

Polymer Reaction Engineering IX

Cancun, Mexico
10-15 May 2015

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Monday, May 11, 2015

06:30 Buffet Breakfast opens (NAOS)

Session 1: Product Engineering I: Advances in Polymer Science (Greco-Dali room)
Co-chairs: **Min Zhang** (DuPont, USA) and **Michael Monteiro** (University of Queensland Australia)

Sponsored by BASF

08:20 - 08:30 Introduction by co-chairs and BASF representative

08:30 - 09:15 **Michael Monteiro (Invited)**
University of Queensland, Australia
Multifunctional nanoworms and nanorods and functional membranes N/A

09:15 - 10:00 **Marc A. Dubé (Invited)**
University of Ottawa, Canada
The challenge of degradative chain transfer in renewable monomer polymerization1

10:00 - 10:20 **Claudia Sayer**
Federal University of Santa Catarina, Brazil
Interfacial step growth polymerization in miniemulsion for the incorporation of magnetic nanoparticles into polyurethane particles N/A

10:20 - 10:40 Coffee break (Lower Foyer)

10:40 - 11:00 **Kiyoshi Suzuki**
University of Fukui, Japan
Reaction loci size effect on reversible deactivation radical polymerization rate N/A

11:00 - 11:20 **Fouad Teymour**
Illinois Institute of Technology, USA
Phosphate-containing poly(ethylene glycol) hydrogel nanoparticles for prevention of gut-derived sepsis N/A

11:20 - 11:40 **Jon Debling**
BASF, USA
Advances in chain extender technology for polyesters N/A

11:40 - 12:00 **Ali Darabi**
Queen's University, Canada
PEGylation of chitosan via nitroxide chemistry in aqueous media N/A

12:00 - 13:55 Lunch at Vento Terrace (use the NAOS buffet)

Monday, May 11, 2015 (continued)

**Session 2: Product Engineering II: Developing Trends in Polymer Chemistry –
Topics in PRE** (Greco-Dali room)

Co-chairs: **Yvon Durant** (Itaconix, USA) and **Marc Dubé** (University of Ottawa, Canada)

- 13:55 - 14:00 Introduction by co-chairs
- 14:00 - 14:45 **Yvon Durant (Invited)**
Itaconix, USA
Emulsion polymerization of 100% biobased itaconate esters N/A
- 14:45 - 15:30 **Miquel Gimeno (Invited)**
Universidad Nacional Autónoma de México, Mexico
Recent developments in enzymatic syntheses of polymers and polymer modifications21
- 15:30 - 16:15 **Etienne Cabane (Invited)**
ETH Zurich, Switzerland
Grafting polymers in the wood structure: towards functional lignocellulosic materials N/A
- 16:15 - 16:35 Coffee break (Lower Foyer)
- 16:35 - 16:55 **Jan-Georg Rosenboom**
ETH Zurich, Switzerland
Ring-opening synthesis of polyethylene furanoate (PEF) as a renewable resource-based substitute for polyethylene terephthalate (PET) N/A
- 16:55 - 17:15 **Bartosz Tylkowski**
Rovira I Virgili University, Spain
Visible light triggered microcapsules N/A
- 17:15 - 17:35 **Ling Zhao**
East China University of Science and Technology, China
New bio-based polymeric thermoset synthesized by ring-opening polymerization of soybean oil-based resin with green curing agent N/A
- 17:35 - 17:55 **Alberto Rosas-Aburto**
Universidad Nacional Autonoma de Mexico, Mexico
Modeling the electrical behaviour of conducting elastomers based on inherent conducting polymers N/A
- 18:30 - 20:30 **Poster Session 1 and Social Hour** (Lanzarote Foyer)
Co-chairs: **Robin Hutchinson** (Queen's University, Canada), **Afsaneh Nabifar** (BASF, USA) and **Helmut Meyer** (THM Nano, Bayer-retired, Germany)
- 20:30 - 22:00 Dinner at Market Grill Terrace (reserved section)

Tuesday, May 12, 2015

06:30 Buffet Breakfast opens (NAOS)

