Gas	526
Miguel A. Pedro, Ana S. Amorim, and Henrique A. Matos	
CFD-based optimal design of a portable and stackable alkaline water electrolyser for hydrogen production ...	534
Akepogu Venkateshwarlu, Gianluca Li-Puma, and Brahim Benyahia	
Modeling and experimental validation of a flat-conduit dense-phase receiver for concentrated solar power ...	543
Mustapha Hamdan, Malak Hamdan, Bogdan Dorneanu, and Harvey Arellano-Garcia	
Section 3: CAPEing with Uncertain Futures	
The Value of Multi-Stage Stochastic Programming in Power Grid Capacity Expansion Planning	550
Sergio Bugosen, Tomas Valencia, Jean-Paul Watson, Chrysanthos E. Gounaris, and Carl D. Laird	
Designing in an Unpredictable World: Novel Methods for Uncertainty Characterization, Quantification, and Optimization in Process Engineering.....	558
Diederik Coppitters, Antoine Laterre, Mahdi Kchaou, Kevin Verleysen, Panagiotis Tsirikoglou, Jerome Stock, Matthias Weigold, Konstantinos Kyprianidis, Ward De Paepe, and Francesco Contino	
Enhancing Interpretability of Stochastic Programming Solutions: A Multiparametric Approach.....	567
Parth Brahmabhatt and Styliani Avraamidou	
Exploring Robust Early-Stage Decisions in Energy Transitions Using Near-Optimal Pathways and Multi-Armed Bandits	574
Mahdi Kchaou, Diederik Coppitters, and Francesco Contino	
Optimization-based Design, Simulation and Data-Driven Learning for Resilient Manufacturing Systems	583
Miriam Sarkis and Efstratios Pistikopoulos	
A Machine Learning Implementation for Fermentation Quality Prediction in Wine Manufacturing.....	592

Matthew A.J. Hill and Dimitrios I. Gerogiorgis

Global Optimization of Robust AC OPF..... 602

Yuhui Yin and Vassilis M. Charitopoulos

Section 4: Pharmaceutical and Biotechnological Systems

Uncertainty-Aware Model Validation Framework for Pharmaceutical Process Development 611

Kensaku Matsunami, Yash Barhate, and Zoltan K. Nagy

Comparison of Centralised and Decentralised Pharmaceutical Manufacturing Paradigms: An Agent-Based Simulation Study..... 618

Farshid Babaei, Mohammad Salehian, David Robins, Cameron J. Brown, Daniel Markl, Alastair J. Florence, and Solomon Brown

Developing predictive models for batch cooling crystallization of APIs with limited data availability..... 625

Mauro Davanzo, Emanuele Tomba, Enrico Carlassare, Riccardo Motterle, Massimiliano Barolo, Zoltan K. Nagy, and Fabrizio Bezzo

An in silico/in vitro approach for uncertainty-aware hybrid models for template-induced protein crystallisation systems 631

Daniele Pessina, Jerry Y. Y. Heng, and Maria M. Papathanasiou

Capturing mixing effects on aggregation kinetics of monoclonal antibodies during viral inactivation 640

T. Marella, F. Cenci, P. Thompson, M. Muhieddine, and F. Bezzo

A Generative AI Approach to Inverse Design for Continuous Pharmaceutical Manufacturing..... 648

Consuelo Del Pilar Vega-Zambrano and Vassilis M. Charitopoulos

Development of Symbolic Regression-Based ATR-FTIR Calibration Models..... 655

Fernando A. R. D. Lima, Inga S. Nordhus, Marcellus G. F. de Moraes, M. Enis Leblebici, Argimiro R. Secchi, Mauricio B. de Souza Jr., and Idelfonso Nogueira

Beyond Solid-Phase: Comparative Assessment of Liquid Phase Oligonucleotide Synthesis with Single- and Dual-Stage Diafiltration..... 664

Alberto Saccardo, Rachel Ha, Zoe Fang, and Benoît Chachuat

In silico solvent selection for green and cost-effective pregabalin crystallisation 672

Matthew Blair and Dimitrios I. Gerogiorgis

Molecular Similarity Coefficient in Chemical Design and Analysis..... 681

Youquan Xu, Zhijiang Shao, Abdulelah S. Alshehri, Mansour S. Alhoshan, and Anjan K. Tula

Pareto Front Guided Sampling for Efficient Bioprocess Experimentation..... 692

Stricker Samuel, Lucas Francisco dos Santos, Claus Wirnsperger, Alessandro Butté, Antonio del Rio Chanona, Mehmet Mercangöz, and Gonzalo Guillén Gosálbez

Sensitivity-Based Comparison of Resource Competition Models for Optogenetic Gene Circuit Design..... 702

Pratham Kapavarapu, Satyajeet S. Bhonsale, Simen Akkermans, and Jan F.M. Van Impe

Genome to Production: A Multiscale Model for Bioprocess Design 709

Rajiv Kailasanathan, Mohammad Reza Boskabadi, Abhishek Sivaram, and Seyed Soheil Mansouri

Modelling & optimization of recombinant protein production in a microbial cultivation with tunable induction .. 714

Philipp Pably, I Gede Eka Perdana Putra, Gerd Seibold, Jakob K. Huusom, and Julian Kager

Automatic kLa determination in stirred tank reactors by model-based design of experiments..... 721

Ana Helena V. Caetano, Krist V. Gernaey, and Julian Kager

Decarbonizing API Manufacturing: Conceptual Design and Scale-up Analysis of Continuous-Flow Electrosynthesis for Ibuprofen Production	727
Tuse Asrav, Merlin Alvarado-Morales, and Gürkan Sin	
A Multi-Level Hybrid EKF–Machine Learning Soft Sensor for Robust Bioprocess Monitoring.....	733
Mohammad Reza Boskabadi, Rajiv Kailasanathan, Luis Ricardez-Sandoval, and Seyed Soheil Mansouri	
Understanding the Impact of Ribbon Splitting on Tablet Properties Using a Hybrid Mechanistic–Machine Learning Framework	742
Shumaiya Ferdoush, Mohammad Shahab, Xinle Zhang, Jayden A. Pierce, Emma Jeffries, Adaugo Ufomba, Zoltan K. Nagy, Gintaras V. Reklaitis, and Marcial Gonzalez	
Physics-Informed Neural Networks for NIR Spectroscopy Analysis of Pharmaceutical Tablet Properties	751
Xinle Zhang, Shumaiya Furdoush, Marcial Gonzalez, and Gintaras V. Reklaitis	
Probabilistic design spaces from small DoEs – A boundary-focused workflow using quantile surrogates.....	756
Tobias Overgaard, Emmanouil Papadakis, Maria-Ona Bertran, and Maria M. Papathanasiou	
(article retracted)	763
Combined PBM-PBPK Modeling for Optimized Integrated Oral Solid Dosage Form and Dosing Strategy Design	769
Meng-Hua Yang, Francesco Rossi, Gintaras V. Reklaitis, and Zoltan K. Nagy	
Experiments & Modelling of Batch Fermentation of Fusarium venenatum on Glucose-Fructose Mixtures	776
Tom Vinestock and Miao Guo	
Towards Digital Threads for FAIR, Trustworthy, and Human-Centric Bioprocess Development	783
Jonas M. Karsten, Ernesto C. Martínez, and Mariano N. Cruz Bournazou	
Safe and Sustainable by Design Pharmaceuticals through Combined Computer-Aided Retrosynthesis, Techno-Economic Analysis, and Life Cycle Assessment	791
Shang Gao and Brahim Benyahia	
 Section 5: Modelling and Simulation	
An Open-Source IDAES Framework for Simulating Inductively Heated Adsorption Processes	802
Sudip Sharma and Thomas A. Adams II	
Development of a Predictive Model for Microbial Growth under Variable Conditions Using a Multilayer Perceptron Neural Network: Application to Candida guilliermondii.....	810
Jazmín Cortez-González, Juan Gabriel Segovia-Hernández, Salvador Hernández, Varinia López-Ramírez, Arturo Hernández-Aguirre, and Rodolfo Murrieta-Deñas	
Dynamic optimization of glucose feed in cell cultivation for monoclonal antibody production process design balancing productivity and impurity generation.....	816
Kosuke Nemoto, Yuki Yoshiyama, Mizuki Morisasa, Junshin Iwabuchi, Yusuke Hayashi, Sara Badr, and Hirokazu Sugiyama	
Development of ANN-based models for dye removal through electrochemical advanced oxidation techniques.....	822
Zaira J. Mosqueda-Huerta, Oscar D. Lara-Montaño, Juan Manuel Peralta-Hernández, and Fernando I. Gómez-Castro	
Model Screening and Identifiability Analysis of Methanol Synthesis Kinetics: Information-Guided Evaluation of Operating Conditions	828
Eblagh Ahmad, Biasin Alberto, Nardi Luca, and Federico Galvanin	

