MaCKiE 2025

3-5 September 2025, Çeşme, İzmir/TÜRKİYE

Technical Program

		WEDNESDAY - September 3rd		
9:00 – 13:30		**Registration** *Hotel Reception*		
13:30 – 14:15		**Opening remarks** **Room Okyanus** Guy B. Marin (MaCKiE Co-Founder) Abhishek Dutta (Conference Chair) Cem Çelebi (IZTECH Vice President) J. Antonio Torres (on behalf of Food MaCKiE organization committee)		
14.15 – 15:15		**Plenary** Stochasticity in Bioreaction Engineering: Opportunities and Challenges for Bioprocess Industries Duygu Dikicioğlu, *University College London, United Kingdom*		
15:15 – 15:40		**25 minutes break – coffee and snacks**		
		Expanding the fundamentals – I Room Gerence 1, Chair: Necip B. Üner		**Resolving complexity – I** Room Okyanus, Chair: Enis Leblebici
15:40 – 16:00	G055	A Reaction Extent-Based Approach to Kinetic Analysis of Reaction Networks - Glycerol Oxidation as a Case Study Akkihebbal K. Suresh, *IIT Madras-IIT Zanzibar*	G004	Multi-Objective Optimization of Electrified Shockwave Turboreactor for Enhanced Heat Transfer and Selectivity Rejish Lal Johnson, *Ghent University*
16:00 – 16:20	G014	Regulation of Micro-Environments by Multi-Metal Promoters: A Theoretical Study on CO_2 Activation over Iron Carbide Catalysts Nan Song, *ECUST*	G006	Artificial Neural Network-Based Modeling and Optimization of Nanofiltration Membranes for Lithium/Magnesium Separation Elif Güngörmüş, *IZTECH*
16:20 – 16:40	G018	Kinetics and Simulation of Polyethylene Liquefaction in Supercritical Water, Sphurti P. Kulkarni, *Ghent University*	G011	Cheminformatics-Driven Automated Kinetic Modeling with Genesys-Py, Lowie Tomme, *Ghent University*
16:40 – 17:00		**20 minutes Stretch-your-legs Break**		
17:00 – 17:20	G032	Optimization of Catalyst Deactivation Based on Mechanistic Analysis: Alkane Dehydrogenation as an Example Zoë J.G. Gromotka, *TU Delft*	G009	Consistency-Regularized Dual-Stage Semi-Supervised Learning for Prediction of Attributes in Chemical Processes with Incomplete Datasets Xiaochen Liu, *ECUST*
17:20 – 17:40	G054	Kinetic Modelling of Acetylene Hydrogenation in Ethylene Production Process Gizem Pınar, *Ege University*	G016	Optimal Microgrid Planning: Integrating Mixed-Integer Programming and Monte Carlo Simulations for Reliable and Cost-Effective Energy Systems Mohammadreza Jahanbakhsh, *Koç University*
17:40 – 18:00	G027	Deactivation of Olivine-derived Catalyst in Non-Oxidative Methane Coupling Ali Cheshmeh Roshan, *Ghent University*	G074	Python-Based Semi-Automated Analysis of Turbidimetric Growth Delay Data to Study Antimicrobial Activity Vahit Köroğlu & Çağatay Gence*, *ITU*
18:00 – 18:20	G044	Steam Cracking Beyond the Plug Flow Assumption Ismaël Amghizar, *AVGI BV*	G092	Advanced Power Law Modeling of Bio-Based Drying Kinetics Robson Pessoa, *NTNU*
18:30 – 20:00		**Welcome reception and cocktail**		