Session 3: Enabling Research in PRE I: Process Modeling, Simulation, Optimization and Control (Greco-Dali room)

Co-chairs: **Kenneth Leffew** (DuPont, USA) and **Alex Penlidis** (University of Waterloo, Canada)

Sponsored by Exxon Mobil Chemicals

08:20 - 08:30 Introduction by co-chairs and Exxon Mobil Chemicals representative

08:30 - 09:15 **Hidetaka Tobita (Invited)**

University of Fukui, Japan

Modeling and simulation method for nonlinear polymer formation N/A

09:15 - 10:00 **Wolfgang Gerlinger (Invited)**

BASF SE, Germany

Model-based product engineering: How can we describe application properties from polymer structure? N/A

10:00 - 10:20 **Daniele Marchisio**

Polytechnic Institute of Turin, Italy

Multiscale modelling of expanding polyurethane foams via computational fluid dynamics and population balance model39

10:20 - 10:40 Coffee break (Lower Foyer)

10:40 - 11:00 **Eduardo Castellanos Sahagún**

Comex, Mexico

Joint control and operation design for alkyd resin polyesterification reactors N/A

11:00 – 11:20 **Benjamin Hosemann**

Technical University Clausthal, Germany

Modeling the degree of branching in VDF/HFP copolymer systems and copolymer analyses applying triple detection SEC N/A

11:20 - 11:40 **Wayne Reed**

Tulane University, USA

Full scale industrial reactor implementation of automatic continuous online monitoring of polymerization reactions (ACOMP) N/A

11:40 - 12:00 **John Tsavalas**

University of New Hampshire, USA

Kinetic Monte Carlo simulation of emulsion copolymerization reactions with divinyl crosslinker monomer: Effect of process parameters on final properties N/A

12:00 - 12:20 **Shaghayegh Hamzehlou**

Polymat UPV/EHU, Spain

Monte Carlo: A versatile tool for modeling complex polymerization processes N/A

12:20 - 14:00 Lunch at the Vento Terrace (use NAOS buffet) /Optional tours and activities begin

14:00 – 20:30 *ad hoc* sessions/Free time/Optional tours/activities

20:30 - 22:00 Dinner at Market Grill Terrace (reserved area)

Wednesday, May 13, 2015

06:30 Buffet Breakfast opens (NAOS)

Session 4: Enabling Research in PRE II: Kinetics, Thermodynamics, and Multi-Scale Modeling (Greco-Dali room)

Co-chairs: **Klaus-Dieter Hungenberg** (BASF-retired, Germany) and **Mike Cunningham** (Queen's University, Canada)

08:25 – 08:30 Introduction by co-chairs

08:30 - 09:15 **Marco Villalobos (Invited)**
Cabot Corporation, USA
Particle design for the synthesis of tailored polymer nano-composites N/A

09:15 – 10:00 **Yuri Orlov (Invited)**
BASF SE, Germany
Polymer thermodynamics: Leverage modeling results for industrial applications N/A

10:00 – 10:45 **Joao B. P. Soares (Invited)**
University of Alberta, Canada
When polymer reactor engineers play dice: An overview of Monte Carlo methods in PRE N/A

10:45 - 11:05 Coffee break (Lower Foyer)

11:05 - 11:50 **Markus Busch (Invited)**
Technical University Darmstadt, Germany
Simulation based product development in high-pressure polymerization technology N/A

11:50 – 12:10 **Dagmar D'hooge**
Ghent University, Belgium
A novel 4-dimensional modeling strategy for optimization of NMP mini- and microemulsion N/A

12:10 – 12:30 **Mayank Kashyap**
SABIC, USA
An approach towards a multi-scale model of the fluidized bed reactor for LLDPE production N/A

12:30 - 14:00 Lunch at the Vento Terrace (use the NAOS buffet)

14:00 – 18:30 *ad hoc* sessions/Free time

18:30 - 20:30 **Poster Session 2** and **Social Hour** (Lanzarote Foyer)
Co-chairs: **Robin Hutchinson** (Queen's University, Canada), **Afsaneh Nabifar** (BASF, USA) and **Helmut Meyer** (THM Nano, Bayer-retired, Germany)