A Process Modeling Approach for Water and Energy Optimization in Geologic Hydrogen Extraction	838
Caroline Kaitano and Thokozani Majazi	
Optimal Simulation of an Electrodialysis Reactor for the Desalination and Regeneration of Multi-Ionic Wastewater	846
Vicent Ayala-Andreu, Miguel A. Montiel, Vicente Montiel, and Juan A. Labarta	
A Data-Efficient Symbolic Regression Framework for Automated Interpretable Bioprocess Modelling	855
Luca Riezzo, Alexander Rogers, Harry Kay, and Dongda Zhang	
Modelling Pressure Effects in Boiling Brazed Aluminum Heat Exchangers: A Software Comparison	861
Hamza Karim, Rim Khodr, Rodolphe Sardeing, and Gaëtan Becker	
From Drift to Adaptation to the failed ML model: Transfer Learning in Industrial MLOps	870
Waqar Muhammad Ashraf, Talha Ansar, Fahad Ahmed, Jawad Hussain, Muhammad Mujtaba Abbas, and Vivek Dua	
Design of a Chemical Heat Pump based on Methylcyclohexane, Toluene and Hydrogen	879
Rajalakshmi Krishnadoss, Félix Le Bot, and Thomas A. Adams II	
An Integrated Process of Multi Effect Distillation Based Desalination with Renewable Energies: Evaluation of Power Generation Efficiency and Freshwater Production Cost.....	886
Mohammed Adam, Mudhar A. Al-Obaidi, and I. M. Mujtaba	
Dynamic Modelling of Renewable-driven CO₂ Methanation using Recurrent Neural Networks	895
M. Andrea Pappagallo, Diego A. Romero Lombo, Mattia Vallerio, and Emanuele Moioli	
Chemical Language Transformers for the Inverse Design of Novel Surfactants.....	903
Alexander W. Rogers, Ruediger Zillmer, Amanda Lane, Adam Kowalski, and Dongda Zhang	
A Modeling Framework Integrating Data Trends and Reference Information for Predicting Temperature-Dependent Thermophysical Properties	910
Shuai Zhang, Abdulelah S. Alshehri, Mansour S. Alhoshan, and Anjan Tula	
Exploring Molecular Pretraining and Mechanism-Aware Modeling for Reaction Yield Prediction	919
Yongkyu Lee, Won Bo Lee, and Lauren Ye Seol Lee	
Synergistic integration of direct air capture in bioenergy systems.....	927
Nor Syuriaty Jaafar, Norhuda Abdul Manaf, Noor Fatina Emelin Nor Fadzil, and Nilay Shah	
An Adaptive Framework for Robust Energy Forecasting under Concept Drift and Feature Uncertainty	934
Francesco Marcato, Alessio Santecchia, Manuel Ruivo de Oliveira, Francesco Silvestri, and Rafael Castro-Amoedo	
Analysis and comparison of technologies for the regeneration of a capture solution in DAC absorption systems	943
Grazia Leonzio and Nilay Shah	
From Plastic Waste to Platform Chemicals: Aspen Plus Modeling of Polystyrene Conversion Through Hydrothermal Processing into Value-added Chemicals	950
MohammadSina HajiHashemi, Corinna Schulze-Netzer, and Thomas A. Adams II	
Uncertainty Prioritisation for Water-Energy-Food-Land Nexus Optimisation.....	958
Md Shamsul Alam, I. David L. Bogle, and Vivek Dua	
Data Transformation Techniques and its Influence in Hybrid Model Performance	964
Juan Federico Herrera-Ruiz, Carlos Eduardo Robles-Rodríguez, Cesar Arturo Aceves-Lara, Javier Fontalvo, and Oscar Andrés Prado-Rubio	

Simulation and analysis of carbon capture process using piperazine for large scale biomass-fired power plant	972
Shengyuan Huang, Olajide Otitoju, Yao Zhang, and Meihong Wang	
Differentiable Programming for Cyclic Adsorption Processes	978
Alex Glover, Maria M. Papathanasiou, and Ronny Pini	
Bayesian Optimization Framework for Agrochemical Formulation Design	986
Yipei Zhao, Robin Wesley, and Joan Cordiner	
Variational Bayesian Neural Networks for Modelling and Uncertainty Quantification in Bioprocessing	992
George Spencer, Harini Narayanan, Claus Wirtensperger, Alessandro Butté, Cleo Kontoravdi, and Maria M. Papathanasiou	
Multi-objective simulation-based optimisation of pharmaceutical process systems	1001
Artemis Tsochatzidi, Francesca Cenci, Magdalini Aroniada, and Lazaros G. Papageorgiou	
Modeling, Simulation, and Optimization of an Anion Exchange Membrane Cell for Ammonia Electrolysis	1007
Laureen E. Hernández Lefrán, Leonardo A. Cáceres Avilez, Antonio E. Bresciani, Claudio A. Oller do Nascimento, and Rita M. Brito Alves	
A Coarse-Graining Algorithm for Complex Chemical Reaction Networks	1014
Yi Tao and Tong Qiu	
Automated Construction of Bayesian Networks of Chemical Process for Dynamic Risk Assessment	1022
Kai Yin, Hao Kang, and Jinsong Zhao	
CO₂ Conversion: Three-Dimensional Modelling of Gas Diffusion Electrodes	1030
Cristina González-Fernández, Camilo Peralta, Jose Antonio Abarca, Esther Santos, Guillermo Díaz-Sainz, and Ángel Irabien	
(article retracted)	1036
Multiscale Modeling of PHBV Production: Explicit Polymerization Modeling and Improved Prediction of Chain Length Distributions	1043
Stefan Hempfling, Rudolph Kok, Stefanie Duvigneau, Achim Kienle, and Robert Dürr	
Evaluating Extrapolation of Modular Hybrid Process Models for Pilot-Scale Batch Separation Processes	1050
Søren Villumsen, Jakob K. Huusom, Xiaodong Liang, and Jens Abildskov	
Exploiting Input-Space Separation in Kolmogorov–Arnold Networks to Prevent Catastrophic Forgetting in Industrial NIR Systems	1058
Imam M. Iqbal, Isabell Viedt, and Leon Urbas	
Renewables to X: Micro-Reactor Pathways towards Methanol and Dimethyl Ether Production	1064
David T. Hren and Andreja Nemet	
Dynamic modeling of fouling development during dead-end filtration of dusty superheated steam	1073
Felipe de Oliveira, Wijtze Nijhuis, Marcel Meinders, and Edwin Zondervan	
Robust Design of Transient Flow Experiments for the Identification of Kinetic Models in Flow Reactor Systems with Catalyst Deactivation	1080
Jinwen Cui and Federico Galvanin	
Process modelling and multi-objective optimisation of solid sorbent-based direct air capture	1088
Toluleke E. Akinola and Meihong Wang	
Uncertainty Quantification of Stochastic Gene Expression	1095
Francisca Pizarro Galleguillos, Satyajeet S. Bhonsale, and Jan F.M. Van Impe	

