

Program

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

May 20 – May 25, 2018

Paradisus Punta Cana Resort, Punta Cana, Dominican Republic

Chair

John Tsavalas

University of New Hampshire, USA

Co-Chairs

Fouad Teymour

Illinois Institute of Technology, USA

Jose R. Leiza

University of the Basque Country, Spain

Jeffrey Stubbs

HP Inc., USA



Engineering Conferences International
32 Broadway, Suite 314 - New York, NY 10004, USA
Phone: 1 - 212 - 514 - 6760
www.engconfintl.org – info@engconfintl.org

**Paradisus Punta Cana Resort
Playa de Bávaro, Punta Cana
Dominican Republic
Tel: +1-809-687-9923
Fax: +1-809-687-0752
paradisus.punta.cana@melia.com**

Engineering Conferences International (ECI) is a not-for-profit global engineering conferences program, originally established in 1962, that provides opportunities for the exploration of problems and issues of concern to engineers and scientists from many disciplines.

ECI BOARD MEMBERS

Barry C. Buckland, President
Mike Betenbaugh
Nick Clesceri
Peter Gray
Michael King
Raymond McCabe
Eugene Schaefer
P. Somasundaran

Chair of ECI Conferences Committee: Nick Clesceri

ECI Technical Liaison for this conference: Bill Sachs

ECI Executive Director: Barbara K. Hickernell

ECI Associate Director: Kevin M. Korpics

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

Conference Sponsors



ExxonMobil



Conference Sponsors

POLYMAT



**Macromolecular
Reaction
Engineering**

سابک
sabic



**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

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
	<u>Session 3: Process Engineering: Production Issues & Process Control</u> 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	<i>ad hoc</i> 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 Hamzehlou, 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

Polymer Reaction Engineering X (PRE 10)

An ECI Conference Series

May 20 – May 25, 2018

Paradisus Punta Cana Resort, Punta Cana, Dominican Republic



Engineering Conferences International

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 Ezenwajaku, 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 Nowotny, 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 AfiBgi-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