Polymer Reaction Engineering VIII

May 6 - 11, 2012

Cancun, Mexico

Conference Chair

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University of Ottawa, Canada

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Sunday, May 6, 2012

16:00 – 18:00	Registration (Hotel Lobby)
18:00 – 19:00	Opening Reception (Terraza Veranda)
19:00 – 20:30	Dinner (Terraza Veranda)

NOTES

- Technical sessions will be held in El Greco room.
- Poster Sessions will be in the Picasso – Murillo – Miro rooms. Although there are two poster sessions, posters will remain mounted for the entire conference. Posters may be hung on Monday prior to 6:30 pm and should be removed after lunch on Thursday.
- Breakfasts are at the main dining hall (Quetzal) and are served buffet style. Breakfast opens at 6:30.
- Lunches will be at the LaPerla Restaurant.
- Dinners on Sunday, Monday, Tuesday and Wednesday will be at Terraza Veranda. The Thursday evening banquet will be in the Picasso – Murillo – Miro rooms.
- Audiotaping, videotaping and photography of presentations are strictly prohibited.
- Speakers – Please leave at least 5 minutes for questions and discussion.
- Please do not smoke at any conference functions.
- Turn your cellular telephones to vibrate or off during technical sessions.
- Be sure to make any corrections to your name/contact information on the Master Participant List or confirm that the listing is correct. A corrected electronic copy will be sent to all participants after the conference.
- The hotel has wi-fi. We recommend using your own ethernet cable should you need a faster speed as most guests bring smart phones, iPads and laptops, thereby slowing access.

Monday, May 7, 2012

06:30 Buffet Breakfast opens (Quetzal)

Session 1: New Trends in Polymer Reaction Engineering
Co-chairs: **Philipp Mueller** (DuPont, USA) & **Giuseppe Storti** (ETH Zurich)

08:15 - 08:25 Conference Welcome/Overview (Marc Dubé, Bill Sachs)

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

08:30 - 09:15 **Marco Lattuada** (University of Fribourg, Switzerland)
Structured polymeric-inorganic nanocomposites via magnetically-driven self-assembly

09:15 - 10:00 **Eugenia Kumacheva** (University of Toronto, Canada)
Microfluidic synthesis of polymer particulate materials: an engineering perspective

10:00 - 10:20 **Rebekka Siegmann** (University of Potsdam, Germany)
Azide-terminated poly(vinylidene fluoride) as building block for nanocomposite materials and amphiphilic block copolymers

10:20 - 10:40 Coffee break

10:40 - 11:25 **Marco Dossi** (Solvay Specialty Polymers, Italy)
Novel characterization techniques to identify and quantify chain ends of vinylidene fluoride/hexafluoropropylene copolymers

11:25 - 11:45 **Eric Neuhaus** (Technische Universitaet Darmstadt, Germany)
Modelling the polymeric microstructure of LDPE with a novel hybrid simulation approach

11:45 - 12:05 **Benoit Lessard** (McGill University, Canada)
Fluorescent, thermo-responsive copolymers synthesized by nitroxide mediated polymerization

12:05 - 13:55 Lunch at LaPerla Restaurant

Session 2: **Polymer Process Monitoring, Control and Simulation**

Sponsored by BASF

Co-chairs: **Klaus-Dieter Hungenberg** (BASF, Germany) & **Alex Penlidis** (University of Waterloo, Canada)

13:55 - 14:00 Introduction by co-chairs

14:00 - 14:45 **Philipp Mueller** (DuPont, USA)
A comprehensive polymerization model for online industrial process control

14:45 - 15:30 **Davide Moscatelli** (Politecnico di Milano, Italy)
QM, a powerful tool in polymer reaction engineering

15:30 - 15:50 **Juraj Kosek** (ICT Prague, Czech Republic)
Mathematical modeling of heat transfer in micro- and nano-cellular polymer foams

Monday, May 7, 2012 (continued)

15:50 - 16:10 Coffee break

16:10 - 16:55 **Ursula Tracht** (Bayer, Germany)
Kinetic modeling from early product development to polymerization process optimization