Practical Identifiability and Optimal Experiment Design for Hybrid Cybernetic Models: An E.Coli Case Study .	1102
Stylianos Floros, Satyajeet S. Bhonsale, Simen Akkermans, and Jan F.M. Van Impe	
Semi-Supervised Generative Augmentation Improves Surfactant Surface Tension Prediction from Limited Experimental Data	1111
Gabriela C. Theis Marchan, Kyle Territo, and Jose A. Romagnoli	
A CFD Analysis of Dielectric Fluid Performance in Thermal Management of Li-ion Cells	1119
Margarita G. Correa-Ibarra, Jorge A. Alfaro-Ayala, Jose de J. Ramirez-Minguela, Zeferino Gamiño-Arroyo, and Agustin R. Uribe-Ramirez	
Simulation of Fixed-Bed Reactor System for Combined Ca–Cu Chemical Looping with Integrated Combustion and CO2 Capture	1127
Levente Biró, Norbert–Botond Mihály, and Ana-Maria Cormos	
Comparison of Various Hydrogen Flux Trajectories in a Catalytic Membrane Reactor Operating Dehydrogenation of Ethylbenzene to Styrene.....	1135
Nabeel S. Abo-Ghander	
A Neural Model of Pinch-Based Multicomponent Distillation for Applications in Flowsheet Synthesis.....	1145
Alexander B. Wolf, Mirko Skiborowski, and Jakob Burger	
Physics-informed Graph Neural Networks to Predict Thermodynamically Consistent Activity Coefficients in Multicomponent Mixtures	1153
Lifeng Zhang, Benoît Chachuat, and Claire S. Adjiman	
SMILE: Smell Maximisation In Low-cost Eau de parfum	1160
Flora Esposito, Ulderico Di Caprio, Mattia Collu, Raffaele Graziano, Vincenzo Guida, Hasan Sildir, Idelfonso B.R. Nogueira, Florence Vermeire, M. Enis Leblebici	
Dynamic Operation of a Haber-Bosch Loop with Quench-Cooled Converter for Power-to-Ammonia Systems	1167
José M. Pires, Diogo A. C. Narciso, Carla I. C. Pinheiro	
A Symbolic Regression-based approach for Modeling Fouling Resistance in Heat Exchangers.....	1175
Fernando A. R. D. Lima, Antonioni B. Campos, Bruna Carla G. de Assis, Livia Pereira L. Costa, Fabio S. Liporace, Mauricio B. de Souza Jr., and Argimiro R. Secchi	
Energy Integration Via Heat Pump in a Simulated Fluidized TSA Column for CO2 Capture from Biomass-Derived Flue Gases.....	1183
Eduardo S. Funcia, Yuri S. Beleli, Enrique Vilarrasa-Garcia, Marcelo M. Seckler, José L. Paiva, and Galo A. C. Le Roux	
Towards White-box Environmental and Economic Process Optimization: Tailoring Modelling Approaches to Multi-scale Simulations.....	1189
Thomas Hietala, Sonja Herres-Pawlis	
Designing MgCl₂-Based Ethanol Dehydration Systems: A Multi-Objective Approach with Open-Loop Controllability	1197
Josué J. Herrera Velázquez, J. Rafael Alcántara Avila, Salvador Hernández, and Julián Cabrera Ruiz	
Addressing Matrix Effects Through A Physical Prior-Informed Calibration Model For Quantitative Analysis ...	1205
Onur C. Boy, Ulderico Di Caprio, Idelfonso Nogueira, and M. Enis Leblebici	
Multi-Objective CAPE Simulation of Agro-Industrial Systems Integrating High-Yield Sugarcane and the Inversion Process.....	1212
Satoshi Ohara, Yoshifumi Terajima, Hiro Tabata, and Yasunori Kikuchi	

Towards the Decarbonization of a Conventional Ammonia Plant by the Gradual Incorporation of Green Hydrogen and Air-Separated Nitrogen	1219
João Fortunato, Diogo A. C. Narciso, and Henrique A. Matos	
Hybrid Modeling of Wastewater Treatment Dynamics Using Hammerstein-Wiener Structures	1226
Arne Tirez, Niels Stevens, Dominik Bongartz, and José Matias Assumpcao	
Re-parametrisation of NRTL model for C1+ organics and alcohols recovery from aqueous phase in pyrolysis oil production	1234
Matteo Gilardi, Filippo Bisotti, Trung Trinh, and Bernd Wittgens	
A Framework based on Population Balance Modeling for Predicting Li-O₂ Battery Discharge and Life Cycle Behavior	1242
Nadia G. Khouri, Jean F. Leal Silva, Letícia M. S. Barros, Viktor O. C. Concha, and Rubens Maciel Filho	
A Computational Framework for Simulation and Energy Evaluation of Sustainable Biodiesel Production Routes	1249
Ian B. B. Batata, Emílio E X. Guimarães Filho, Victor H. S. Ramos, Maria R. Wolf Maciel, Nadia G. Khouri, and Rubens Maciel Filho	
(article retracted)	1256
Enhancing Pharmaceutical Supply Chain Robustness via Simulated Annealing	1262
Nelson Chibeles-Martins, Maria A. Monge, and Tânia Pinto-Varela	
Assessing the Impact of Thermodynamic and other Modelling Choices in MEA-based CO₂ Capture Simulations	1269
Hassan Khaled Hassan Baabbad, Alberto Fernández, Fèlix Llovel, and Carlos Pozo	
Experimental and Kinetic Study of Iron Oxide Reduction in a Fixed Bed Reactor using a Dynamic Shrinking Core Model	1277
Emiliano Salucci, Antonio D'Angelo., Vincenzo Russo, Henrik Grénman, and Henrik Saxén	
A General Framework for Model Recognition in Chemical Reactor Systems Using Artificial Neural Networks Classifiers	1285
Emmanuel Agunloye, Asterios Gavriilidis, and Federico Galvanin	
Predicting Flow Regimes in a Wiped Film Evaporator Using the Volume of Fluid Method	1292
Gonçalo V.L. Pardal and Fernando P. Bernardo	
Modelling of fouling dynamics in a falling-film evaporator	1298
Johanne L. Christensen, Lukas S. Theisen, Kevin Feldmann, and Jakob K. Huusom	
Modeling Slug Flow Dynamics in Offshore Wells using Universal Differential Equations	1306
Gustavo Luís Rodrigues Caldas, Giovani Gerevini, Fábio C. Diehl, Idelfonso B. R. Nogueira, Maurício B.de Souza Jr., and Argimiro R. Secchi	
Estimation of Thermodynamic Properties for Cellulosic Biomass-Derived Compounds: Application to Heat and Work Balances in Process Simulation	1318
Anthony D. Anastasi, Cornelius M. Masuku, Praveen Ravikumar, Shishir P.S. Chundawat, and Diane Hildebrandt	
Municipal Solid Waste Valorization into Chemical Solvents for Industrial Symbiosis: Techno-Economic and Environmental Assessment	1328
Oktay Boztas, Daniel A. Flórez-Orrego, Meire E. G. R. Domingos, and François Maréchal	
Energy Baseline Surrogates for Modular Reactors from Generated Recipe-Based Process Data	1336
Shreyas Parbat, Greeshmanth Rajanala, Isabell Viedt, and Leon Urbas	

Evaluation of dual pressure low-temperature distillation for LNG Production in CO₂-rich fields	1345
Victor S. V. Mercado, Dirceu Noriler, Laura Plazas Tovar, Radin Suhaib Salihuddin, Amiza Bt Surmi, Fadhli Hadana Rahman, and Jean F. Leal Silva	
Multi-scale Metabolic Modeling and Simulation	1353
Peter E. Carstensen, Teddy Groves, Lars K. Nielsen, Ulrich Krühne, Krist V. Gernaey, and John B. Jørgensen	
Enhancing Parameter Identifiability in Capacitive Deionization: A Model-Based Design of Experiments Approach	1360
Yuxuan Yang and Federico Glavanin	
Process Intensification for LNG Purification: Modeling CO₂ Separation in a Rotating Packed Bed.....	1366
Alexander A. Zerwas, Bruna L. V. Maia, Wilson Santos Neto, Radin Suhaib Salihuddin, Amiza Bt Surmi, Fadhli Hadana Rahman, Jean F. Leal Silva, and Dirceu Noriler	
Desing and optimization of a multi-objective plant to obtain the best furfural derivates	1374
Melanie Coronel Muñoz, Brenda Huerta Rosas, Eduardo Sánchez Ramírez, Juan Gabriel Segovia Hernández, and Juan José Quiroz Ramírez	
Multi-Level Optimization of Crane Scheduling	1383
Sophia Onyshkevych, Bianca Springub, and Christos Galanopoulos	
Modelling of carbon dioxide methanation in radial flow reactor	1391
Salvatore Capasso, Vincenzo Russo, and Henrik Grénman	
Dynamic Modeling of a Biomass Fluidized-Bed Gasifier	1398
Jefferson D. C. Araujo, Frédéric Marias, and Sabine Sochard-Reneaume	
Comprehensive Framework for Model Discovery and Discrimination Based on Symbolic Regression and Structural Identifiability - Application to a Partially Observed Chemical Reaction System	1406
Xuming Yuan and Brahim Benyahia	
SEMPRE-BIO project: comparison of three innovative scaled up and optimised technologies for biomethane production and its purification.....	1414
Filippo Bisotti, Matteo Gilardi, and Bernd Wittgens	
Modeling and Simulation of Nitrogen Generation by Pressure Swing Adsorption for Power-to-Ammonia	1422
Marcus J. Schytt, Lorenz T. Biegler, and John B. Jørgensen	
Energy recovery from process purges: steam turbine integration and operation optimisation in biogas upgrading within SEMPRE-BIO project.....	1431
Filippo Bisotti, Matteo Gilardi, and Bernd Wittgens	
ProcessSimulator.jl: A Symbolic-Numeric Open-Source Framework for Process Simulation in Julia Language.....	1439
Vinicius V. Santana, Christopher V. Rackauckas, and Idelfonso Nogueira	
Nanoparticle Nucleation and Growth Model Exploration with Perturbative Analysis.....	1445
Stephen T. King, Antonios Armaou, Themis Matsoukas, Griffin A. Canning, and Robert M. Rioux	
Sustainable and Optimized Biorefinery Design for the Production of High-Value Catechol Derivatives from Lignin	1455
Alden Paul Rangel-López, Eduardo Sánchez-Ramírez, Maricruz Juarez-García, Jesús Manuel Núñez-López, and Juan Gabriel Segovia-Hernández	
Integrated Data-Driven Optimisation of LNG Hot Section for Energy Efficiency and Decarbonization.....	1461
Aisha Al-Hammadi, Dr Tareq Al-Ansari, Dr Ahmed AlNouss, and Abdul Aziz Shaikh	
Modeling and Optimization of Sonochemical Reactors through simulations	1467