		THURSDAY - September 4th		
8:30 – 9:00		**Keynote 1:** Nanoconfinement Effects on Diffusion and Reaction in Porous Materials, Heterogeneity, and What We Could Learn from Nature for Applications Marc-Olivier Coppens - *University College London, United Kingdom*		
		Expanding the fundamentals – II Room Gerence 1, Chair: Gregory S. Yablonsky	**Resolving complexity – II** Room Okyanus, Chair: Zhongmei Li	
9:10 – 9:30	G013	Kinetic Analysis in Reaction Networks: Elucidation of Reaction Mechanisms in Asymmetric Autocatalysis Oliver Trapp, *LMU Munich*	G089	AI-Enhanced Modeling of Flavor Release and Sensory Dynamics in Complex (Bio)Chemical Systems Idelfonso Nogueira, *NTNU*
9:30 – 9:50	G031	Entropy Production Extrema for Systems Constrained to Operature Far from Local Equilibrium (COFFE) Elijah Thimsen, *Washington University in St. Louis*	G033	Learning to Optimize: Application to Two-Stage Stochastic Pooling Problem Seyyid Eren Çamurcu, *Koç University*
9:50 – 10:10	G010	A Critical Evaluation of the Critical Lines of Water-Hydrocarbon Systems Gust Popelier, *Ghent University*	G073	Interpretable Machine Learning Models for Quantitative Structure–Property Relationships in Aviation Fuels Xiaomeng Zhao, *Ghent University*
10:10 – 10:30	G057	Conservatively Perturbed Equilibrium and Perturbation (Linear Case, Gibbs Free Energy Analysis) Jonah M. Sachs, *Washington University in St. Louis*	G034	Advanced Digital Solutions Through Operational Excellence Fatih Alperen Güler, *SOCAR Türkiye R&D*
10:30 – 11:00		**30 minutes break – coffee and snacks**		
11:00 – 11:30		**Keynote 2:** Physics-Informed Transfer Learning and Machine Learning based Optimization in Chemical Engineering Erdal Aydın, *Koç University, Türkiye*		
11:40 – 12:00	G076	Quantifying Dye-Sensitized Photocatalysis: A Kinetic Study with Oxygen-Deficient ZnO Philippe Heynderickx, *Ghent University Glob. Camp.*	G090	Hybrid Modelling and Its Automation: A Paradigm Shift in Chemical Engineering Enis Leblebici, *KU Leuven*
12:00 – 12:20	G071	An Absolutely-Calibrated Integrating Cylinder for Studying Photochemical Reactions AbdelAziz Hamza, *METU*	G082	Mathematical Modelling and Multi-Parameter Optimization of Phosphate Removal from Water Using Polymer Enhanced Ultrafiltration Yaşar Kemal Recepoğlu, *IZTECH*
12:20 – 12:40	G091	Kinetics-Informed Neural Networks for Post-Equilibrium Dynamics in Thermodynamically Constrained Systems, Abhishek Dutta, *IZTECH*	G067	Condition Recognition Method for Organosilicon Monomer Synthesis Process Based on Autoencoder and Nonlinear Clustering Jionghao Lou, *ECUST*
12:40 – 14:00		**Lunch break (complementary – Altın Yunus)**		
14:00 – 14:30		**Keynote 3:** Top-Down and Bottom-Up Multiscale Methodology for Modeling an Industrial-Scale Catalytic Reactor Carlos Omar Castillo-Araiza - *Metropolitan Autonomous University-Iztapalapa, Mexico*		
		Application to New Processes – I Room Gerence 1, Chair: Subramaniam Pushpavanam	**Resolving complexity – III** Room Okyanus, Chair: Guy B. Marin	
14:40 – 15:00	G059	A Computational Model to Analyze the Impact of Endothelial Dysfunction on H_2O_2 Biotransport Saptarshi Kar, *AUM Kuwait*	G012	Multi-scale Modeling of Calcium-Looping in Super-Dry Reforming Robin Vercauteren, *Ghent University*
15:00 – 15:20	G048	Modelling of Microfluid Siphons for High-Performance Point of Care Diagnostics and Near-the-source DNA Purification, Nuno M. Reis, *University of Bath*	G019	Multi-Stage Gas-Liquid Vortex Reactor with a Cyclone for Process Intensification: CFD-Based Design For Mass Transfer and Separation Siyuan Chen, *Ghent University*
15:20 – 15:40	G005	Particle-Scale Modeling of Joule Heating in Electrified Fluidized Beds Hamed Hoorijani, *Ghent University*	G093	Core-Annular Flow for Bioprocess Pipelines: Reducing Pressure Drop with Aqueous Film Lubrication Patrick Lima, *NTNU*
15:45 – 16:15		MaCKiE 2025 Welcome - Yusuf Baran, Rector of Izmir Institute of Technology Coffee and snacks will be available		
16:20 – 16:40	G069	Assessing Stability and Hydrogen Yield of Carbon Catalysts for Methane Decomposition Spyridon Fragkiskatos, *Ghent University*	G035	Predicting Lipid Nanoparticles Size Distribution Using a CFD-PBM Approach Fernando P. Bernardo, *University of Coimbra*
16:40 – 17:00	G075	Characterization and Operation of a Gliding Arc Plasma Reactor for Methane Pyrolysis Hüseyin Öztürk, *METU*	G046	Transport Enhancement of Accessible Porous Carbon in PEMFCS: A Multiscale Modelling Approach Yang Daoming, *ECUST*
17:00 – 17:20	G053	Modeling and Experimental Study of an Integrated Post-Plasma Catalyst Victor Rosa, *Ghent University*	G037	Population Balance Model (PBM) Including Nucleation and Size-Concentration Dependent Growth for Crystallization Process Özkan Avit, *NKU Tekirdağ*
17:20 – 17:40	G056	Hydroconversion of Vegetable- and Lignin-based feeds: Modeling the Impact of Co-Processing Arij Ben Hassine, *Instituto Superior Técnico*	G039	Two to Jive: Accelerating Numerical Reactive Flows in Turboreactors Mike Bonheure, *Ghent University*
17:45 – 18:45		**Joint Roundtable Conversation** Navigating the Crisis of Scientific Publishing Ethics: What Can Authors Do Now? Marc-Olivier Coppens, *UCL*; Ferruh Erdoğdu, *Ankara University*; Necip B. Üner, *METU*; J. Antonio Torres, *Tecnologico de Monterrey*		
17:40 – 19:30		**Poster session** Conference Hallway		