20:30 - 22:00 Dinner at Market Grill Terrace (reserved area)

Thursday, May 14, 2015

06:30 Buffet Breakfast opens (NAOS)

Session 5: Process Engineering I: Production issues of polymerization processes

(Greco-Dali room)

Co-chairs: **Thomas Karjala** (Dow Chemical, USA) and **Enrique Saldivar-Guerra** (CIQA, Mexico)

08:05 - 08:10 Introduction by co-chairs of Sessions 5

08:10 - 08:15 Introduction by co-chairs of Sessions 6

08:15 - 09:00 **Walter Kaminsky (Invited)**

University of Hamburg, Germany

Production of polyolefins by metallocene catalysts and their recycling by pyrolysis N/A

09:00 - 09:45 **Timothy F.L. McKenna (Invited)**

University of Lyon (CNRS), France

The impact of induced condensing agents in the gas phase polymerization of ethylene N/A

09:45 - 10:05 **Weiwei Yang**

Queen's University, Canada

The effectiveness of reactive dispersants in non-aqueous dispersion polymerization N/A

10:05 - 10:25 **Daniel Arriola**

The Dow Chemical Company, USA

MWD instability of divinyl and monovinyl addition copolymerization in continuous-flow stirred reactors N/A

10:25 - 10:45 Coffee break (Lower Foyer)

10:45 - 11:05 **Marzieh Riahinezhad**

University of Waterloo, Canada

Can copolymerization kinetics help tailor properties of poly (acrylamide/acrylic acid) for enhanced oil recovery? N/A

11:05 - 11:25 **Sebastian Fries**

Technical University Darmstadt, Germany

Fouling in the high pressure LDPE process: experimental and computational investigation approach52

11:25 - 11:45 **Enrique Saldivar-Guerra**

CIQA, Mexico

Mathematical modeling of a catalytic pyrolysis depolymerization process N/A

11:45 - 12:05 **Danilo Cuccato**

ETH Zurich, Switzerland

Experimental and modeling study of acrylamide copolymerization with cationic monomers in aqueous medium N/A

12:05 - 13:55 Lunch at Vento Terrace (use the NAOS buffet)

Thursday, May 14, 2015 (continued)

Session 6: Process Engineering II: Sustainability, Innovation, Intensification of Polymer Processes and Future Trends¹ (Greco-Dali room)

Co-chairs: **Philip Nising** (Sulzer, Switzerland) and **Christophe Serra** (University of Strasbourg, France)

- 14:00 - 14:45 **Hans-Ulrich Moritz (Invited)**
University of Hamburg, Germany
Process intensification of continuous emulsion polymerization in smart scale tubular reactors N/A
- 14:45 - 15:30 **Fabio Codari (Invited)**
Sulzer Ltd., Switzerland
Enhanced Process Sustainability in Polymerization and Devolatilization Technologies N/A
- 15:30 - 16:15 **Michael Bartke (Invited)**
Fraunhofer Polymer Pilot Plant Center, Germany
Polymer isolation as important step in synthetic rubber production processes N/A
- 16:15 - 16:40 Coffee break (Lower Foyer)
- 16:40 - 17:00 **F. Joseph Schork**
Georgia Institute of Technology, USA
Polycondensation in the primordial world: A hypothesis for the evolution of the first biopolymers N/A
- 17:00 - 17:20 **Binjie Hu**
University of Nottingham Ningbo, China
Study of room temperature ionic liquid on miniemulsions polymerization for application in low-emitting waterborne coating products N/A
- 17:20 - 17:40 **Jose Ramon Leiza**
University of the Basque Country, Spain
Tracking droplet nucleation in seeded semibatch miniemulsion polymerization63
- 18:00 – 19:00 Reception (Foyer outside Greco-Dali-Goya rooms)
- 19:00 - 22:00 Conference Banquet (Greco-Dali-Goya rooms)
Poster Awards

¹ The objectives and opening remarks for this session will be presented by Philip Nising at 8:10 a.m. since he must leave early that day and C. Serra is not attending. One of the conference organizers will moderate the session in the afternoon.