16:55 - 17:40 **Vincent Gomes** (University of Sydney, Australia)
Living emulsion polymerization with RAFT: Modelling and optimal operating strategies

17:40 - 18:00 **Peter Singstad** (Cybernetica, Norway)
A Mechanistic Modelling Suite for Nonlinear Model Predictive Control of Emulsion Polymerization Reactors

18:30 - 20:30 **Poster Session 1 and Social Hour**
Co-chairs: **Jon Debling**, BASF, USA**; Milan Maric**, McGill Univ., Canada; **Davide Moscatelli**, Politecnico di Milano, Italy

20:30 - 22:00 Dinner at Terraza Veranda

Tuesday, May 8, 2012

06:30 Buffet Breakfast opens (Quetzal)

Session 3: Sustainable Polymer Reaction Engineering
Co-chairs: **John Eng** (DuPont, USA) & **Mike Cunningham** (Queen's University, Canada)

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

08:30 - 09:15 **John Eng** (DuPont, USA)
Process Development Aspects of Cerenol® Polymer

09:15 - 10:00 **James Rawlins** (University Southern Mississippi, USA)
Emulsion copolymerization of vegetable oil macromonomers possessing both acrylic and allylic functionality

10:00 - 10:20 **Roque Minari** (INTEC (Universidad Nacional del Litoral), Argentina)
Production of acrylic-casein hybrid latices by emulsion polymerization

10:20 - 10:40 Coffee break

10:40 - 11:25 **Jean Bouchard** (FP Innovations, Canada)
Industrialization of nanocrystalline cellulose

11:25 – 11:45 **Pascale Champagne** (Queen's University, Canada)
Graft modification of cellulose in ionic liquids via living radical polymerization

11:45 - 12:05 **Claudia Sayer** (Federal University of Santa Catarina, Brazil)
Encapsulation of vegetable oils by miniemulsion polymerization. Effect on molar mass distribution

12:05 - 14:00 Lunch at LaPerla Restaurant /Tour to Tulum departs

14:00 – 20:30 *ad hoc* sessions/Free time/Return from Tulum

20:30 - 22:00 Dinner at Terraza Veranda

Wednesday, May 9, 2012

06:30 Buffet Breakfast opens (Quetzal)

Session 4: Industrial Process Innovation in Polymer Reaction Engineering

Sponsored by CONACYT

Co-chairs: Min Zhang (DuPont, USA); *the late George Kalfas* (DuPont, USA)

08:25 - 08:40 Remembering Drs. George Kalfas & Tuyu Xie

08:40 – 08:45 Introduction by co-chair

08:45 - 09:25 **Dan Arriola** (Dow, USA)
Engineering of Polymer Chain Shuttling Systems

09:25 – 09:45 **Zhen Liu** (Karlsruhe Institute of Technology (KIT), Germany)
Continuous free radical polymerization in a Taylor-Couette reactor

09:45 – 10:05 **Christian H. Hornung** (CSIRO Materials Science & Engineering, Australia)
Sequential continuous flow polymerization for the synthesis of RAFT block copolymers

10:05 - 10:45 **Masoud Soroush** (Drexel University, USA)
Lasting Academia-Industry Collaboration: Challenges and Rewards

10:45 - 11:05 Coffee break

11:05 - 11:25 **Isabel Kadel** (Technische Universitaet Darmstadt, Germany)
Modelling the effect of functionalized co-monomers in tubular LDPE reactors

11:25 – 11:45 **Andreas Daiss** (BASF, Germany)
Process analysis in an early development phase by modeling and simulation

11:45 – 12:05 **Ivano Costa** (Sulzer Chemtech Ltd., Switzerland)
Industrial PLA production by bulk ring-opening polymerization of lactides in a continuous process

12:05 - 14:00 Lunch at LaPerla Restaurant

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

18:30 - 20:30 **Poster Session 2 and Social Hour**

Co-chairs: **Jon Debling**, BASF, USA**; Milan Maric**, McGill University, Canada; **Davide Moscatelli**, Politecnico di Milano, Italy