		**FRIDAY - September 5th**
8:30 – 9:00		**Keynote 4:** Multiscale Modeling of Zeolite Catalytic Process: From Crystal to Reactor Xinggui Zhou - *East China University of Science and Technology (ECUST), China*
		**Application to New Processes – II** Room Gerence 1, Chair: Fernando P. Bernardo		**Resolving Complexity – IV** Room Okyanus, Chair: Idelfonso Nogeira
9:10 – 9:30	G007	A Reaction-Advection-Diffusion Model to Describe Non-Uniformities in Colorimetric Sending Using µPADs S. Pushpavanam, *IIT Madras*	G058	Low-Order Modeling of a Shock Wave Turboreactor for Steam Cracking Diego Castellanos, *Ghent University*
9:30 – 9:50	G066	Green Synthesis of Ru/CeO2 nanoparticles FOR dehydrogenation of Ethylenediamine Bisborane S. Türk, *Ankara University*	G065	Robust Few-Shot Time Series Modeling for Silicone Monomer Synthesis via Task-Aware Temporal Fusion Zhongmei Li, *ECUST*
9:50 – 10:10	G068	Application of Symmetry and Topology for Engineering New Carbon Materials Alexey V. Ignatchenko, *St. John Fisher University*	G087	Accelerating the Moment Inversion Procedure in Quadrature-Based Population Balance methods Meltem Turan, *Simuligence*
10:10 – 10:30	G025	Exploiting a Mass Transfer Paradox for Optimal Scale-up of a Pharmaceutical Debenzylation Reaction Wout Callewaert, *Ghent University*	G078	Modeling Polyethylene Pyrolysis: A Comparison Between Kinetic Monte-Carlo and Method of Moments *(WITHDRAWN)* Laura Pires Costa, *Ghent University*
10:30 – 11:00		**30 minutes break – coffee and snacks**
11:00 – 11:30		**Keynote 5:** On the Interplay of Spatio-Temporal Gradients in Catalytic Kinetics Evgeniy Redekop - *University of Oslo, Norway*
		**Career Development Tips & Talks**
11:40 – 12:00	E001		Guiding Energy – Supporting Great Minds to Flourish Christoph Sprung, *Active-Sites Consulting*
12:00 – 12:20	E002		Inherent Trademarks of an Academic Career Mikhail Kurushkin, *ITMO University*
12:20 – 12:40		Q&A and Discussion
12:40 – 14:00		**Lunch break**
14:00 – 14:30		**Keynote 6:** Synergistic Modeling of Multiphase Reactors: Blending CFD, Machine Learning and Data Shantanu Roy - *Indian Institute of Technology Delhi-Abu Dhabi, UAE*
		**Expanding the fundamentals – III** Room Gerence 1, Chair: Saptarshi Kar		**Resolving Complexity – V** Room Okyanus, Chair: Nuno Reis
14:40 – 15:00	G020	Catalytic Pyrolysis of LDPE using Gallium Doped and Structural Modified Zeolite Qing He, *Ghent University*	G038	Holistic Design and Assessment of e-fuels Manufacturing: The Case of e-Methanol and e-Ammonia Fabio Cameli, *National Technical University of Athens*
15:00 – 15:20	G022	Modeling of Momentum Transfer at Complex Spatiotemporal Scales in Siemens Reactor Fanzheng Meng, *ECUST*	G029	Stochastic Optimization of Water-Energy Networks with Renewable Energy Integration Kaan Altaş, *Koç University*
15:20 – 15:40	G002	Development of a Rational Kinetic Model for the Steady-State Conversion of Dimethyl Ether over ZSM-5 Catalysts Toyin Omojola, *University of Bath*	G028	Cradle-to-Gate Life Cycle Assessment of Light Olefin Production Using Steel Mill Off-Gases for Feedstock Oleksii Mynko, *Ghent University*
15:40 – 16:00		**20 minutes break – coffee and snacks**
16:00 – 16:20	G072	Solvent-Mediated Dehydrogenation of Ethylenediamine Bisborane using Pd/RGO Catalysts: A Comparative Study of Hydrolysis and Ethanolysis Bensu Naz Örs, *Ankara University*	G051	Pykinemod: A Software Tool for Automated Modeling of Reaction Systems from Data Tirthankar Sengupta, *IIT Madras*
16:20 – 16:40	G017	Pilot-Scale Vortex Reactor for Efficient Thermal Pyrolysis of Polystyrene and Polyethylene Rohit Kumar, *Ghent University*	G085	A Feature Selection Methodology for Scarce Data Scenarios Flora Esposito, *KU Leuven*
16:40 – 17:00	G023	Methoxy Intermediates: Key to Xylene Formation in Benzene-Ethylene Alkylation Jundi Wong, *ECUST*	G086	Biologically Informed Artificial Intelligence Models for Predicting Human Sensory Perception of Scents and Flavors Luana P. Queiroz, *University of Porto*
17:00 – 17:20	G003	Mathematical Modeling and Simulation of Steam Cracking of Plastic-Waste Pyrolysis Oils: Overcoming Kinetic and Computational Challenges Tamás Buzogány, *Ghent University*	G094	Scents of AI: Utilising Graph Neural Networks and Optimisation to Reproduce Aromas Bruno Rodrigues, *NTNU*
17:30 – 18:00		**Pre-Epilogue** The MaCKiE Workshop - From Foundational Theory to the Future of Sustainable Processes Kevin Van Geem, *Ghent University*
18:00 – 18:45		**Epilogue** Time: The Main Mystery of Chemical Kinetics Gregory S. Yablonsky, *Washington University in St Louis, USA*
18:45 – 20:00		**Break**
20:00 – 23:00		**Gala Dinner, Award ceremony &** **Birthday Celebration of Prof. Gregory S. Yablonsky**

