# **Polymer Reaction Engineering X** (PRE 10)

An ECI Conference Series Volume 18AB

Punta Cana, Dominican Republic 20-25 May 2018

**Editors:** 

John Tsavalas Jeffrey Stubbs Fouad Teymour Jose R. Leiza

ISBN: 978-1-5108-7019-2

Printed from e-media with permission by:

Curran Associates, Inc. 57 Morehouse Lane Red Hook, NY 12571



Some format issues inherent in the e-media version may also appear in this print version.

Copyright© (2018) by Engineering Conferences International All rights reserved.

Printed by Curran Associates, Inc. (2018)

For permission requests, please contact Engineering Conferences International at the address below.

Engineering Conferences International 32 Broadway, Suite 314 New York, NY 10004 USA

Phone: (212) 514-6760 Fax: (212) 514-6030

info@engconfintl.org

#### Additional copies of this publication are available from:

Curran Associates, Inc. 57 Morehouse Lane Red Hook, NY 12571 USA Phone: 845-758-0400 Fax: 845-758-2633 Email: curran@proceedings.com Web: www.proceedings.com

#### 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 dispersions1 Devon Shipp, Clarkson University, USA
09:15 – 10:00	Functional nanomaterials from single chain nanoparticles2 Erik Berda, University of New Hampshire, USA
10:00 – 10:25	Synthesis and characterization of CO <sub>2</sub> responsive cellulose nanocrystals via RAFT-mediated graft modification3 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 tailings4 Georges Younes, Queens University at Kingston, Canada
11:20 – 11:45	SI-ARGET-ATRP grafting of block copolymers with amphiphilic properties on lignocellulosic materials5 Marta Vidiella del Blanco, ETH Zürich, Switzerland
11:45 – 12:10	<b>Click chemistry within LDPE6</b> 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 catalyst7 Joao Soares, University of Alberta, Canada
14:45 – 15:30	The influence of (macro) monomer functionality on reactivity in radical (co)polymerization8 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-polymerization9 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 oligomers10 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 acid11 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 evolution12 F. Joseph Schork, Georgia Institute of Technology, USA
18:40 – 20:40	<b>Poster Session 1</b> 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/CI13 Wayne F. Reed, Tulane University, USA
09:15 – 10:00	Condensed mode cooling for PE: Importance of thermodynamics in reactor and particle modelling34 Timothy McKenna, Université Claude Bernard Lyon 1, France
10:00 – 10:25	Modelling and control of the microstructure of MAA-co-PEGMA water soluble copolymers35 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 Process36 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 spectroscopy37 Roland Hass, University of Potsdam, Germany
11:45 – 12:10	Rational design of polymerization systems: Perspectives from computational chemistry and reaction engineering38 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 behavior39 Michael F. Cunningham, Queen's University, Canada
09:15 – 10:00	Micron sized colloids for effect coatings: Haptic response40 Ad Overbeek, DSM Coating Resins, Netherlands
10:00 – 10:45	Role of dispersed polymeric nanoparticles in the bulk polymerization of methyl methacrylate41 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 nanocomposites42 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 polymerization66 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 liquid67 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 copolymerization68 Dagmar R. D'hooge, Ghent University, Belgium
09:00 – 09:45	Modeling and characterization of the morphology of multiphase polymeric nanoparticles69 Shaghayegh Hamzehlou, University of the Basque Country, Spain
09:45 – 10:10	Modeling polycondensation equilibrium for Nylon 6 and Nylon 6,670 Fei Liu, Queen's University, Canada
10:10 – 10:35	A novel interpretation of measured and simulated PLP data71 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 reactor72 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 approach73 Amin Nasresfahani, Queen's University, Canada
11:55 – 12:20	Living apart together: On graph theory and polymer chemistry74 Ivan Kryven, University of Amsterdam, Netherlands
12:20 – 14:00	Lunch
	<u>Session 6: PRE in Biomedical &amp; Pharmaceutical Applications</u> 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 tissues75 Georgia Papavasiliou, Illinois Institute of Technology, USA
14:50 – 15:15	Synthesis of "clickable" macro-porous materials for ultrafast purification of monoclonal antibodies76 Marcel Lorenz, ETH Zurich, Switzerland
15:15 – 15:40	Nanoparticles for intestinal sepsis prevention synthesized via inverse miniemulsion polymerization77 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 lesions78 Costas Kiparissides, Aristotle University of Thessaloniki, Greece
16:35 – 17:20	Nanostructured polymers for targeted and responsive drug delivery: Exploitations of RAFT and click chemistries79 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	<u>Closing Plenary Talk</u> Versatile macromolecules and their biomedical applications80 Massimo Morbidelli, ETH Zürich, Switzerland
19:30 – 20:00	Reception
20:00 – 22:30	Conference Banquet
	Poster Awards

