Program

Polymer Reaction Engineering XII

June 1 – 6, 2025
Clearwater Beach, Florida

Conference Co-Chairs

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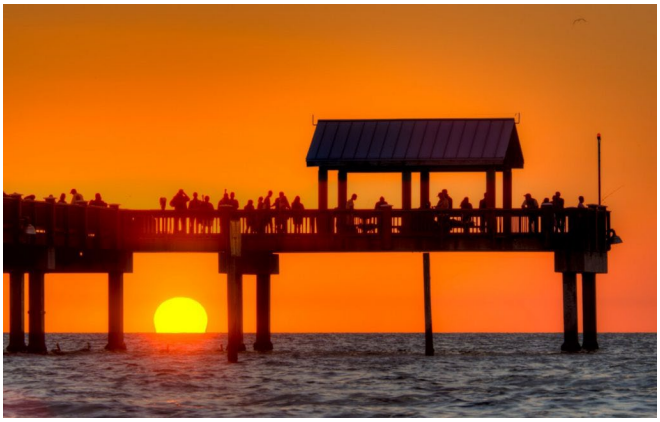
The Dow Chemical Company

Piet Iedema
University of Amsterdam

Mike Grady
Axalta Coating Systems



ECI Engineering Conferences International

Engineering Conferences International
369 Lexington Ave., Suite 389 - New York, NY 10017, USA
Phone: 1 - 212 - 514 - 6760
www.engconfintl.org – info@engconfintl.org

Clearwater Beach Marriott Resort on Sand Key

1201 Gulf Boulevard

Clearwater Beach, Florida, USA, 33767

Toll Free: +1-800-228-9290

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Sunday June 1, 2025

17:30 – 18:30	Conference check-in (Sand Key Ballroom Foyer)
18:30 – 19:00	Welcome reception (Veranda)
19:00 – 20:30	Dinner (Veranda)

NOTES

- *Technical sessions will be in the Sand Key Ballroom.*
- *Poster sessions will be in the Longboat Key Room.*
- *Breakfasts will be in the Siesta Key.*
- *Lunches will be in the Watercolour Restaurant.*
- *Dinner locations are noted in the program.*
- *Audio, still photo and video recording by any device (e.g., cameras, cell phones, laptops, watches) is **strictly prohibited** during the technical sessions, unless the author and ECI have granted prior permission.*
- *Speakers – Please have your presentation loaded onto the conference computer prior to the session start (preferably the day before).*
- *Speakers – Please leave at least 5 **minutes** for questions.*
- *Please do not smoke at any conference functions.*
- *Turn your cellular telephones to vibrate or off during technical sessions.*
- *After the conference, ECI will send an updated participant list to all participants. Please check your listing now and if it needs updating, you may correct it at any time by logging into your ECI account.*

Monday, June 2, 2025

07:30 – 08:30	Breakfast
08:30 – 08:45	Conference Welcome – Conference Liaison and Chairs
	Session 1: Advances in PRE
08:45 – 09:30	**Keynote: Design of New Ethylene Based Terpolymer: Structure Property Relationships** Hadi Mohammadi, Braskem, USA
09:30 – 10:00	**Model-Based Analysis And Design For Mechanical And Chemical Recycling** (Remote Presentation) Francisco Arraez, Polinivo, Belgium
10:00 – 10:45	Coffee Break and Networking
	Session 2: Model development, simulation and optimization I
10:45 – 11:30	**Keynote: Experimental and modelling approach to triboelectric charging of rough polyolefin particles** Juraj Kosek, University of Chemistry and Technology Prague, Czech Republic
11:30 – 12:00	**Toward faster kinetic Monte Carlo solvers to enhance polymer reaction engineering simulations** Freddy L, Figueira, Ghent University, Belgium
12:00 – 12:30	**Diffusion in Semi-Crystalline Polyolefins: Experiments and Models** Jakub Klimošek, University of Chemistry and Technology Prague, Czech Republic
12:30 – 14:00	Lunch
	Session 3: Data Science in PRE
14:00 – 14:45	**Keynote: Application of machine learning methods for reverse engineering of polymers** Marco Drache, TU Clausthal, Institute of Technical Chemistry, Germany
14:45 – 15:15	**Machine learning algorithms for improving semi-batch solution radical copolymerization recipes using a comprehensive stochastic model** (Remote Presentation) Amin Nasresfahani, Axalta, Canada
15:15 – 15:45	**Automated digital design of homogeneous polymerization catalysts** Pavel Dub, Schrödinger, Inc., USA
15:45 – 17:00	Coffee Break
17:00 – 18:00	Flash Poster Presentations
18:00 – 19:00	Social Hour / Networking (Longboat Key)
19:00 – 20:30	Dinner (Siesta Key)