Poster Session	Thursday - September 4th
Conference Hallway	

G021	A Diffusion Approach to Kinetic Model Discrimination in Heterogeneous Catalysis Oleksii Zhokh, *L.V. Pisarzhevskii Institute of Physical Chemistry of National Academy of Sciences of Ukraine*
G042	Coupled and De-coupled Active Sites in Catalytic Reactions Christoph Sprung, *Active-sites Consulting*
G047	Use of Spectroscopy, Machine Learning and Chemical Speciation Models to Determine Chromium Concentration in Aqueous Solutions Divyang Deep Tiwari, *IIT Madras*
G060	Uncertainties in Net Zero Roadmap Using Monte Carlo Technique Miray Kaya & Srijita Bhattacharyya, *Izmir Institute of Technology & Jadavpur University*
G061	Physics-Informed Neural Network (PINN) for a Particulate Aggregation-Breakage System Sk. Aftab Hosen, *Jadavpur University*
G062	A Physics-Informed Neural Network (PINN) Approach to Over-Equilibrium Dynamics in Conservatively Perturbed Equilibrium Systems Bitan Mukherjee, *Jadavpur University*
G063	A Kinetic Monte Carlo Simulation on Fischer-Tropsch Synthesis to Model the Effect of Hydrogen Dynamics on Product Selectivity Merve Ceren Uyhan, *METU*
G077	Kinetic Modeling of Malondialdehyde Reactivity: Is This a True Lipid Oxidation Marker? Philippe Heynderickx, *Ghent University Global Campus*
G080	Particle-Resolved Simulations for the Catalytic Dehydrogenation of Ethane to Produce Ethylene Carlos O. Castillo-Araiza, *Universidad Autónoma Metropolitana-Iztapalapa*
G081	Kinetics of Carboxylic Acid Enolization on Metal Oxides in Vapor Phase Alexey V. Ignatchenko, *St. John Fisher University*
G083	Surrogate Superstructure Optimization Based on Machine Learning and Mixed Integer Programming Fatih Alperen Güler, *SOCAR Türkiye R&D*
G088	Optimal Operation Strategy for Koç University Campus Energy System: Enhancing Energy Efficiency Sunoy Sanyal, *Koç University*