Program

Polymer Reaction Engineering X (PRE 10)
An ECI Conference Series

May 20 – May 25, 2018
Paradisus Punta Cana Resort, Punta Cana, Dominican Republic

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University of New Hampshire, USA

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Previous conferences in this series:

Polymer Reaction Engineering
March 10-15, 1991
Santa Barbara, California
Conference Chairs:
Charles Cozewith, Exxon Chemical, USA
Charles Barren, Clemson University, USA

Polymer Reaction Engineering II
February 13-18, 1994
Palm Coast, Florida
Conference Chairs:
Eugene P. Dougherty, Rohm & Haas, USA
Joseph Schork, Georgia Institute of Technology, USA

Polymer Reaction Engineering III
March 16-21, 1997
Palm Coast, Florida
Conference Chairs:
Kyu Yung Choi, University of Maryland, USA
Dr. Michael E. Muhle, Exxon Chemical, USA
Michael Cunningham, Xerox, USA

Polymer Reaction Engineering IV
March 19-24, 2000
Palm Coast, Florida
Conference Chairs:
Michael Cunningham, Queens University, Canada
K.W. Leffew, DuPont Central R&D, USA
K.B. McAuley, Queens University, Canada

Polymer Reaction Engineering V
May 18-23, 2003
Quebec City, Canada
Conference Chairs:
Joao B.P. Soares, University of Waterloo, Canada
Rafael Galvan, Johnson Polymer, UK
Robin A. Hutchinson, Queen's University, Canada

Polymer Reaction Engineering VI
May 21-26, 2006
Halifax, Nova Scotia, Canada
Conference Chairs:
Robin A. Hutchinson, Queen's University, Canada
Michael Muhle, ExxonMobil Chemical Co., USA
Alexander Penlidis, University of Waterloo, Canada
Previous conferences in this series:

**Polymer Reaction Engineering VII**
May 3-8, 2009  
Niagara Falls, Ontario, Canada  
Conference Chairs:  
Alexander Penlidis, University of Waterloo, Canada  
John R. Richards, DuPont, USA  
Marc A. Dube, University of Ottawa, Canada

**Polymer Reaction Engineering VIII**
May 6-11, 2012  
Cancun, Mexico  
Conference Chairs:  
Marc A. Dube, University of Ottawa, Canada  
Marco Villalobos, Cabot Corp., USA  
Eduardo Vivaldo-Lima, UNAM, Mexico

**Polymer Reaction Engineering IX**
May 10-15, 2015  
Cancun, Mexico  
Conference Chairs:  
Eduardo Vivaldo-Lima, UNAM, Mexico  
Jon Debling, BASF, USA  
Fernando Zaldo-Garcia, COMEX, Mexico  
John Tsavalas, University of New Hampshire, USA
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Macromolecular
Reaction
Engineering

سابك

University of New Hampshire
**Sunday, May 20, 2018**

16:00 – 18:00    Conference check-in (Grill Steakhouse and next to Naos)

18:00 – 19:00    Opening Reception (Beach in front of Naos)

19:00 – 20:30    Dinner on the Beach in front of Naos

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**Room locations and notes**

- General Sessions and Poster Sessions will be in Caney I, II and III.
- Breakfast and Lunches will be at Gabi Beach and Naos.
- ECI office is in Karaya (across foyer from Caney).
- Audio, still photo and video recording by any device (e.g., cameras, cell phones, laptops, PDAs, 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 discussion time as previously directed by your session chair.
- Please do not smoke at any conference functions.
- Turn your mobile telephones to vibrate or off during technical sessions.
- Please write your name on your program so that it can be returned to you if lost or misplaced.
- 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.
- Emergency Contact Information: Because of privacy concerns, ECI does not collect or maintain emergency contact information for conference participants. If you would like to have this information available in case of emergency, please use the reverse side of your name badge.
Monday, May 21, 2018

07:00 Breakfast

08:15 – 08:25 Conference Welcome/Overview
Conference Chair: John Tsavalas, University of New Hampshire, USA
ECI Technical Liaison: Bill Sachs, Princeton Polymer Consultants, USA