Friday, May 15, 2015

06:30 Buffet breakfast opens (NAOS)

Steering Committee and Organizing Committee meeting (May take place on Wednesday, before poster session 2)

Free time for networking activities, followed by departures

Polymer Reaction Engineering IX (PRE 9)

May 10-15, 2015

Cancun, Mexico

Poster List

Monday, May 11, 2015

Biomonomers and Biopolymers

1. **Copolymerization of limonene: Experimental kinetics and modeling** N/A
Yujie Zhang, University of Ottawa, Canada
2. **Mathematical modelling of polyether production from bio-sourced 1,3-propanediol: Accounting for cyclic oligomers** N/A
Kim B. McAuley, Queen's University, Canada
3. **d-Limonene/n-butyl acrylate copolymer synthesized by free-radical polymerization and nitroxide-mediated polymerization** N/A
Shanshan Ren, University of Ottawa, Canada
4. **Synthesis and characterization of n-butyl acrylate/butyl methacrylate/d-limonene terpolymers** N/A
Shanshan Ren, University of Ottawa, Canada
5. **From laboratory to industrial continuous production of low residual monomer polylactic acid** N/A
Fabio Codari, Sulzer Chemtech, Switzerland
6. **Synthesis and characterization of a new biopoly-urethane-ester from ricinoleic acid and its use as biopolymeric matrix for magnetic nanocomposites** N/A
Paulo Suarez, University of Brasilia, Brazil
7. **Production and characterization of deconstructed biopolymers and second generation bioethanol from lignocellulosic biomasses** N/A
Diana Orea-Cortina, Universidad Nacional Autónoma de México, Mexico
8. **Ring-opening polymerization (ROP) of polybutylene terephthalate (PBT) as a model system for renewable polymer synthesis** N/A
Jan-Georg Rosenboom, ETH Zurich, Switzerland
9. **PLP-SEC study of the propagation rate of N-(2-hydroxypropyl)-methacrylamide in aqueous solution** N/A
Umberto Capasso Palmiero, Politecnico di Milano, Italy

Free Radical Polymerization

10. **The effect of head-to-head addition on vinyl acetate radical polymerization kinetics** N/A
Otlaatla Monyatsi, Queen's University, Canada
11. **Modelling of the auto-acceleration effect in free-radical polymerization: A new approach** N/A
David Victoria Valenzuela, Centro de Investigación en Química Aplicada, Mexico

12. **Production of terminally unsaturated acrylic resins through free-radical polymerization at elevated temperatures** N/A
Wolfgang Gerlinger, BASF SE, USA
13. **Monte Carlo simulations of free radical polymerizations with divinyl crosslinker: Pre- and post-gel simulations of reaction kinetics and molecular structure** N/A
John Tsavalas, University of New Hampshire, USA
14. **Effect of crosslinking monomer type on network formation efficiency in free-radical copolymerization: A kinetic Monte Carlo study** N/A
John Tsavalas, University of New Hampshire, USA
15. **A hybrid algorithm for accurate and efficient Monte Carlo simulations of free-radical polymerization reactions** N/A
Amit Tripathi, University of New Hampshire, USA
16. **Raman spectroscopy monitoring of acrylic acid and trimethylolpropane triacrylate copolymerization on inverse suspension** N/A
Maria Veronica Carranza Oropeza, University of São Paulo, Brazil
17. **The effect of pH on the polymerization and properties of poly(acrylic acid) synthesized via redox polymerization** N/A
Marc A. Dubé, University of Ottawa, Canada