20:30 - 22:00 Dinner at Terraza Veranda

Thursday, May 10, 2012

06:30 Buffet Breakfast opens (Quetzal)

Session 5: Novel Polymer Applications
Co-chairs: Timothy Klots (BASF, USA) & Tim Bender (Univ. of Toronto, Canada)

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

08:30 - 09:15 **Karl Matos** (BASF, USA)
Organoborane as very effective polymer initiators to enable bonding of low energy surface olefins

09:15 - 10:00 **Tim Bender** (University of Toronto, Canada)
Polymer design and processing considerations for organic light emitting diodes and organic solar cells

10:00 - 10:20 **Jens Buller** (University of Potsdam, Germany)
Protein recognition by responsive polymers

10:20 - 10:40 Coffee break

10:40 - 11:20 **Ernesto Rivera-García** (UNAM, Mexico)
Synthesis and NLO Properties of Poly(Ethylene Glycol) Diacrylate Copolymers Containing Azobenzene Groups Prepared by Frontal Polymerization

11:20 - 11:40 **Daisuke Kobayashi** (Tokyo University of Science, Japan)
Design of new reaction fields for spherical polypyrrole particle synthesis

11:40 - 12:00 **Katherine M. E. Stewart** (University of Waterloo, Canada)
A polymeric sensor for the detection of formaldehyde

12:00 - 12:20 **Giuseppe Storti** (ETH Zurich, Switzerland)
Novel Functional Macroporous Supports: from Preparation to Application

12:20 - 13:55 Lunch at LaPerla Restaurant

Session 6: Recent Advances in Heterogeneous Polymerization
Co-chairs: **Isabel Saenz de Buruaga** (Comex, Mexico) & **Jose Ramon Leiza** (University of the Basque Country UPV/EHU, Spain)

13:55 - 14:00 Introduction by co-chairs

14:00 - 14:45 **Aitziber Lopez** (University of the Basque Country UPV/EHU, Spain)
Design and production of waterborne polyurethane/acrylic hybrid PSAs

14:45 - 15:30 **Harm Wiese** (BASF SE)
Nanocomposite dispersions - From basic research to large scale applications

15:30 - 15:50 **Pedro Henrique Hermes de Araújo** (Federal University of Santa Catarina, Brazil)
Encapsulation of nickel nanoparticles in polystyrene via miniemulsion polymerization

Thursday, May 10, 2012 (continued)

15:50 - 16:10 Coffee break

16:10 - 16:55 **John Tsavalas** (University of New Hampshire, USA)
Morphology development of structured latex particles as influenced by water content and water-interacting functional groups

16:55 - 17:40 **Isabel Saenz de Buruaga** (Comex, Mexico)
Environmentally friendly paint using controlled radical polymerization in emulsion polymerization

17:40 - 18:00 **Kathleen Krüger** (Max Planck Institute, Germany)
The Role of Gas in Radical Heterophase Polymerization

18:00 - 19:00 **Social Hour**

19:00 - 22:00 Conference Banquet (Picasso – Murillo – Miro rooms)

Guest Speaker: Jesús Álvarez-Calderón, Professor, Universidad Autónoma Metropolitana, Plantel Iztapalapa (UAM-I), Mexico City, Mexico. National Researcher, Level III, Sistema Nacional de Investigadores (S.N.I.), México.S.N.I. Director, CONACYT, México
Control of batch emulsion polymerization reactors

Friday, May 11, 2012

06:30 Buffet breakfast opens (Quetzal)

Polymer Reaction Engineering VIII
Poster List

1. **Simultaneous *in situ* sorption and swelling of polymers with gases and supercritical fluids 2: Measurements and modeling with the Sanchez-Lacombe equation of State**
   Philipp Mueller, E. I. du Pont de Nemours and Company, USA

2. **The influence of different operating conditions on the performance of the living free radical polymerization (LFRP) in emulsion**
   Eduardo Galhardo, University of Campinas, Brazil

3. **Individual rate coefficients for homogeneous phase copolymerization of fluorinated olefins in supercritical CO_2**
   Rebekka Siegmann, University of Potsdam, Germany