Nikolaos I. Vittas and Antonios Armaou

MCSGP dynamic simulation for peptides separation using Aspen Chromatography1476

Ivan Chóez-Guaranda, Emmanuel Appiah-Danquah, Bogdan Dorneanu, and Harvey Arellano-García

Multisectorial Energy Integration of Low-Temperature Brewery Process, Manufacturing Industry and District Heating Network 1483

Pullah Bhatnagar, Daniel Florez-Orrego, Oktay Boztas, Meire Ribeiro Domingos, Manuele Margni, and Francois Marechal

Process-Intensified Oscillatory Opposed-Jet Mixers: Mixing Quantification and Operational Guidelines 1494

Sofia P. Brandão, Ricardo J. Santos, Madalena M. Dias, José C. Lopes, and Margarida S. C. A. Brito

Section 6: Concepts, Methods and Tools

A Multimodal Framework Integrating Procedural Texts and Visual Perception for Laboratory Safety Monitoring 1503

Shuo Xu and Jinsong Zhao

Optimal Stopping of Batch Processes with Stochastic Dynamics – A Study of When to Act under Uncertainty 1513

Rafif S. Ramadhan, Luca Grebe, Maximilian Maschmeier, Johannes Pastoors, and Eike Cramer

A Multi-objective Experimental Design Framework Leveraging Hybrid Modelling and Gaussian Process Optimization.....1520

Michael Aku, Solomon Gajere Bawa, Ye Seol Lee, and Federico Galvanin

A Universal Framework for Automated Reaction Network Identification and Interpretable Rate Model Generation1529

Harry Kay, Alexander Rogers, and Dongda Zhang

Unveiling Reaction Patterns in Thermal and Catalytic Biomass Pyrolysis Using PCA and Multivariate Analysis1539

Martín Rodríguez-Fragoso, Sandro González-Arias, Octavio Elizalde-Solis, and Edgar Ramírez-Jiménez

Optimisation of Synthetic Natural Gas Production via Direct Air Capture and Utilisation using Reduced Models under a Novel Trust-Region Funnel Method 1551

Gul Hameed, Tao Chen, Antonio del Rio Chanona, Lorenz T Biegler, and Michael Short

Control-Guided Reinforcement Learning for Cooperative Energy Management.....1558

Isabela Fons Moreno-Palancas, Raquel Salcedo Díaz, Rubén Ruiz Femenía, José A. Caballero, and Antonio del Río Chanona

New tools, new thinking: Biomimetic Process Design through Parametric Modelling and Simulation.....1565

Alix Saury, Thibaut Houette, Pierre-Emmanuel Fayemi, Jean-Matthieu Cousin, Jérôme Fortin, and Arnaud Dujany

A Comparative Analysis of Sequential Active Learning Approaches: Statistical Design of Experiments versus Bayesian Optimisation..... 1573

Daniel V. Batista and Marco S. Reis

Advancing Industrial Fermentation across scales: Model Development, Cost Analysis, and Predictive Control1582

Marc Lemperle, Pedram Ramin, Julian Kager, Benny Cassells, Stuart Stocks, and Krist V. Gernaey

Predicting Ecotoxicity (HC50) Values Using Symbolic Regression for Transparent Life Cycle Assessment1592

Abdulhakeem Ahmed, Nitya Kasera, and Ana I. Torres

Adaptive soft sensor to estimate alite fraction in clinker production through quasi-ensemble PLS modelling . 1601

Mihnea Stefan, Wilson R. Leal da Silva, Fabrizio Bezzo, and Pierantonio Facco

Semantic PEA Datasheets for digitalised modular plant documentation	1608
Sascha Lamm, Sebastian Tecl, Ingo Dietrich, Sissy Sommer, Markus Heinbücher, and Peter F. Pelz	
libDIPS: An Open-Source Platform for Global Optimization of Hierarchical Optimization Problems	1617
Adrian W. Lipow, Daniel Jungen, Aron Zingler, Hatim Djelassi, and Alexander Mitsos	
Model verification and Uncertainty Quantification methods using the CCSI simulation model for CO2 capture	1626
Jessica V. Scheffer, Serena Delgado, Olivier Authier, Valentin Loubière, Franchine Ni, Christophe Castel, and Jean-Marc Commenge	
An End-to-End Pure Component Property Prediction Framework Based on a Hierarchical Molecular Fragmentation Method	1634
Jianfeng Jiao and Jie Li	
Global Optimization of a Hydrodealkylation Flowsheet through Spatial Decomposition with SNoGloDe	1643
Madeline Leppla, Georgia Stinchfield, Norman Tran, and Carl D. Laird	
Superstructure Framework for Feasibility and Flexibility Analysis Methods in Modular Plant Design	1650
Julian Pamperin, Jonathan Mädler, Amy Koch, Isabel Viedth, and Leon Urbas	
Process Flowsheet Synthesis via Quantum Reinforcement Learning with Improved Scalability	1659
Austin Braniff, Fengqi You, and Yuhe Tian	
A Unified Multi-Scale TCN Framework for Batch Manufacturing Soft Sensing and Monitoring	1666
Yee Hung Hong and Zhao Jinsong	
Optimizing the Solubility of Organic Molecules in Mixed Solvents Using Bayesian Optimization and Multicomponent Directed-Message Passing Neural Networks	1679
Simona Buzzi, Ulderico Di Caprio, Dominik Bongartz, and Florence Vermeire	
Coupling Analytical Derivatives with Adjoint Automatic Differentiation in a Modular Process Simulator	1687
Andrés Piña-Martinez and Jean-Marc Commenge	
Hand-crafted Feature Fusion for Deep Learning-Based Instance Segmentation in Microfluidics	1696
Wenle Xu, Lin Sheng, Qichen Shang, Mengqi Liu, Tong Qiu, Kai Wang, and Guangsheng Luo	
Methodology to assess the integrity of Water and Energy Integration Systems (WEIS) models using the ThermWatt computational tool	1705
Miguel Castro Oliveira, Rita Castro Oliveira, and Henrique A. Matos	
Targeted Olfactory Molecule Generation for Vanilla Scents Using Generative Flow Networks	1713
Bruno C. L. Rodrigues, Paul J. Groening, Laura Sisson, Mumin Enis Leblebici, and Idelfonso B. R. Nogueira	
A Strategy for Limiting the Effects of Nonconvexities in Mixed-Integer Nonlinear Programming Reformulation of Nonconvex Generalized Disjunctive Programs	1721
Miloš Bogataj, Chiara Železnik, and Zdravko Kravanja	
Beyond Tennessee Eastman: Benchmarking Deep Anomaly Detection on Real-World Pilot-Scale Continuous Distillation Data	1728
Fabian Hartung, Aparna Muraleedharan, Marius Kloft, and Jakob Burger	
From P&ID Drawings to Process Graphs: A Multimodal Language Model Approach	1737
Baikai Zhu, Samuel Duong, Javal Vyas, and Mehmet Mercangöz	
Task-Conditioned Hierarchical Representations for Controllable AI-Assisted Process Synthesis	1746
Ali Tarik Karagoz, Omar Alqusair, and Jie Li	
Recommendation System for Prediction of Adsorption Properties using Kernelized Probabilistic Matrix Factorization	1754