Product Characterization and Optimization

18. **In-line conversion monitoring of poly (sodium acrylate)/nanosilver nanocomposites** N/A
Marc A. Dubé, University of Ottawa, Canada
19. **Development of solid super desiccants based on superabsorbent hydrogel composite** N/A
Yifan Yang, University of Ottawa, Canada
20. **Porosity characterization of polyacrylamide hydrogels templated with SDS micelles through thermoporometry technique** N/A
Maria Veronica Carranza Oropeza, Tennessee Tech University, USA
21. **Heat and mass transfer analysis in dead-end vacuum membrane distillation process** N/A
Yifan Yang, University of Ottawa, Canada
22. **Sulfonated block copolymer technology for coatings applications** N/A
Guy A. Cordonier, Kraton Polymers LLC, USA
23. **Selecting polymeric sensing materials for the detection of ethanol** N/A
Katherine M. E. Stewart, University of Waterloo, Canada
24. **Evaluation of UV radiation for improving polypropylene melt strength: Imparting long chain branches** N/A
Alex Penlidis, University of Waterloo, Canada
25. **Thermal behaviour of poly(lactic acid)/polypropylene blends** N/A
Rodrigo Aire Torres, Universidad Anáhuac México Norte, Mexico
26. **Evaluation of compatibilizers for improving dispersion in polypropylene matrix** N/A
Andres Behnsen Garza, Universidad Anahuac México Norte, Mexico
27. **Study on PA-MXD6/PET copolymer by copolycondensation** N/A
Dongdong Hu, East China University of Science and Technology, China

28. **Kinetics of melt transesterification of bisphenol-A and diphenyl carbonate to polycarbonate with tetraethyl ammonium hydroxide catalyst** N/A
Dongdong Hu, East China University of Science and Technology, China

Foaming

29. **Polymer foaming – nucleation vs spinodal decomposition** N/A
Andra Nistor, University of Chemistry and Technology, Prague, Czech Republic
30. **Modeling of heat insulation properties of polystyrene and polyurethane foams** N/A
Pavel Ferkl, University of Chemistry and Technology, Prague, Czech Republic
31. **Challenges in meso-scale modeling of polymeric foam evolution** N/A
Pavel Ferkl, University of Chemistry and Technology, Prague, Czech Republic
32. **Curing kinetics and chemorheology analysis during rigid polyurethane foaming process using carbon dioxide as the foaming agent** N/A
Dongdong Hu, East China University of Science and Technology, China

Wednesday , May 13, 2015

Coordination Polymerization

33. **Influence of activation conditions on the gas phase polymerisation of propylene** N/A
Timothy F.L. McKenna, C2P2 - UMR 5265, Université de Lyon, France
34. **Role of silica particle size in the catalytic activity of supported (n-BuCp)₂ZrCl₂/methylaluminoxane metallocene system** N/A
Timothy F.L. McKenna, C2P2 - UMR 5265, Université de Lyon, France
35. **Kinetic study of the bulk polymerization of propylene with metallocene catalyst using reaction calorimetry** N/A
Joana Kettner, Martin-Luther University Halle-Wittenberg, Germany
36. **Single-reactor dual-catalyst model for the effect of branching on the polyolefin properties** N/A
Ivan Konstantinov, The Dow Chemical Company, USA
37. **High impact polypropylene: Morphology generation during homo-stage** N/A
Miguel Plata, Martin Luther University, Germany
38. **Coupled deterministic and stochastic modeling of an industrial multi-zone LDPE autoclave reactor¹** N/A
David Eckes, Technische Universität Darmstadt, Germany
39. **Continuous polymerization for gas-phase propylene in a pilot plant using an improved Ziegler-Natta catalyst (BCM)** N/A
Luqiang Yu, Sinopec, China
40. **Monte Carlo simulation of ethylene/diene copolymerization with single-site catalysts** N/A
Joao B. P. Soares, University of Alberta, Canada
41. **Sorption of organic gases and vapours in polyethylene** N/A
Andra Nistor, University of Chemistry and Technology, Prague, Czech Republic
42. **The modeling and scale-up of a metallocene copolymerization—predicting long chain branching with mechanisms for terminal double bond formation and reincorporation** N/A
Jay Reimers, ExxonMobil, USA

CRP/Living Polymerization

43. **Parallel models for arborescent polyisobutylene synthesized in batch reactor** N/A
Kim McAuley, Queen's University, Canada
44. **Nitroxide mediated polymerization at elevated temperatures** N/A
Kevin A. Payne, Queen's University, Canada
45. **Design and synthesis of CO₂-philic poly(vinyl acetate)-based copolymers—simulations and dissolution behaviors in CO₂** N/A
Dongdong Hu, East China University of Science and Technology, China
46. **Semibatch copolymerization Of 2-hydroxyethyl methacrylate And ethylene glycol dimethacrylate** N/A