4. **Towards network homogeneity indicators in crosslinking nitroxide-mediated radical copolymerization of styrene and divinylbenzene**
   Afsaneh Nabifar, University of Waterloo, Canada

5. **Experimental and theoretical investigation of acrylic copolymer reactivity and solvent effect**
   Danilo Cuccato, Politecnico di Milano, Italy

6. **Synthesis of functionalized nanoparticles for detection and characterization of amyloid fibrils**
   Davide Moscatelli, Politecnico di Milano, Italy

7. **Polyesters through free radical polymerization: A new synthesis route for biodegradables nanoparticles**
   Davide Moscatelli, Politecnico di Milano, Italy

8. **Converting PET to a glass-like water barrier for flexible photovoltaics**
   Kenneth W. Leffew, DuPont Central Research & Development, USA

9. **Detailed microstructure investigation of homo and copolymers of acrylate monomers by kinetic Monte Carlo simulation**
   Shaghayegh Hamzehlou, University of Basque Country, Spain

10. **Continuous free radical polymerization in a Taylor-Couette reactor**
    Zhen Liu, Karlsruhe Institute of Technology (KIT), Germany

11. **Model based design of controlled radical polymerization**
    Dagmar R. D'hooge, Ghent University, Belgium

12. **Kinetic modeling as a tool to evaluate the importance of diffusional limitations and nitroxide partitioning in styrene nitroxide mediated miniemulsion polymerization**
    Dagmar R. D'hooge , Ghent University, Belgium

13. **Optimization of ICAR ATRP of styrene at low catalyst ppm levels**
    Dagmar D'hooge, Ghent University, Belgium

Polymer Reaction Engineering VIII
Poster List

14. **Synthesis of core-shell particles of polystyrene and polymethylmethacrylate using emulsion photopolymerization**
Reinaldo Giudici, Universidade de São Paulo, Brazil

15. **Azide-terminated poly(vinylidene fluoride) as building block for nanocomposite materials and amphiphilic block copolymers**
Rebekka Siegmann, University of Potsdam, Germany

16. **A polymeric sensor for the detection of formaldehyde**
Katherine M. Stewart, University of Waterloo, Canada

17. **Modeling of reactive extrusion: Application of a new method to MMA polymerization**
Jean-Pierre Puaux, Universite Claude-Bernard Lyon 1, France

18. **Kinetic modeling of the full molecular weight distribution (FMWD) in addition polymers**
Ivan Zapata, Universidad Autónoma de Coahuila, Mexico

19. **The effect of polymer microstructure and thermal post-treatment on latex-based pressure sensitive adhesive performance**
Marc A. Dubé, University of Ottawa, Canada

20. **Stimuli-responsive polyglycerol hydrogels from renewable feedstocks**
Marc A. Dubé, University of Ottawa, Canada

21. **Kinetic study of anionic ring opening polymerization of octamethylcyclotetrasiloxane in emulsion**
Ines Mohoric, Hidria Institute for Materials and Technologies, Slovenia

22. **Mass transfer and kinetics in heterophasic copolymerization of propylene**
Thomas Kröner, University of Halle-Wittenberg, Germany

23. **A semi-analytical model predicting MWD and branching distribution of terminally branched polymers undergoing random scission**
Piet D. Iedema, Universiteit van Amsterdam, The Netherlands

24. **Modeling interchange reactions between linear and branched polycondensates of the AB2-type**
Piet D. Iedema, Universiteit van Amsterdam, The Netherlands

25. **Modelling the effect of functionalized co-monomers in tubular LDPE reactors**
Isabel Kadel, Technische Universitaet Darmstadt, Germany

26. **Modelling the polymeric microstructure of LDPE with a novel hybrid simulation approach**
Eric Neuhaus, Technische Universitaet Darmstadt, Germany

27. **Modelling topological scission in ldPE**
Nazila Yaghini, Universiteit van Amsterdam, The Netherlands

Polymer Reaction Engineering VIII
Poster List

28. **Efficient treating convolutions in multi-dimensional population balance modelling of polymer modification**
Ivan Kryven, University van Amsterdam, The Netherlands