Gnaneshwar Sampathirao, Sasidhar Gumma, and Nabil Magbool Jan

Optimizing MIP-Heuristics: Generic Formulation and Code	1761
Sophie Hildebrandt, Meik Franke, Edwin Zondervan, and Guido Sand	
A Large Language Model Enhanced Fault Diagnosis Framework for Chemical Processes	1769
Jingkang Liang and Gürkan Sin	
A Unified Python/JAX Framework for Thermodynamic Modeling, Nonlinear Solvers, and DAE Solution of Hydrocarbon Systems	1776
Carlos C. Sanz and Galo Le Roux	
Digital Twin Supported FAIR Electronic Lab Notebooks for Simulated Experiments	1786
Amy Koch, Isabell Viedt, and Leon Urbas	
Nonconvex Robust Optimization for Process Design with Artificial Neural Networks Embedded	1793
Diego Izquierdo González, Basit Adeogun, Yuhui Yin, and Vassilis M. Charitopoulos	
Using Active Learning to Efficiently Calibrate Foundation Models on Raman Spectra in Upstream Bioprocess Fermentations	1801
Christoph Lange, Ernesto Martínez, Peter Neubauer, and Mariano Nicolas Cruz Bournazou	
Utilizing Machine Learning for Phenomena-based Synthesis of Intensified Process Flowsheets	1809
Omar Alqusair and Jie Li	
Separation of Concern Capabilities of Information Model Candidates for Modular Plant System Engineering Lines	1817
Tobias Kock, Isabell Viedt, Amy Koch, and Leon Urbas	
A Framework for Flexible Start/Stop Operation of Electrified Chemical Processes	1825
Samuel Mercer and Michael Baldea	
PhoSim V.0 - Towards A Digital Twin for an Industrial Wet-Process Phosphoric Acid Production	1833
Ilias Bouchkira, Sanae Elmisaoui, and Abderrazak Latifi	
MatStudio: A Human-in-the-Loop Framework for Microstructure Segmentation with SAM-Guided Refinement	1841
Yao Xue, Yanhu Wang, and Antonios Armaou	
Hybrid Multi-Task Learning for Sustainability-Aware Pharmaceutical Molecular Design	1847
Yiming Ma, Shang Gao, and Brahim Benyahia	
Machine Learning-Assisted Multi-PAT Data Fusion for Physics Consistent Crystallization Monitoring	1856
Yiming Ma, Xuming Yuan, and Brahim Benyahia	
Analysis of Ultrasound-Assisted Transesterification for Sustainable Biodiesel Production via Inline Raman spectroscopy	1866
Ilias Bouchkira and Adel Mhamdi	
Evaluating and adapting modelling strategies for data-driven prediction of solvent effects on reaction barriers	1876
Daeun Shin, Lingfeng Gui, Jonggeol Na, Won Bo Lee, and Lauren Ye Seol Lee	
GlycoPy: An Equation-Oriented and Object-Oriented Python Framework for Process Modeling, Optimization and Optimal Control	1884
Yingjie Ma, Jing Guo, and Richard D. Braatz	
Automated workflow for the configuration of modular plants and HAZOP analysis by utilizing DEXPI P&ID	1891
Mathias Schmitz, Janis Weber, and Norbert Kockmann	

(article retracted)	1899
Accelerating Efficient Dimethyl Ether Synthesis through Machine Learning-Based Process Optimization	1908
Mitra Jafari, Jefferson Santos da Silva, Wilson Sousa Mercês Neto, Lucas Fonseca Couto, Bogdan Dorneanu, Karen Valverde Pontes, and Harvey Arellano-García	
Decomposition of MINLP Formulations in Process Family Design using Progressive Hedging	1916
Ali Asger, Bernard Knueven, and Carl Laird	
Physics Constrained Machine Learning for Modeling and Optimization of Chemical Process Systems	1925
Rahul Golder, Bimol Nath Roy, and M. M. Faruque Hasan	
Section 7: Process Design, Scheduling and Optimisation	
Effect of the feed composition on the performance of a double-dividing wall distillation column	1933
Carlos E. Guzmán-Martínez, Araceli G. Romero-Izquierdo, Claudia Gutiérrez-Antonio, Salvador Hernández, Massimiliano Errico, and Fernando I. Gómez-Castro	
System-Level CO₂ Allocation under Supply Constraints in Industrial Clusters	1943
Razan Sawaly, Ahmad Abushaikha, and Tareq Al-ansari	
Virtual Plant–Model Pair as a Step Towards Real-Time Optimization of a Simulated Moving Bed System	1950
Guilherme C. Amaral, Alexandre F. P. Ferreira, Ana M. Ribeiro, Idelfonso B. R. Nogueira, and Diogo Rodrigues	
Rolling-Horizon Scheduling for Dynamic Market-Driven Operation of an Air Separation Plant	1958
Kieran McKenzie and Christopher L. E. Swartz	
Deep Kernel Learning with Kolmogorov–Arnold Networks for Bayesian Optimization	1967
Zhongtao Shang, Zhihong Yuan, Lifeng Zhang, and Yiyang Dai	
Machine Learning and Adaptive Sampling Powered Feasible Path Algorithm for Black-box Optimization	1974
Zixuan Zhang, Xiaowei Song, Jiaming Li, Yujiao Zeng, Yaling Nie, Min Zhu, Dongyun Lu, Yibo Zhang, Xin Xiao, and Jie Li	
Work and Heat Exchanger Networks as a General Energy-Integration Strategy for Chemical Processes	1986
José A. Caballero, Zinet Mekidiche-Martínez, and Juan A. Labarta	
Designing a Load-Flexible Renewable Ammonia Plant for Variable Green Hydrogen Supply	1992
Niklas Groll and Gürkan Sin	
A framework for dynamic rescheduling under disruptions and resource constraints	2001
David Robins, Farshid Babaei, Joan Cordiner, and Solomon F. Brown	
Optimization of Large-Scale Lycopene Production from Tomato Waste: A Comparative Study of Different Processing Technologies	2008
Nereyda V. Hernández-Camacho, Fernando I. Gómez-Castro, Mariano Martín, Ehecatl A. del Rio-Chanona, and Oscar D. Lara-Montaño	
Auxiliary flexibility in an integrated green steel plant participating in Day-ahead and Intra-day electricity markets	2015
Santeri Vaara and Iiro Harjunkoski	
Development of a process modeling library for the design and optimization of beverage production plants ...	2023
Valentin Becher, Christian Prommesberger, Ulrike Paap, Anna Afanasev, Anna Bechtold, and Jörg Zacharias	
Discrete multi-criteria optimisation of a modular heterogeneous electrolysis system	2029
Hannes Lange, Lukas Furtner, Michael Große, Isabell Viedt, and Leon Urbas	

Optimizing Flexible Operation of Grid-Connected Electrolyzers: Storage Capacity as the Key to Economic Viability	2036
Julian Pamperin, Hannes Lange, Michael Große, and Leon Urbas	
Comparative Techno-Economic Assessment of Hybrid-Green Ammonia Layouts for Available-to-Date Decarbonization of the Fertilizer Industry.....	2045
Andrea Isella and Davide Manca	
Optimizing Steam flux for Energy efficiency in Ammonia Recovery during Sodium carbonate production	2051
Ediane S. Alves, Mohamad A. Chahine, Denis Guillaume, and Julien Gornay	
Structural Constraints with the P-graph Framework: Application to an Ammonia Synthesis Process	2058
Darrick Hillaby, Andrés Piña Martínez, Jean-François Portha, and Laurent Falk	
High Performance Heat Pumps Using Tailored Refrigerants	2066
Finlay M. Sandham, Andrew Muumbo, Kenneth Mathew, Sarthak Sinha, and Smitha Gopinath	
Generative AI for the optimal design of seawater desalination processes	2074
Valentin ZARLENGA, Antonio ROCHA AZEVEDO, Alvaro MARTINEZ-TRIANA, and Thibaut NEVEUX	
Assessing the Impact of Solvent Recycling in Cooling Crystallization using Computer-Aided Molecular and Process Design	2082
Gaurav Seth, Saman Naseri Boroujeni, Shubhani Paliwal, Amparo Galindo, George Jackson, and Claire S. Adjiman	
Reinforcement Learning-driven Process Intensification Synthesis – Design and Optimization of Reaction/Separation Systems	2091
Dylan Nice, Daniel Wenck Ribeiro, Kristina Savitskaya, Rahul Bindlish, Efstratios N. Pistikopoulos, and Yuhe Tian	
A Graph Reinforcement Learning Framework for Batch Process Scheduling in State-Task Networks.....	2099
Syu-Ning Johnn, Victor-Alexandru Darvariu, and Vassilis M. Charitopoulos	
Two-stage stochastic programming optimization of natural gas pipeline network under cost and carbon emission reduction.....	2107
Huiyu Hao and Bohong Wang	
Optimization-based design of distillation processes with embedded pressure drop and HETP correlations....	2115
Sina Bertram, Jonas Schnurr, and Mirko Skiborowski	
Data-Driven Multi-Objective Optimization of Energy, Environmental, and Economic Performances in Manufacturing with Physics-Consistent Deep Learning.....	2123
Hyeonrok Choi, Jaewook Lee, Won Yang, and Seong-il Kim	
Joint Optimization of Feedstock Procurement and Production Planning in AD: A Deep Learning-Integrated Stochastic Programming Framework	2131
Ruosi Zhang and Michael Short	
A Method for Uniquely Determining Robust Operating Conditions in Simulated Moving Bed Chromatography	2140
Kensuke Suzuki, Tomoyuki Yajima, and Yoshiaki Kawajiri	
Design of Fluid Distribution Devices Using Topology Optimization	2145
Osamu Tonomura, Shunya Doi, Naohiro Akashi, and Ken-ichiro Sotowa	
An Extended Superstructure Formulation for Non-Isobaric Flowsheet Synthesis	2152
Harrison A. Fraser, Smitha Gopinath, Jan Sefcik, George Jackson, Amparo Galindo, and Claire S. Adjiman	
Superstructure Optimization of CCUS Value Chain: Case Study on Sohar Freezone in Oman	2161
Shaima Al-Salmani and Muhammad Abdul Qyyum	