¹ This contribution belongs to the “free-radical” session on Wednesday

Carlos Hipólito Antonio-Hernández, Universidad Nacional Autónoma de México, Mexico

47. **The RAFT copolymerization and its use for the production of SEC copolymer standards: Procedure and case studies** N/A
Umberto Capasso Palmiero, Politecnico di Milano, Italy
48. **Modeling of RAFT copolymerization with crosslinking of vinyl/divinyl monomers in supercritical carbon dioxide** N/A
Porfirio López-Domínguez, Universidad Nacional Autónoma de México, Mexico
49. **Controlled release of vitamin B-12 using hydrogels synthesized by RAFT copolymerization with crosslinking in scCO₂** N/A
Patricia Pérez-Salinas, Universidad Nacional Autónoma de México, Mexico

Emulsion Polymerization

50. **A novel approach to determine partition coefficients of monomers in polymer dispersions via headspace gas chromatography** N/A
Eric Jean Fischer, ETH Zurich / ICB, Switzerland
51. **A new method for measuring the stability of emulsion polymer particles using turbidity measurements** N/A
Timothy F.L. McKenna, C2P2 - UMR 5265, Université de Lyon, France
52. **Latex polymer property modification using cellulose nanocrystals** N/A
Zahra Dastjerdi, University of Ottawa, Canada
53. **Acrylic-graphene oxide latexes prepared by semicontinuous emulsion polymerization** N/A
Maria Esther Trevino, CIQA, Mexico
54. **The dynamics of phase separation within latex particles during emulsion polymerization** N/A
John Tsavalas, University of New Hampshire, USA
55. **Acyclic diene and triene metathesis polymerization in miniemulsion** N/A
Pedro Henrique H. Araujo, Federal University of Santa Catarina, Brazil
56. **Polymeric surfactants based on maleamic acid copolymers** N/A
Odilia Perez, Centro de Investigacion en Quimica Aplicada, Mexico

Free Radical Polymerization

57. **From plant to lab scale: Challenges and solutions for semi-batch experiments to determine homo- and copolymerization kinetics** N/A
Kaytlin M. Henry, The Dow Chemical Company, USA
58. **Microgels based on N-isopropylacrylamide and acrylic acid: Study of stability and pH sensitivity** N/A
Esmar Faben Souza, Universidade de São Paulo, Brazil
59. **Modeling and measurement of aqueous phase non-ionized acrylic acid/ acrylamide copolymerization** N/A
Calista Preusser, Queen's University, Canada
60. **Kinetics of copolymerization of acrylamide and MADAMBQ** N/A
Arkom Drawpateep, Martin Luther University, Germany

61. **Radical copolymerization of hydroxy-functional monomers: Kinetic and semibatch studies** N/A
Jan E. S. Schier, Queen's University, Canada
62. **Molecular Weight Distribution (MWD) of low-density PE near gel regime** N/A
Piet D. Iedema, Universiteit van Amsterdam, Netherlands
63. **Composition drift in copolymer microstructure** N/A
Piet D. Iedema, Universiteit van Amsterdam, Netherlands
64. **On the minimal number of molecules used in kinetic Monte Carlo simulations of free radical polymerization** N/A
Hanyu Gao, Northwestern University, USA

Combined Topics

65. **Kinetic modeling of ethylene/1-octene living copolymerization catalyzed by fluorinated FI-Ti** N/A
Bo-Geng Li, Zhejiang University, China
66. **CO₂/N₂ triggered switchable surfactants** N/A
Bo-Geng Li, Zhejiang University, China
67. **Miniemulsion polymerization Of styrene: Modeling and experimental validation** N/A
Esmar Souza, University of Sao Paulo, Brazil
68. **Encapsulation of thermochromic pigment using miniemulsion polymerization** N/A
Maria Veronica Carranza Oropeza, University of São Paulo, Brazil