Session 1: Product Engineering I: Developing Trends in Polymer Chemistry in PRE
Chairs: Michael Cunningham, Queen's University, Canada
Jan Duchateau, Saudi Basic Industries Corporation Europe, Netherlands

08:25 – 08:30 Session introduction by co-chairs

08:30 – 09:15 Step-growth radical-mediated thiol-ene polymerizations in water-borne systems: Emulsions, suspensions and dispersions
Devon Shipp, Clarkson University, USA

09:15 – 10:00 Functional nanomaterials from single chain nanoparticles
Erik Berda, University of New Hampshire, USA

10:00 – 10:25 Synthesis and characterization of CO₂ responsive cellulose nanocrystals via RAFT-mediated graft modification
Pascale Champagne, Queen's University, Canada

10:25 – 10:55 Coffee break

10:55 – 11:20 Structure modifications of hydrolytically degradable polymer flocculant for improved water recovery from mature fine tailings
Georges Younes, Queens University at Kingston, Canada

11:20 – 11:45 SI-ARGET-ATRP grafting of block copolymers with amphiphilic properties on lignocellulosic materials
Marta Vidiella del Blanco, ETH Zürich, Switzerland

11:45 – 12:10 Click chemistry within LDPE
Jan Duchateau, Saudi Basic Industries Corporation Europe, Netherlands

12:10 – 13:55 Lunch

Session 2: Enabling Research in PRE I: Kinetics and Thermodynamics
Chairs: Massimo Morbidelli, ETH Zürich, Switzerland
Jeffrey Stubbs, HP Inc., USA

13:55 – 14:00 Session introduction by co-chairs

14:00 – 14:45 The curious case of the molecular catalysts that behaved like a dual-site catalyst
Joao Soares, University of Alberta, Canada

14:45 – 15:30 The influence of (macro) monomer functionality on reactivity in radical (co)polymerization
Robin A. Hutchinson, Queen's University, Canada
Monday, May 21, 2018 (continued)

15:30 – 16:15  **Mechanistic insights into topological network formation in free radical co-polymerization**  
Amit Tripathi, University of New Hampshire, USA

16:15 – 16:45  Coffee break

16:45 – 17:10  **Understanding of cyclodepolymerization kinetics for the production of cyclic polyethylene furanoate oligomers**  
Peter Fleckenstein, ETH Zürich, Switzerland

17:10 – 17:35  **Effect of solution properties on the terpolymerization of 2-acrylamido-2-methylpropane sulfonic acid, acrylamide and acrylic acid**  
Alison J. Scott, University of Waterloo, Canada

17:35 – 17:40  Introduction to Opening Plenary Talk  
John Tsavalas, University of New Hampshire, USA

17:40 – 18:40  **Opening Plenary Talk**  
**Polymer reaction engineering in the origins of life: How to get from synthetic rubber to chemical evolution**  
F. Joseph Schork, Georgia Institute of Technology, USA

18:40 – 20:40  **Poster Session 1** and Social Hour  
Chairs:  F. Joseph Schork, Georgia Institute of Technology, USA  
Jay Reimers, ExxonMobil, USA

20:45  Dinner
**Tuesday, May 22, 2018**

07:00  Breakfast

**Session 3: Process Engineering: Production Issues & Process Control**
Chairs: Timothy McKenna, Université Claude Bernard Lyon 1, France
        Ivan Konstantinov, Dow Chemical Company, USA

08:25 – 08:30  Session introduction by co-chairs

08:30 – 09:15  **Automatic, simultaneous control of molar mass and composition in free radical copolymerization using ACOMP/Ci**
                Wayne F. Reed, Tulane University, USA

09:15 – 10:00  **Condensed mode cooling for PE: Importance of thermodynamics in reactor and particle modelling**
                Timothy McKenna, Université Claude Bernard Lyon 1, France

10:00 – 10:25  **Modelling and control of the microstructure of MAA-co-PEGMA water soluble copolymers**
                Jose Ramon Leiza, University of the Basque Country, Spain