Design Optimization of Shell-and-Tube Heat Exchangers Under Operational Uncertainty: A Comparative Study Across Three Paradigms	2170
Fernando Israel Gómez-Castro, Sergio Iván Martínez-Guido, Claudia Gutiérrez-Antonio, and Oscar Daniel Lara-Montaño	
Reactor network synthesis of enzymatic cascades using superstructure optimization	2176
Swastik Chandra, Leandros Paschalidis, Siv Kinau, and Mirko Skiborowski	
Designing Multi-Objective Optimization Models for Vaccine Supply Chains: Economic, Environmental, and Social Trade-offs in the COVID-19 Context	2183
Jonathan Jair Cuevas Lopez, Sofía De-León Almaraz, Alberto A. Aguilar Lasserre, and Catherine Azzaro-Pantel	
Multiperiod optimisation of a European CCS supply chain under capture-cost uncertainty	2191
José A. Álvarez-Menchero, Rubén Ruiz-Femenia, Raquel Salcedo-Díaz, and José A. Caballero	
Optimal Operation of an Alkaline Electrolyzer in an Industrial Setting Using Effective Linearization Techniques	2201
Jonaed Bin Mustafa Kamal, Loukas Kyriakidis, Saskia Bublitz, Bogdan Dorneanu, and Harvey Arellano-García	
Set-based Formulations for the State Task Network Scheduling Problem	2209
David A. Liñán, Georgia Stinchfield, Carl D. Laird, and Jan Kronqvist	
Ammonia as Fuel for Gas Turbines – The Impact of Heat Integrated Partial Decomposition	2218
Julian Straus, John C. Morud, and Elettra Vantaggiato	
Research on Dynamic Scheduling of Multi-line Polyolefin Production Based on Deep Reinforcement Learning	2226
Zhineng Tao, Tong Qiu, Zhenzhi Gong, Fenglian Dong, Zhi Wei, and Yunlong Guan	
Multi-Objective Optimisation of Pressure Swing Adsorption Systems via Symbolic Regression	2234
Carine Menezes REBELLO, Amilton Barbosa BOTELHO JUNIOR, Anderson Rapello DOS SANTOS, and Idelfonso B. R. NOGUEIRA	
GPU-Accelerated Nonlinear Multi-Period AC Optimal Power Flow for Large-Scale Power-Hydrogen Systems	2243
Geunseo Song, Dirk Lauinger, Sungho Shin, and Jonggeol Na	
Foundation Model-Guided Optimization of Chemical Reaction Spaces for Autonomous Experimentation	2252
Youhyun Kim and Jonggeol Na	
Techno-Economic Optimization of Electrified Airports as Collaborative Energy Hubs	2261
Mohammadreza Babaei, Stavros Vouros, Konstantinos Kyprianidis, and John D. Hedengren	
Particle Swarm Optimization for simultaneous design and optimization of heat pumps considering Mixed Integer problems	2272
Beatriz C. da Silva, Ana M. Ribeiro, Alírio E. Rodrigues, Alexandre F.P. Ferreira, Diogo Rodrigues, and Idelfonso B.R. Nogueira	
Techno-economic analysis of hydrogen refueling station with on-site production from a novel blue H₂ and N₂ production system	2280
Adrian R. Irhamna and George M. Bollas	
Distributed low-carbon hydrogen for freight corridors: siting hydrogen refueling station with onsite production on New England highways	2288
Adrian R. Irhamna, Burcu Beykal, and George M. Bollas	
Superstructure Modelling of Membrane Systems for the Optimization and Flexible Design of Post-combustion Carbon Capture Processes	2297

Multi-scenario Optimization of Groundwater-Sourced Water Production Networks With Daily Well Shutdown Requirements.....	2303
Pedro H. CALLIL-SOARES, René P. SCHNEIDER, and Galo A. CARRILLO LE ROUX	
Towards the Resilient Design of Power-to-Ammonia Systems via Linear Optimization Tools.....	2311
José M. Pires, João Fortunato, Henrique A. Matos, and Diogo A. C. Narciso	
Transfer Learning-Enhanced Deep Probabilistic Surrogates for Scalable Multi-Fidelity Bayesian Optimisation in Process Design	2320
Jaewook Lee, Ethan Errington, and Miao Guo	
Optimal Biogas Utilization Planning in a Pig Farm Under Sustainability Indicators	2327
Jaime David Ponce-Rocha, Martín Picón-Núñez, César Ramírez-Márquez, José María Ponce-Ortega, and Ricardo Morales-Rodríguez	
Process design for the recovery of valuable organic compounds from pyrolysis oil aqueous phase.....	2334
Matteo Gilardi, Filippo Bisotti, Stefan Schmidt, Rune Myrstad, Camilla Otterlei, Trung Trinh, and Bernd Wittgens	
Intensified liquid-liquid process design for critical metals extraction from e-waste.....	2340
Konstantinos Katsoulas, Arun Pankajakshan, Malik Olasinde, Cong Chao, Federico Galvanin, Panagiota Angeli, and Eric S. Fraga	
(article retracted)	2349
A novel decomposition-based approach to solve heterogeneous capacitated vehicle routing problems	2355
Vakil Vamsi Krishna, Mangesh Kapadi, Pankaj Verma, and Shamik Misra	
(article retracted)	2362
Simulation-Optimization vs. MILP Approaches for Real-Time Scheduling of Multiproduct Batch Plants.....	2370
Engelbert Pasieka and Sebastian Engell	
Design and Optimization of Supply Chain for Citrus Biorefineries: A Regional Approach for Waste Valorization in Brazil.....	2377
Marilia G. L. Cavenaghi, Larissa T. Bruschi, and Moises T. dos Santos	
Logistics Management of Agri-Industrial Waste for Energy Valorization in Uruguay	2386
Milena Lagarmilla, Ivan Guchin, Mauro Gambetta, Darío Huelmo, Adrián Ferrari, and Soledad Gutierrez	

Section 8: Process Control and Operation

Design and Control of Heat Pump Assisted Distillation Processes for Flexible E-methanol Production.....	2393
Lucas A.T. Poker, Marija Saric, Jan Wilco Dijkstra, Vladimir Dikic, and Anton A. Kiss	
Long-Cycle Operation for Residue Hydrotreating Processes with Bayesian Optimization	2400
Pengcheng Zhu, Han Wang, Gang Chen, Bo Chen, Fei Zhao, and Xi Chen	
Decentralized Causal Monitoring in High-Dimensional Systems: Revealing the Topological Drivers behind Fault Detection Performance	2406
Rodrigo Paredes and Marco S. Reis	
Control Structure Design of Novel Microwave-Catalyzed Process for Simultaneous Production of Ammonia and Ethylene	2418
Md Mizanur Rahman, Omar Almaraz, Snehittha Baddam, Jianli Hu, and Srinivas Palanki	
Towards Safety-Intelligent Cyber-Physical Systems: A Real-time Monitoring and Control Framework.....	2425

Zhane Ann Tizon, Yuanxing Liu, Sahithi Srijana Akundi, Austin Braniff, Beatriz Dantas, Yuhe Tian, Faisal I. Khan, and Efstratios N. Pistikopoulos

Extremum seeking control by perturb and observe applied to dividing wall column pilot 2433

Ivar J. Halvorsen, Bart M. A. Bergers, Giovanni Merlo, Leontine I.M. Aarnoudse, Mark A.M. Haring, and Sigurd Skogestad

Managing Renewable Energy Uncertainty in Green Hydrogen Production Systems 2441

Matteo Lea Casagrande, Andrea Isella, and Davide Manca

Forecasting Time-to-Cyclic Steady State in Periodic Bioprocesses via a Multi-Feature k-Nearest Neighbours Framework 2449

Yasser Algoufily, Foteini Michalopoulou, Maria M. Papathanasiou, and Mehmet Mercangöz

Enhancing Control in Chemical Processes using Reinforcement from Human Feedback 2457

Hilde Gerold, Dean Bradner, and Sergio Lucia

Open-Source Optimization Algorithm for the Simulated Moving Bed Process using CasADi 2466

João Nunes, Ana M. Ribeiro, Alexandre Ferreira, Diogo Rodrigues, and Alírio E. Rodrigues

Connecting the Dots: A Graph-based Approach for Unsupervised Learning and Adaptive Process Monitoring with LLM-assisted Fault Diagnosis 2473

Kyle Territo and Jose Romagnoli

A Hybrid Data-Driven Approach for the Optimization of an Industrial Alkylation Unit2481

Rastislav Fáber, Karol Lubušký, and Radoslav Paulen

Energy Management of a Renewable-Powered Alkaline Electrolyzer System: A Comparative Study of Nonlinear Optimization Methods 2488

Loukas Kyriakidis, Jonaed Bin Mustafa Kamal, Saskia Bublitz, Bogdan Dorneanu, and Harvey Arellano-Garcia

Real-Time Estimation and Optimal Control of Supersaturation in Sugar Crystallization using Model-based Soft Sensor 2497

Ananya Lohani, Adam Fedor, Július Kurucz, and Radoslav Paulen

Data Reconciliation for Inventory Monitoring in a Petrol Refinery 2505

Jakub Gaborčík, Karol Lubušký, and Radoslav Paulen

Advanced Process Control Structures for Energy-Efficient Downstream Processing in HMF Biorefineries..... 2511

Norbert B. Mihály, Miruna Prodan, Vasile M. Cristea, and Anton A. Kiss

CMLM: A Cascade of Machine Learning Models to detect and diagnose the performance of model predictive controllers2518

Elizabeth V. Melo, Argimiro R. Secchi, and Maurício B. de Souza Jr.