Tuesday, June 3, 2025

07:30 – 08:30	Breakfast
	Session 4: Kinetics, thermo and microstructure
08:30 – 09:15	**Keynote: Effect of Solvent Polarity on Radical Copolymerization Kinetics of Functional Acrylate/methacrylates** Robin A. Hutchinson, Queen's University, Canada
09:15 – 09:45	**Opening Pandora's Box to Reveal the Key Role of the Aqueous Phase in Emulsion Polymerization with Allyl Methacrylate as a co-Monomer Crosslinker** John Tsavalas, University of New Hampshire, USA
09:45 – 10:15	**A heterogeneous kinetic Monte Carlo model of maleic anhydride grafting onto polypropylene** Tomás Romero Pietrafesa, Planta Piloto de Ingeniería Química (PLAPIQUI), Universidad Nacional del Sur-CONICET, Argentina
10:15 – 10:45	Coffee Break
	Session 5: Process Developments
10:45 – 11:30	**Keynote: Acetoacetoxy ethyl methacrylate (AAEMA) hydrolysis rate kinetics and subsequent hazards in adiabatic scenarios** Jonathan Antonucci, BASF, USA
11:30 – 12:00	**The Synthesis of Acrylate-Based Macromonomers and Structured Copolymers by High-Temperature Semi-Batch Radical Polymerization** Elizabeth Bygott, Queen's University, Canada
12:00 – 12:30	**Application of a novel rapid-heating reactor system for kinetic studies of catalytic pyrolysis of PE** Abdulrahman Alzailaie, SABIC, Saudi Arabia
12:30 – 14:00	Lunch
	Session 6: New processes for circular economy and recycling of polymers II
14:00 – 14:45	**Keynote: Understanding poly(ethylene terephthalate) deconstruction and structure-property effects in glycolysis for recycling** Gorugantu Sribala, University of Houston, USA
14:45 – 15:15	**Modeling the Thermal Degradation of Vinyl-Alcohol Containing Polymers** Alexander Best, Northwestern University, USA
15:15 – 15:45	**Hybrid Deterministic and Monte Carlo Modeling of Controlled Degradation of Polypropylene** Jakob Straznicky, Queen's University, Canada

Tuesday, June 3, 2025 (continued)

15:45 – 16:15	Coffee Break
16:15 – 18:00	Networking / Free time
18:00 – 19:00	**Poster Session** and Social Hour (Longboat Key)
19:00 – 20:30	Dinner (Siesta Key)

Wednesday, June 4, 2025

07:30 – 08:30	Breakfast
	Session 7: Structure-property relationships and multi-scale modeling
08:30 – 09:15	**Industry disruption through innovation** (Remote Presentation) Rajen Patel, Dow Chemical, USA
09:15 – 09:45	**Cyclization in Random Graph modeling of acrylate polymerization** Piet Iedema, Universiteit van Amsterdam, the Netherlands
09:45 – 10:15	**A unified and versatile kMC framework for polymer networks modeling** Alessandro D. Trigilio, Ghent University, Belgium
10:15 – 10:45	Coffee Break
	Session 8: Model development, simulation and optimization II
10:45 – 11:30	**Keynote: Selected topics from daily-life modeling practice** Michael Wulkow, CiT GmbH & Co. KG, Germany
11:30 – 12:00	**Designing AA-co-HPEG superplasticizers with tailored microstructure using a kinetic modelling approach** Kevin Palma, POLYMAT-University of the Basque Country, Spain
12:00 – 12:30	**Vinyl Acetate Polymerization over a Broad Temperature and Pressure Range – Experiments and Modeling** Kristina Zentel, TU Darmstadt, Germany
12:30 – 14:00	**Lunch**
	Free afternoon / Dinner on your own