## **Poster Presentations**

- Pressure sensitive adhesives produced by in-situ emulsion polymerization of cellulose nanocrystal-poly(nBA-VAc) .....81 Amir Saeid Pakdel, University of Ottawa, Canada
- 2. **Molecular modeling of free radical polymerization of diacrylates .....82** Ariana Torres Knoop, University of Amsterdam, Netherlands
- Predicting average molecular weights and branching level for self-condensing vinyl copolymerization in a CSTR .....83 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 .....84 Costas Kiparissides, CERTH/CPERI, AUTh, Greece
- Designing controlled radical polymerization: A selection of a terminal or penultimate model for the intrinsic reactivities .....85 Dagmar R. D'hooge, Ghent University, Belgium
- 6. **Designing polymer-based piezoresistive strain sensors .....86** Dagmar R. D'hooge, Ghent University, Belgium
- 7. Model-based design of MADIX under bulk and solution conditions ....87 Dagmar R. D'hooge, Ghent University, Belgium
- 8. **Modeling and parameter estimation in a PO3G Polyether process with time delay .....88** Duong Vo, Queen's University, Canada
- 9. **Synthesis of waterborne degradable polyester nanoparticles .....89** 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 .....90 Ikenna Henry Ezenwajiaku, Queen's University, Canada
- 11. Synthesis of novel double metal cyanide catalysts and polymerization of PO and CO<sub>2</sub> .....91 Jakob Marbach, University of Hamburg, Germany
- 12. **High-pressure calorimetry: Thermophysical properties of gases and polymers .....92** Jonas Nowottny, TU Darmstadt, Germany
- 13. **Prepolymerization for the gas phase polymerization of propylene .....93** Jorik Hill, Martin-Luther-University Halle-Wittenberg, Germany
- 14. Linking process conditions with polymer properties for the LDPE process .....94 Kristina Maria Pflug, TU Darmstadt, Germany
- 15. **Phase equilibria effect on catalytic olefin polymerization .....95** Lenka Krajáková, UCT Prague, Czech Republic
- 16. **Evolution of high impact polypropylene morphology upon thermal treatment .....96** Lenka Krajáková, UCT Prague, Czech Republic

- Effect of reaction conditions on the distribution of hydroxyl functional groups in HEA-BMA copolymer .....97 Loretta A. Idowu, Queens University, Canada
- 18. Solvent-controlled modification on lignocellulosic materials via SI-ATRP .....98 Marta Vidiella del Blanco, ETH Zürich, EMPA, Switzerland
- Poly(HPMA)-based copolymers with biodegradable side chains able to self-assemble into nanoparticles .....99 Mattia Sponchioni, Politecnico di Milano, Italy
- A process for the production of bottle grade polyethylene furanoate by ring-opening polymerization .....100
  Peter Fleckenstein, ETH Zürich, Switzerland
- 21. **Method of moments in nonlinear free radical polymerization .....101** Rolf Bachmann, Covestro Deutschland AG, Germany
- 22. Acrylic-melamine latex with controlled crosslinking capability .....102 Roque Minari, INTEC (CONICET - Universidad Nacional del Litoral), Argentina
- 23. **Film-forming thermoresponsive nanogels for dermal protein delivery .....103** Roque Minari, INTEC (CONICET - Universidad Nacional del Litoral), Argentina
- 24. Characterizing catalyst performance of DMCs on PO homopolymerization .....104 Sarah-Franziska Stahl, University of Hamburg, Germany
- 25. Nitroxide-mediated polymerization of bio-based farnesene and glycidyl methacrylate .....105 Sharmaine Luk, McGill University, Canada
- 26. Effect of hydrogen partioning on homo-propylene polymerization kinetics .....106 Sina Valaei, Martin Luther University Halle-Wittenberg, Germany
- 27. The combination of ROP and RAFT polymerization for the synthesis of polymeric nanoparticles .....107 Umberto Capasso Palmiero, Politecnico di Milano, Italy
- 28. General model for step-growth polymerization of hyperbanched AfiBgi-type polymers .....108 Verena Schamboeck, University of Amsterdam, Netherlands
- 29. Reactivity ratio estimation for co- and terpolymerization of n-butyl acrylate, methyl methacrylate and 2-ethylhexyl acrylate .....109 Vida A. Gabriel, University of Ottawa, Canada
- 30. Starch nanoparticle-based latexes for pressure-sensitive adhesive applications .....110 Yujie Zhang, University of Ottawa, Canada
- 31. **Auto-generated chemical reaction networks for polymerization processes .....111** Yuliia Orlova, University of Amsterdam, Netherlands
- A simple Monte Carlo method for modeling arborescent polymer production in continuous stirred tank reactor .....112 Yutian Zhao, Queen's University, Canada
- 33. **ROP of vic-disubstituted lactones: A diastereoselective way to polymerize .....113** Francesco Distante, ETH Zurich, Italy

- Biocompatible superparamagnetic poly(thioether-ester) nanoparticles via miniemulsion technique .....114
  Pedro Henrique Hermes de Araújo, Universidade Federal de Santa Catarina, Brazil
- 35. Contrasting acrylate versus methacrylate crosslinking reactions and the impact of temperature .....115 Chang Liu, University of New Hampshire, USA
- 36. **Kinetics of PE crystallization .....116** Fabiana N. Andrade, <u>Timothy McKenna</u>, CNRS/ESCPE Lyon, France
- A new approach to stopped-flow reactions for slurry and gas-phase olefin polymerization .....117 Yashmin Rafante Blazzio, <u>Timothy McKenna</u>, CNRS/ESCPE Lyon, France
- High impact polypropylene: Influence of copolymerization conditions on powder and polymer properties .....118
  Aarón J. Cancelas, <u>Timothy McKenna</u>, CNRS/ESCPE Lyon, France
- 39. **Impact of geometric properties of silica supports on metallocene catalyst behavior .....119** Barbara Rezende Lara, <u>Timothy McKenna</u>, CNRS/ESCPE Lyon, France
- 40. **Need and potential of digitalization in the development and production of polymers .....120** Wolfgang Gerlinger, BASF SE, Germany