10:25 – 10:55  Coffee break

10:55 – 11:20  **Multi-Scale, Multi-Phase Modelling of a Slurry-Phase Catalytic Ziegler-Natta HDPE Continuous Process**
                Costas Kiparissides, Aristotle University of Thessaloniki, Greece

11:20 – 11:45  **In-line monitoring of polymer nanoparticle growth during synthesis in concentrated systems by photon density wave spectroscopy**
                Roland Hass, University of Potsdam, Germany

11:45 – 12:10  **Rational design of polymerization systems: Perspectives from computational chemistry and reaction engineering**
                Ivan Konstantinov, Dow Chemical Company, USA

12:10 – 14:00  Lunch

14:00 – 18:30  

**ad hoc sessions/Networking OPTIONAL tours and activities**

Evening  Dinner
Wednesday, May 23, 2018

07:00 Breakfast

Session 4: Product Engineering II: Heterogeneous Polymerizations & Processes
Chairs: Ad Overbeek, DSM Coating Resins, Netherlands
       Hans-Ulrich Moritz, University of Hamburg, Germany

08:25 – 08:30 Session introduction by co-chairs

08:30 – 09:15 Amphiphilic block copolymers as stabilizers in emulsion polymerization: Effects of molecular weight dispersity and evidence of self-folding behavior
       Michael F. Cunningham, Queen's University, Canada

09:15 – 10:00 Micron sized colloids for effect coatings: Haptic response
       Ad Overbeek, DSM Coating Resins, Netherlands

10:00 – 10:45 Role of dispersed polymeric nanoparticles in the bulk polymerization of methyl methacrylate
       Hua Wu, ETH Zurich, Switzerland

10:45 – 11:15 Coffee break

11:15 – 12:00 The effect of cellulose nanocrystals on latex and adhesive properties in emulsion-based polymer nanocomposites
       Marc A. Dubé, University of Ottawa, Canada

12:00 – 12:25 Synthesis and utilization of low dispersity acrylic macromonomer as dispersant for non-aqueous dispersion polymerization
       Mingmin Zhang, Queen's University, Canada

12:25 – 12:50 High molecular weight polystyrene particles by cationic miniemulsion polymerization catalyzed by an iron-containing imidazolium-based ionic liquid
       Claudia Sayer, Federal University of Santa Catarina, Brazil

12:50 – 14:00 Lunch

14:00 – 18:30 ad hoc sessions/Networking

18:30 – 20:30 Poster Session 2 and Social Hour
Chairs: F. Joseph Schork, Georgia Institute of Technology, USA
       Jay Reimers, ExxonMobil, USA

20:30 Dinner
Thursday, May 24, 2018

07:00 Breakfast

**Session 5: Enabling Research in PRE II: Advances in Polymerization & Process Modeling**
Chairs: Dagmar R. D'hooge, Ghent University, Belgium  
Rolf Bachmann, Covestro Deutschland AG, Germany

08:10 – 08:15 Session introduction by co-chairs

08:15 – 09:00 A detailed characterization and design of copolymerization  
Dagmar R. D'hooge, Ghent University, Belgium

09:00 – 09:45 Modeling and characterization of the morphology of multiphase polymeric nanoparticles  
Shaghayegh Hamzelou, University of the Basque Country, Spain

09:45 – 10:10 Modeling polycondensation equilibrium for Nylon 6 and Nylon 6,6  
Fei Liu, Queen's University, Canada

10:10 – 10:35 A novel interpretation of measured and simulated PLP data  
Yoshi W. Marien, Ghent University, Belgium

10:35 – 11:05 Coffee break

11:05 – 11:30 Modeling possible long chain branching reactions for polyethylene in a semi-batch reactor  
Abdulrahman Albeladi, University of Alberta, Canada

11:30 – 11:55 Distribution of functional groups in starved-feed semi-batch free radical copolymerization: An accelerated stochastic modeling approach  
Amin Nasresfahani, Queen's University, Canada

11:55 – 12:20 Living apart together: On graph theory and polymer chemistry  
Ivan Kryven, University of Amsterdam, Netherlands