Thursday, June 5, 2025

07:30 – 08:30	Breakfast
	Session 9: New monomers, comonomers and chemistries
08:30 – 09:15	**Keynote: Reaction Principles for in-Situ Functionalization of Ion Chromatography Columns** Bastian Brand, ZHAW, Switzerland
09:15 – 09:45	**Ethylene/1-Hexene Copolymerization Kinetics and Microstructure of Copolymers Made with a Supported Metallocene Catalyst** Saeid Mehdiabadi, Formosa Plastics USA
09:45 – 10:15	**Mathematical Modeling of 1,6-Hexanediol Diacrylate Photopolymerization with Spatial Gradients and Film Shrinkage** Kim B. McAuley, Queen's University, Canada
10:15 – 10:45	Coffee Break
	Session 10: Structure-property relationships
10:45 – 11:30	**Keynote: Properties to process in silico, using PolyFTS as a tool for driving process conditions in polymer synthesis** Marc Charendoff, Verdant Solutions, USA
11:30 – 12:00	**Engineering Dynamic Non-Covalent Interactions for High-Performance Adhesives** Qi Zhang, The Chinese University of Hong Kong, Shenzhen, China
12:00 – 12:30	**Fracture-resistant stretchable materials** He Zhu, The Chinese University of Hong Kong, Shenzhen, China
12:30 – 14:00	**Lunch**
14:00 – 14:45	**Keynote: Oxygen Threshold in Free Radical and RAFT Polymerization with Potential for Molecular Weight Control** Wayne Reed, Tulane University, USA
15:00 – 18:00	**Workshop: Using Predici for Parameter Estimation** Facilitator: Michael Wulkow, CiT GmbH & Co. KG, Germany
18:15 – 19:15	Reception (Sand Key Ballroom Foyer)
19:15 – 21:00	Conference banquet (Siesta Key)

Friday, June 6, 2025

07:30 – 08:30	Breakfast
08:30 – 09:30	PRE Working Team Meeting
	Departures

Poster Presentations

1. **Upcycling polyolefins via oxidation: mechanistic modeling of decane oxidation as a model compound**
   Tung Nguyen, Northwestern University, USA

2. **Modeling n-Butyl Acrylate Polymerization using Complementary Modeling Techniques**
   Kristina Zentel, TU Darmstadt, Germany

3. **Design and Evaluation of Polymers for Gas Sensing Applications**
   Bhoomi Mavani, University of Waterloo, Canada

4. **Multiscale kinetic Monte Carlo simulation of styrene / butyl methacrylate emulsion polymerization**
   Marco Drache, Clausthal University of Technology, Germany

5. **Modeling Molecular Weight Distributions by Coupling Cfd and Monte-carlo Simulations in the High-pressure Polymerization of Ethene**
   Emil Schwarz, TU Darmstadt, Germany

6. **Zone-Specific Effects on LDPE Production in a High-Pressure Multizone Autoclave**
   Christoph Weigel, TU Darmstadt, Germany

7. **Application of a Reactor Cascade Model for the Investigation of the Oxygen Kinetics on the High-Pressure Polymerization of Ethene**
   Joshua Stahl, TU Darmstadt, Germany

8. **Modeling assisted mini-plant tool for kinetic evaluations of catalytic solution polymerizations**
   Phillip Weigmann, TU Darmstadt, Germany

9. **Ethylene/1-hexene copolymerization kinetics and microstructure of copolymers made with homogeneous single-site metallocene catalysts**
   Juraj Kosek, University of Chemistry and Technology Prague, Czech Republic

10. **Morphology of heterophase polymers: Relation to thermodynamics and properties**
    Juraj Kosek, University of Chemistry and Technology Prague, Czech Republic

11. **Understanding Recycling of Plastics Waste by Solvent-Based Methods and COSMO-SAC Modeling**
    Jakub Klimošek, University of Chemistry and Technology Prague, Czech Republic

12. **Investigation into radical copolymerizations of itaconates with acrylates**
    Marco Drache, TU Clausthal, Germany

13. **Optimizing Redox Ratios and Biocide Stability in Emulsion Polymerization**
    Maggie White, BASF, USA

14. **TBD**
    Yan Jiang, SABIC