

***Program***

***Polymer Reaction Engineering XII***

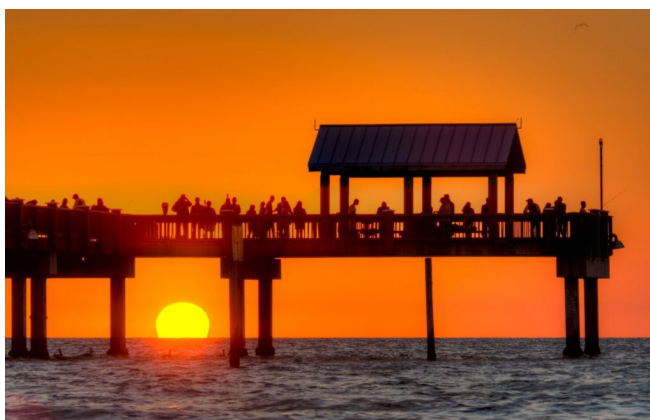
**June 1 – 6, 2025  
Clearwater Beach, Florida**

**Conference Co-Chairs**

**Ivan Konstantinov**  
The Dow Chemical Company

**Piet Iedema**  
University of Amsterdam

**Mike Grady**  
Axalta Coating Systems



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## Sunday June 1, 2025

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

## NOTES

- *Technical sessions will be in the Sand Key Ballroom Redington and Belleair sections.*
- *Poster sessions will be in the Longboat Key Room.*
- *Breakfasts will be in the Sand Key Ballroom Medeira and Indian Shores sections.*
- *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**  
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 (Sand Key Ballroom)

## **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	<b>Poster Session</b> and Social Hour ( <b>Longboat Key</b> )
19:00 – 20:30	Dinner ( <b>Sand Key Ballroom</b> )

**Wednesday, June 4, 2025**

07:30 – 08:30 Breakfast

**Session 7: Structure-property relationships and multi-scale modeling**

08:30 – 09:15 TBA

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 (**Sand Key Ballroom**)

**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