12:20 – 14:00 Lunch

**Session 6: PRE in Biomedical & Pharmaceutical Applications**
Chairs: Georgia Papavasiliou, Illinois Institute of Technology, USA  
Fouad Teymour, Illinois Institute of Technology, USA

14:00 – 14:05 Session introduction by co-chairs

14:05 – 14:50 Hydrogel biomaterials with independent and combined variations in modulus and cell adhesion ligand gradients for guided neovascularization of engineered tissues  
Georgia Papavasiliou, Illinois Institute of Technology, USA

14:50 – 15:15 Synthesis of "clickable" macro-porous materials for ultrafast purification of monoclonal antibodies  
Marcel Lorenz, ETH Zurich, Switzerland

15:15 – 15:40 Nanoparticles for intestinal sepsis prevention synthesized via inverse miniemulsion polymerization  
Fernando T. P. Borges, Illinois Institute of Technology, USA
Thursday, May 24, 2018 (continued)

15:40 – 16:10 Coffee break

16:10 – 16:35 **Injectable hyaluronic acid based hydrogels for the repair of cartilage lesions**
Costas Kiparissides, Aristotle University of Thessaloniki, Greece

16:35 – 17:20 **Nanostructured polymers for targeted and responsive drug delivery: Exploitations of RAFT and click chemistries**
Danielle Benoit, University of Rochester, USA

17:20 – 17:25 Introduction to Closing Plenary Talk
John Tsavalas, University of New Hampshire, USA

17:25 – 18:25 **Closing Plenary Talk**
**Versatile macromolecules and their biomedical applications**
Massimo Morbidelli, ETH Zürich, Switzerland

19:30 – 20:00 Reception

20:00 – 22:30 Conference Banquet
Poster Awards
Friday, May 25, 2018

07:00
Breakfast

Free time for networking activities

Lunch and departures
Posters

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May 20 – May 25, 2018

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**Poster Presentations**

1. **Pressure sensitive adhesives produced by in-situ emulsion polymerization of cellulose nanocrystal-poly(nBA-VAc)**
   Amir Saeid Pakdel, University of Ottawa, Canada

2. **Molecular modeling of free radical polymerization of diacrylates**
   Ariana Torres Knoop, University of Amsterdam, Netherlands

3. **Predicting average molecular weights and branching level for self-condensing vinyl copolymerization in a CSTR**
   Bradley D. Buren, Queen's University, Canada

4. **An advanced model-based strategy to optimize the microbial production of biodegradable polymers under fed-batch conditions**
   Costas Kiparissides, CERTH/CPERI, AUTh, Greece

5. **Designing controlled radical polymerization: A selection of a terminal or penultimate model for the intrinsic reactivities**
   Dagmar R. D'hooge, Ghent University, Belgium

6. **Designing polymer-based piezoresistive strain sensors**
   Dagmar R. D'hooge, Ghent University, Belgium

7. **Model-based design of MADIX under bulk and solution conditions**
   Dagmar R. D'hooge, Ghent University, Belgium

8. **Modeling and parameter estimation in a PO3G Polyether process with time delay**
   Duong Vo, Queen's University, Canada

9. **Synthesis of waterborne degradable polyester nanoparticles**
   Fabian Wenzel, Polymat, University of the Basque Country, Spain

10. **Effect of functional groups and ionization on the radical copolymerization of acrylic acid and cationic monomers in aqueous solution**
    Ikenna Henry Ezenwajiaku, Queen's University, Canada

11. **Synthesis of novel double metal cyanide catalysts and polymerization of PO and CO₂**
    Jakob Marbach, University of Hamburg, Germany

12. **High-pressure calorimetry: Thermophysical properties of gases and polymers**
    Jonas Nowottny, TU Darmstadt, Germany

13. **Prepolymerization for the gas phase polymerization of propylene**
    Jorik Hill, Martin-Luther-University Halle-Wittenberg, Germany

14. **Linking process conditions with polymer properties for the LDPE process**
    Kristina Maria Pflug, TU Darmstadt, Germany