Utilization of Additional Equipment Information for Drift Diagnosis in Chemical Plants 2527

Linda Eydam, Julius Lorenz, and Leon Urbas

Reinforcement Learning Supervisory Control with Fuzzy-Logic Reward for Multistage Gas Compression 2534

José R. Torracca Neto, Sergio A. C. Giraldo, Mario C. M. Campos, Gustavo L. R. Caldas, Bruno D. O. Capron, and Argimiro R. Secchi

Relating Loss Geometry to Empirical Generalization in Recurrent Neural Net Surrogates: Three Tanks Case Study 2542

Ricardo M. Roxas II and Karl Ezra Pilario

Active-Constraint Regions and Power Distribution in Multi-Stack PEM Water Electrolysis Systems.....2551

Marius Fredriksen and Johannes Jäschke

Exploiting the line pack potential of gaseous CO₂ pipelines 2558

Archana Kumaraswamy and Johannes Jäschke

Causal Discovery for the Spatial Autoregressive Model: Application to Defect Analysis in the Plastic Injection Molding Process 2565

Ryosuke Tanaka and Koichi Fujiwara

Industrial batch process online fault detection using machine learning..... 2572

Oliver Pennington, Adam Wilson, Carolina Cruz, and Dongda Zhang

Enhancing plasma etching efficiency via physics-based modeling and machine learning 2578

Eneri Boniakou, Yao Xue, Tzannis Vasileiadis, Sotiris Mouchtouris, Katerina Oikonomou, Chloi Zormpa, Antonios Armaou, Vassilios Constantoudis, Evangelos Gogolides, and George Kokkoris

Identification and Self-optimization of Robust Nominal Operating Ranges Using Proximal Policy Optimization.....2587

Ashish Yewale and Brahim Benyahia

Hybrid Physics-Informed Neural Networks for Thermal Process Identification and Control..... 2594

Sahar Hemmati, Mohammadreza Babaei, and John Hedengren

Section 9: CAPE in Education, Knowledge Transfer and Entrepreneurship

Benchmarking generative AI on fermentation knowledge 2600

Fiammetta Caccavale, Ulrich Krühne, Krist V. Gernaey, and Carina L. Gargalo

Assessing Workflow Automation Platforms in Engineering Education: Towards an Ethical, Technical, and Pedagogical Framework..... 2607

Daniela Galatro, Stuart Grey, and Sourojeet Chakraborty

Artificial Intelligence (AI) Usage in an Undergraduate Chemical Engineering Course: Strengths, Pitfalls, and Future Insights.....2613

Sourojeet Chakraborty, Stuart Grey, and Daniela Galatro

LLM-Based Intelligent Data Extraction System for Industrial Equipment..... 2622

Zean Chen, Kaicheng Song, Lingyu Zhu, Anjan Kumar Tula, and Xi Chen

The Imperial College Integrated Design Project2631

Paul S. Fennell, Klaus Hellgardt, and Daniel R. Lewin

Generative AI in Process Design Instruction: A Survey of Students and Faculty 2638

Daniel R. Lewin, Thomas A. Adams II, Dominik Bongartz, Seyed Soheil Mansouri, and Edwin Zondervan

Understanding Student's Preferences for Computational Tools in Chemical Engineering Assessment 2646

Sakiru Badmos

Empirical survey among experts on the relevance of various criteria for optimizing modular electrolysis systems 2652

Hannes Lange, Lucien Beisswenger, Daniel Erdmann, Isabell Viedt, and Leon Urbas

Mapping "Digital Chemical Engineering" in the UK: A Sector-Level Audit of IChemE MEng Curricula 2658

E. Routoula, M. Mohammad Zadeh, M. Granollers Mesa, M. Malekshahian, D. Dikicioglu, M. Pollock, and M. Zandi

Enhancing Robotics and Automation Education Through the Development of Simulation Tool for Material Synthesis 2666

Hsuan Chang, Adedayo Ogunnoiki, and Solomon Gajere Bawa

A Techno-economic Analysis of Simulated Wind Farms 2674

Isaac N. James, Laura Edwards, and Dhurjati Chakrabarti

An Engineering Clinic-Based Approach to Teaching Process Design and Modeling: Bridging Theory and Practice 2680

Barnabas Gao, Thien An Pham, Amarelys Rios, Corbin Tinker, Saugat Bhandari, Robert Hesketh, C. Stewart Slater, and Kirti M. Yenkie

A pedagogical framework for sustainability learning : the case of Industrial Ecology 2689

Marianne Boix, Sydney Thomas, Lea van der Werf, and Ludovic Montastruc

Closing the Digital Gap: A Scaffolded Pathway for Developing Digitalisation Skills in Undergraduate Chemical Engineering Curricula..... 2696

E Routoula, J Bestenlehner, and M Zandi

INDEX

Author Index Index 1

Keyword IndexIndex 9

Introduction

Solomon Brown, Maria Papathanasiou, David Bogle, Joan Cordiner, Michael Fairweather (eds.)

The 36th European Symposium on Computer Aided Process Engineering (ESCAPE|36) was held in the UK from Sunday 21 June to Wednesday 24 June 2026 at the University of Sheffield. The organisation was led by members of the University's School of Chemical, Materials and Biological Engineering, in collaboration with the Institution of Chemical Engineers (IChemE) and the Grantham Centre for Sustainable Futures.

Since it began, ESCAPE has become a prestigious platform for the process systems engineering community to connect with experts, share innovative ideas, and explore latest advancements. Spread across four days, researchers, industry professionals, and students, will enjoy a wide range of presentations, posters, plenary speakers, workshops, panel discussions, networking opportunities, and social events.

In an era defined by climate challenges, resource constraints, and rapid technological advancement, the need for sustainable practices has never been more urgent or complex. The main theme of this year's conference, Resilient Sustainability through CAPE, reflects the shift toward integrating resilience through design and the critical role computer-aided process engineering has when developing innovative tools and adaptive, efficient systems that can withstand uncertainty while minimising environmental impact. This conference brings together leading minds to explore how advanced modelling, simulation, optimisation, and data-driven decision-making can drive sustainable transformation across sectors.

ESCAPE|36 received 687 abstract submissions, of which 654 were invited for a 5-to-8 page full paper or a 2-page short paper after a first round review. Upon rigorous re-review of all papers submitted, 331 conference papers have been published in full open access by PSE Press as a volume of the *Systems & Control Transactions* series. Another 162 contributions being made available as short papers separately.

The scientific contributions were organised into oral sessions, poster presentations, workshops and demonstrations, within nine thematic areas:

1. CAPE in Circular Economy
2. CAPE in Clean Energy Systems
3. CAPEing with Uncertain Futures
4. Pharmaceutical and Biotechnological Systems
5. Modelling and Simulation
6. Concepts, Methods and Tools
7. Process Design, Scheduling and Optimisation
8. Process Control and Operation
9. CAPE in Education, Knowledge Transfer and Entrepreneurship

We would like to extend our sincere thanks to all authors, reviewers, topic coordinators, plenary and keynote speakers, and members of the Scientific and Organizing Committees. We gratefully acknowledge the University of Sheffield and the IChemE for their support and express our heartfelt appreciation to our numerous sponsors. This edition marks the second volume with PSE Press as the official publisher of the ESCAPE proceedings (full papers volume) – continuing this important collaboration in promoting high-quality, open access dissemination of PSE research.

We hope this volume captures the scientific excellence, collaborative spirit, and forward-looking vision that defined ESCAPE|36 and continue to serve as a valuable reference for researchers and practitioners in the years ahead.

ESCAPE|36 - European Symposium on Computer Aided Process Engineering

Sheffield, UK. 21-24 June 2026

Peer Review Policy

TERMINOLOGY

- **Conference Paper:** This is a peer-reviewed research paper describing an **original** research contribution and published in the conference proceedings.

APPLICATION

- All conference papers are subject to peer review.

PUBLICATIONS

- All conference papers which have passed peer review and have been accepted by the conference chairs will be published in the conference proceedings.