29. **Initiating species in spontaneous thermal free-radical polymerization of alkyl acrylates**
Masoud Soroush, Drexel University, USA

30. **Quantitative NMR spectroscopy analysis for determination of polymer microstructure**
Ruzica Kasalo, Technische Universitaet Darmstadt, Germany

31. **Relating environmental stress cracking resistance (ESCR) of polyethylene with microstructural properties using tensile and extensional flow methods**
Pouyan Sardashti, University of Waterloo, Canada

32. **How micromixing of peroxides into ethylene affects the operation of industrial tubular reactors for high-pressure radical polymerisation of ethylene**
Christoph J. Dittrich, SABIC Technology Center, The Netherlands

33. **A framework for kinetic modeling of aqueous-phase acrylic acid / acrylamide copolymerization**
Calista Preusser, Robin Hutchinson, Queen's University, Canada

34. **Free radical copolymerization kinetics of hydroxy-functional monomers for application in the automotive coatings industry**
Kun Liang, Queen's University, Canada

35. **Investigation of the devolatilization behavior in twin-shaft kneader-processors**
Oliver Seck, Institute of Polymer Materials and Processes, Germany

36. **Impact of torque and stress on kneader-processors**
Oliver Seck, Institute of Polymer Materials and Processes, Germany

37. **Kinetics of ring-opening polymerization of L,L-lactide**
Giuseppe Storti, ETH Zurich, Switzerland

38. **Degradation kinetics of poly(lactic acid) oligomers in solution**
Giuseppe Storti, ETH Zurich, Switzerland

39. **Novel functional macroporous supports: From preparation to application**
Giuseppe Storti, ETH Zurich, Switzerland

40. **Polyacrylamide hydrogels with gradients in mechanical stiffness for differential cell response**
Marco Lattuada, ETH Zurich, Switzerland

41. **Carbazole containing poly(4-acryloylmorpholine) amphiphilic statistical copolymers and block copolymers by nitroxide mediated polymerization**
Benoît Lessard, McGill University, Canada

Polymer Reaction Engineering VIII
Poster List

42. **Fluorescent, thermo-responsive copolymers synthesized by nitroxide mediated polymerization**
Benoît Lessard, McGill University, Canada

43. **Poly(methacrylates) by nitroxide-mediated controlled radical polymerization**
Benoît Lessard, McGill University, Canada

44. **Poly cyanoacrylate-based biodegradable copolymers**
Evangelos Mavroudakis, Politecnico di Milano, Italy

45. **State estimation in polymer processes using delayed measurements**
Mariano Asteasuain, Planta Piloto de Ingeniería Química (PLAPIQUI), Argentina

46. **Industrial PLA production by bulk ring-opening polymerization of lactides in a continuous process**
Liborio Ivano Costa, Sulzer Chemtech Ltd, Switzerland

47. **Thermal properties of Sulzer polylactides**
Liborio Ivano Costa, Sulzer Chemtech Ltd, Switzerland

48. **Mathematical modelling of response of polyacrylamide gel dosimeters to brachytherapy radiation**
Kim B. McAuley, Queen's University, Canada

49. **Kinetic model for non-oxidative thermal degradation of Nylon 66**
Kim B. McAuley, Queen's University, Canada

50. **Model development and parameter estimation for styrene polymerization**
Kim B. McAuley, Queen's University, Canada

51. **Micromixing effects on the dynamic behavior of continuous free-radical solution polymerization reactors**
Priamo Melo, Universidade Federal do Rio de Janeiro, Brazil

52. **Analysis of tubular solution polymerization reactors with the help of CFD tools**
Priamo Melo, Universidade Federal do Rio de Janeiro, Brazil

53. **Analysis of gradient effects on polymerizations performed in stirred tank reactors with the help of CFD tools**
Priamo Melo, Universidade Federal do Rio de Janeiro, Brazil

54. **Modeling of free-radical solution styrene polymerization reactors using multifunctional initiators**
Priamo Melo, Universidade Federal do Rio de Janeiro, Brazil