15. **Phase equilibria effect on catalytic olefin polymerization**
    Lenka Krajáková, UCT Prague, Czech Republic

16. **Evolution of high impact polypropylene morphology upon thermal treatment**
    Lenka Krajáková, UCT Prague, Czech Republic
17. Effect of reaction conditions on the distribution of hydroxyl functional groups in HEA-BMA copolymer 
   Loretta A. Idowu, Queens University, Canada

18. Solvent-controlled modification on lignocellulosic materials via SI-ATRP 
   Marta Vidiella del Blanco, ETH Zürich, EMPA, Switzerland

19. Poly(HPMA)-based copolymers with biodegradable side chains able to self-assemble into nanoparticles 
   Mattia Sponchioni, Politecnico di Milano, Italy

20. A process for the production of bottle grade polyethylene furanoate by ring-opening polymerization 
   Peter Fleckenstein, ETH Zürich, Switzerland

21. Method of moments in nonlinear free radical polymerization 
   Rolf Bachmann, Covestro Deutschland AG, Germany

22. Acrylic-melamine latex with controlled crosslinking capability 
   Roque Minari, INTEC (CONICET - Universidad Nacional del Litoral), Argentina

23. Film-forming thermoresponsive nanogels for dermal protein delivery 
   Roque Minari, INTEC (CONICET - Universidad Nacional del Litoral), Argentina

24. Characterizing catalyst performance of DMCs on PO homopolymerization 
   Sarah-Franziska Stahl, University of Hamburg, Germany

25. Nitroxide-mediated polymerization of bio-based farnesene and glycidyl methacrylate 
   Sharmaine Luk, McGill University, Canada

26. Effect of hydrogen partitioning on homo-propylene polymerization kinetics 
   Sina Valaei, Martin Luther University Halle-Wittenberg, Germany

27. The combination of ROP and RAFT polymerization for the synthesis of polymeric nanoparticles 
   Umberto Capasso Palmiero, Politecnico di Milano, Italy

28. General model for step-growth polymerization of hyperbranched AfBiBgi-type polymers 
   Verena Schamboeck, University of Amsterdam, Netherlands

29. Reactivity ratio estimation for co- and terpolymerization of n-butyl acrylate, methyl methacrylate and 2-ethylhexyl acrylate 
   Vida A. Gabriel, University of Ottawa, Canada

30. Starch nanoparticle-based latexes for pressure-sensitive adhesive applications 
   Yujie Zhang, University of Ottawa, Canada

31. Auto-generated chemical reaction networks for polymerization processes 
   Yuliia Orlova, University of Amsterdam, Netherlands

32. A simple Monte Carlo method for modeling arborescent polymer production in continuous stirred tank reactor 
   Yutian Zhao, Queen's University, Canada

33. ROP of vic-disubstituted lactones: A diastereoselective way to polymerize 
   Francesco Distante, ETH Zurich, Italy
34. Biocompatible superparamagnetic poly(thioether-ester) nanoparticles via miniemulsion technique  
   Pedro Henrique Hermes de Araújo, Universidade Federal de Santa Catarina, Brazil

35. Contrasting acrylate versus methacrylate crosslinking reactions and the impact of temperature  
   Chang Liu, University of New Hampshire, USA

36. Kinetics of PE crystallization  
   Fabiana N. Andrade, Timothy McKenna, CNRS/ESCPE Lyon, France

37. A new approach to stopped-flow reactions for slurry and gas-phase olefin polymerization  
   Yashmin Rafante Blazzio, Timothy McKenna, CNRS/ESCPE Lyon, France

38. High impact polypropylene: Influence of copolymerization conditions on powder and polymer properties  
   Aarón J. Cancelas, Timothy McKenna, CNRS/ESCPE Lyon, France

39. Impact of geometric properties of silica supports on metallocene catalyst behavior  
   Barbara Rezende Lara, Timothy McKenna, CNRS/ESCPE Lyon, France

40. Need and potential of digitalization in the development and production of polymers  
    Wolfgang Gerlinger, BASF SE, Germany