PEER REVIEW PROCESS

Initial Screening

The conference chairs will screen the initial submissions (one-page abstracts) of contributed papers. At their option, chairs may choose to reject these submissions for any reason, but the primary reasons for rejection at this stage are (a) subject does not match conference themes and topics; (b) in appropriate, unprofessional, unethical, or dishonest material; (c) duplicate submissions; (d) abandoned submissions; (e) multiple submissions from same presenter; (f) obvious poor quality; (g) reasonable suspicion of machine-generated text; (h) need to limit acceptances because of conference space constraints. Chairs may also transfer papers between sessions at this stage.

Conference chairs will then invite authors of the one-page abstracts that have passed the initial screening to submit a conference paper for peer review.

Conference Paper Peer Review

Conference chairs act as editors. They will assign peer reviewers to assess the quality of the conference papers and manage the peer review process for each paper. Peer reviewers are generally selected from the International Scientific Committee who are scientists, engineers, or researchers with technical expertise in the conference topic. Peer reviewers must be considered technical experts in their field, hold a PhD, and have published peer reviewed scientific works previously. Each work must be reviewed by a minimum of two peer-reviewers.

A “single-blind” peer review system is used, in which the peer reviewers have access to the identities of the authors, but the authors are never given the identities of the peer reviewers. This is consistent with most journal peer-review procedures in our field.

Peer reviewers will be given a set of quality criteria that may include scientific and technical quality, quality of writing, originality and novelty, appropriateness for the conference topic and theme, interest to the community, and other factors of merit. Peer reviewers are expected to be rigorous and critical in their technical assessments and adhere to the highest standards in the field in order to ensure high quality. Peer reviewers are asked to comment on their assigned conference papers and issue a recommendation to the conference chairs based on this quality criteria. Reviewers may recommend one of the following:

- **Accept Paper.** No technical changes are necessary before publication. Only typographical, spelling, grammar, or other minor changes are necessary which do not require technical review.
- **Accept Paper with Minor Revisions.** Some minor technical issues need to be addressed either through technical changes to the manuscript or through rebuttal to reviewer comments. The reviewer does not believe the issues are significant enough to require additional technical review by the reviewers. The reviewer has provided enough commentary such that the editor can decide if the minor issues have been addressed in a future revision.
- **Reject Without Reconsideration.** The technical issues are so significant that it is unlikely that an acceptable

manuscript could be produced by the deadline; or, the manuscript is out of scope, inappropriate, or computer-generated.

Peer reviewers may be asked to provide numerical scores or rankings, as well as provide written comments intended for the chairs and/or the authors. Peer reviewers are encouraged to provide specific and constructive feedback that will aid the authors in improving the work and provide advice to the chairs.

The conference chairs are responsible for making the final decision on each paper and may require several rounds of author changes if necessary to meet quality standards. Conference chairs are not required to follow the recommendations of the peer reviewers in making these decisions. It is possible that conference chairs will choose to not accept some papers that still pass through rigorous technical peer review, especially when limited by available space or when papers do not sufficiently promote conference objectives. Conference chairs may also transfer papers between sessions as desired.

CONFLICTS OF INTEREST AND ETHICAL GUIDELINES

The chairs and peer reviewers must ensure they do not have a conflict of interest that may bias their decisions, such as ensuring that authors are at “arm’s length” and have no financial conflicts of interest. Peer reviewers and chairs must disclose if they have such a conflict of interest with a specific submission, and if so, a different chair and/or peer reviewer should be assigned to handle that submission.

To help determine conflicts of interest, and for all other ethical guidelines, we use the Systems and Control Transactions ethical guidelines described at: <https://psecommunity.org/contributor-guidelines>

International Scientific Committee

Antonis Kokossis	National Technical University of Athens
Daniel Lewin	Technion - Israel Institute of Technology
Dominik Bongartz	KU Leuven
Grégoire Léonard	University of Liège, Liège, Belgium
Gürkan Sin	Technical University of Denmark
Ludovic Montastruc	INP Toulouse
Miroslav Fikar	Slovak University of Technology in Bratislava
Seyed Soheil Mansouri	Technical University of Denmark
Solomon Brown	University of Sheffield
Vasileios Charitopoulos	University College London
Abderrazak Latifi	Université de Lorraine
Alessandro Di Pretoro	Laboratoire de Génie Chimique de Toulouse
Alexander Mitsos	RWTH Aachen University
Ana Barbosa-Povoa	Instituto Superior Técnico
Andrea Bernardi	Imperial College London
Andrea Galeazzi	Imperial College London
Andrzej Kraslawski	LUT University
Antoine Rouxhet	University of Liège
Antonio Del Rio	Imperial College London
Antonio Sánchez García	Universidad de Salamanca
Artur Schweidtmann	Delft University of Technology
Athanasios Papadopoulos	Centre for Research and Technology Hellas
Bogdan Dorneanu	Brandenburg University of Technology Cottbus-Senftenberg
Borja Hernández	Universidad Rey Juan Carlos
Brahim Benyahia	Loughborough University
Catinca Secuianu	Norwegian University of Science and Technology
Cristhian Molina Fernández	University of Liège
Daniel Alexander Florez Orrego	Ecole Polytechnique Fédérale de Lausanne
Daniel Cristiu	Imperial College London
David Bogle	University College London
Deenesh K Babi	Novo Nordisk
Dimitrios Gerogiorgis	University of Edinburgh
Eike Cramer	University College London
Eleni Routoula	University of Sheffield
Emilia Kondili	University of West Attica
Emmanouil Papadakis	Novo Nordisk
Eoin Syron	University College Dublin
Erdal Aydın	Koç University
Erik Resendiz Mora	University of Sheffield
Ezio Nicola D'addario	AIDIC Sezione Centro
Farshid Babaei	University of Sheffield
Fabrizio Bezzo	University of Padova
Fernando Martins	University of Porto
Ferrasse Jean-Henry	Aix Marseille University
Filip Logist	BASF Antwerpen NV
Filippo Bisotti	SINTEF Industry
Flavio Manenti	Politecnico di Milano
Florence Vermeire	KU Leuven
Francois Marechal	Ecole Polytechnique Fédérale de Lausanne
Gendebien Samuel	University of Liège
Grazia Leonzio	University of Cagliari
Henrique Matos	Instituto Superior Técnico

Hirokazu Sugiyama	The University of Tokyo
Iqbal Mujtaba	University of Bradford
Jan Verstraete	IFP Energies Nouvelles
Joan Cordiner	University of Sheffield
Johannes Jäschke	Norwegian University of Science and Technology
Laura Helleckes	Imperial College London
Lidija Čuček	University of Maribor, Maribor, Slovenia
Luigi Piero Di Bonito	University of Naples Federico II
Manuel Rodrigo	University of Castilla la Mancha
Marco Vaccari	University of Pisa
Maria Papathanasiou	Imperial College London
Maria-Ona Bertran	Novo Nordisk
Marianne Boix	Université de Toulouse
Mariano Martin	Universidad de Salamanca
Marija Tasic	University of Nis
Massimiliano M Villone	University of Naples Federico II
Mathew Wilkes	University of Sheffield
Matteo Gazzani	Utrecht University
Michael Fairweather	University of Leeds
Michael Georgiadis	Aristotle University of Thessaloniki
Mo Zandi	University of Sheffield
Monika Bakosova	Slovak University of Technology in Bratislava
Monika Dokl	University of Maribor, Maribor, Slovenia
Muhammad Salman	University of Liège
Mumin Enis Leblebici	KU Leuven
Niki Triantafyllou	Imperial College London
Olga Arsenyeva	University Paderborn
Paulina Quintanilla	University College London
Philippe Nimmegeers	University of Antwerp
Pullah Bhatnagar	Ecole Polytechnique Fédérale de Lausanne
Radoslav Paulen	Slovak University of Technology in Bratislava
Ranjith Chiplunkar	Imperial College London
Ronny Pini	Imperial College London
Sabla Alnouri	Qatar University
Satyajeet Bhonsale	KU Leuven
Sebastian Engell	TU Dortmund
Sergio Lucia	TU Dortmund University, Dortmund, Germany
Sigurd Skogestad	Norwegian University of Science and Technology
Simon Harvey	Chalmers University of Technology
Smitha Gopinath	University of Sheffield
Somnath Nandi	Savitribai Phule Pune University
Sönke Bröcker	Evonik Operations GmbH
Stavros Papadokonstantakis	Technische Universität Wien
Stefan Radl	TU Graz
Stratos Pistikopoulos	Texas A&M
Theodoros Damartzis	Aristotle University of Thessaloniki
Thomas Adams	Norwegian University of Science and Technology
Ulderico Di Caprio	KU Leuven
Vasile Mircea Cristea	Babes-Bolyai University
Vibhu Baibhav	Ecole Polytechnique Fédérale de Lausanne