55. **Sequential continuous flow polymerization for the synthesis of RAFT block copolymers**
Christian H. Hornung, CSIRO Materials Science & Engineering, Australia

Polymer Reaction Engineering VIII
Poster List

56. **Design of new reaction fields for spherical polypyrrole particle synthesis**
Daisuke Kobayashi (Tokyo University of Science, Japan)

57. **A mechanistic modelling suite for nonlinear model predictive control of emulsion polymerization reactors**
Peter Singstad, Cybernetica, Norway

58. **Kinetics of the aqueous phase polymerization of N-Vinylformamide**
Julieta Zataray, University of the Basque Country, Spain

59. **Mathematical modeling of styrene/divinylbenzene copolymerization comprising diffusional effects and cyclization kinetics**
Leandro G. Aguiar, Univ. S. Paulo, Brazil

60. **Polymer nanoparticles for biomedical application**
Marco Dossi, Politecnico di Milano, Italy

61. **Simulation study of the nitroxide mediated copolymerization of styrene and alpha-methyl styrene under different reactor configurations**
Mariano Asteasuain, Planta Piloto de Ingenieria Quimica (PLAPIQUI), Argentina

62. **On-line control of polyethylene production by Raman spectroscopy and chemometrics**
Patice Bourson, Laboratoire Matériaux Optiques, France

63. **Mathematical modeling of heat transfer in micro- and nano-cellular polymer foams**
Juraj Kosek, ICT Prague, Czech Republic

64. **Detecting decomp precursor events in a tubular LDPE reactor**
Craig Hulet, Nova Chemicals, Canada

65. **Experimental study and PC-SAFT simulations of sorption equilibria in polyethylene**
Juraj Kosek, ICT Prague, Czech Republic

66. **Dynamic model of SBR production by emulsion polymerization**
Josef Chmelar, ICT Prague, Czech Republic

67. **Mapping of the high-impact polypropylene morphology**
Juraj Kosek, ICT Prague, Czech Republic

68. **Pseudo-solid state polymerization in amorphous polymer micro-layers: A novel route to produce ultra-high molecular weight polycarbonate**
Kyu Yong Choi, University of Maryland, USA

69. **Polybutadiene incoporation during styrene miniemulsion polymerization**
Pedro Henrique Hermes de Araujo, Federal University of Santa Catarina, Brazil

Polymer Reaction Engineering VIII
Poster List

70. **Design of a copper tubular reactor for continuous controlled radical polymerization of acrylic polymers**
Nicky Chan, Queen's University, Canada

71. **Low catalyst concentration atom transfer radical polymerization in a CSTR**
Nicky Chan, Queen's University, Canada

72. **Synthesis of PS hybrid nanoparticles with preformed polymers of varied compatibility by miniemulsion polymerization**
Luis Gugliotta, INTEC, Universidad Nacional del Litoral, Argentina

73. **Production of acrylic-casein hybrid latices by emulsion polymerization**
Roque Minari, INTEC, Universidad Nacional del Litoral, Argentina

74. **Improving the properties of styrene - acrylic oligomers**
Timothy Klots, BASF Corporation, USA

75. **Polymerization and drying of levitated droplets**
H.-U. Moritz, University of Hamburg, Germany

76. **Modeling of network formation in the production of hydrogels in the presence of RAFT controllers**
Eduardo Vivaldo-Lima, Universidad Nacional Autónoma de México, Mexico

77. **RAFT copolymerization of methyl methacrylate and ethylene glycol dimethacrylate in supercritical carbon dioxide**
Eduardo Vivaldo-Lima, Universidad Nacional Autónoma de México, Mexico

78. **An experimental study on the NMRP copolymerization of styrene and divinylbenzene in supercritical carbon dioxide**
Gabriel Jaramillo-Soto, Universidad Nacional Autónoma de México, Mexico

79. **Modeling the molecular weight distribution of XSBR latexes produced in a seeded semibatch emulsion pilot plant reactor**
Jose Ramon Leiza, University of the Basque Country (UPV/EHU), Spain

80. **Real-time compositional control of semibatch copolymerizations**
Kenneth W. Leffew, DuPont Central Research & Development, USA