

Program

Polymer Reaction Engineering VI

May 21 - 26, 2006

Delta Halifax Hotel
1990 Barrington Street
Halifax, Nova Scotia, Canada B3J 1P2
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Co-sponsored by AIChE

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Robin A. Hutchinson
Queen's University

Conference Co-Chairs

Michael Muhle
ExxonMobil Chemical Co.

Alex Penlidis
University of Waterloo

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The conference chairs and organizers would like to thank the following for their generous support of this conference:

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Sunday, May 21, 2006

16:00 – 18:00	Registration
18:00 – 18:30	Welcome Reception
18:30 – 20:00	Dinner
20:00 – 21:00	Social Hour

Important Notes

All oral sessions will be held in Baronet 1, 2, 5 and 6.

Poster sessions will be held in Baronet 2, 3, 4 and 5. (Room is being re-set after oral session.)

Posters in Session I should be mounted on Monday.

Posters in Session II should be mounted on Wednesday.

Meals will be held in the following areas:

Sunday dinner – Bluenose Ballroom

Monday – breakfast, lunch and dinner – Bluenose Ballroom

Tuesday – breakfast, lunch and dinner – Bluenose Ballroom

Wednesday breakfast – Baronet 3 and 4

Wednesday lunch – on your own

Wednesday dinner – Bluenose Ballroom

Thursday breakfast – Baronet 3 and 4

Thursday lunch – Baronet 3 and 4 (and possibly Mayflower, depending on the number of people who order boxed lunches) – Be sure to be at the Tall Ship Silva for 1:30 boarding. You will find the ship at Queen's Wharf, at the foot of Prince Street, on the Halifax waterfront. Drinks will be available for purchase on the ship. Return to pier at 3:30.

Thursday dinner – on your own

Friday breakfast – Baronet 3 and

Audio taping, videotaping and photography of presentations are prohibited.

Please do not smoke at any conference functions.

Turn your cell phones to *vibrate* or *off* during technical sessions.

Monday, May 22, 2006

07:00 – 08:15 Breakfast

08:15 – 08:30 Conference Welcome and Overview
Conference Chair and ECI Representative

Session I: Polymerization Fundamentals

Chairs: **M. Cunningham** and **J. Kosek**

08:30 – 09:15 *Fundamentals and Reaction Engineering Aspects of ATRP*
Shipping Zhu, McMaster University, Canada

09:15 – 10:00 *Fundamental Aspects of Nanometer Scale Morphology Development in Synthetic Latex Particles*
Don Sundberg, University of New Hampshire, USA

10:00 – 10:20 *PLP Investigations into the Kinetics of Free-Radical Homopolymerizations of Water-Soluble Monomers in Aqueous Phase*
Sabine Beuermann, University of Göttingen, Germany

10:20 – 10:45 Coffee Break

10:45 – 11:30 *Hydrodynamics of Polyolefin Fluidized Bed Reactors*
Apostolos Kantzas, University of Calgary, Canada

11:30 – 12:15 *Real-Time FTIR Monitoring of the Carbocationic Copolymerization of Isobutylene with Styrene*
Judit Puskaş, University of Akron, USA

12:15 – 14:00 Lunch

17:00 – 19:00 **Poster Session I (with social hour)**

19:00 - **Dinner**

Tuesday, May 23, 2006

07:00 – 08:30 Breakfast

Session II: New Mathematical Modeling

Chairs: **J. Asua** and **K.Y. Choi**

08:30 – 09:20 *Modeling of Polymerization Reactors using CFD Techniques*
Nitin Kolhapure, DuPont, USA

09:20 – 10:10 *Modeling of Polyolefin Particle Morphology*
Juraj Kosek, Prague ICT, Czech Republic

10:10 – 10:40 Coffee Break

10:40 – 11:00 *Dynamic Monte Carlo Simulation of Olefin Polymerization with Coordination Catalysts: Applications in High-Throughput, Semi-Batch Stop-Flow, and Tubular Reactors*
Joao Soares, University of Waterloo, Canada

11:00 – 11:50 *Kinetic Modeling of Nonlinear Free Radical Polymerizations*
Mário Rui Costa, University of Porto, Portugal

11:50 – 12:10 *Prediction of MWDs based on ab initio Calculations: Application to the High Temperature Styrene Polymerization*
Davide Moscatelli, Politecnico di Milano, Italy

12:15 – 15:00 Lunch

Session III: Measurement and Control

Chairs: **T.F. McKenna** & **J.C. Pinto**

15:00 – 15:50 *Automatic Continuous Online Monitoring of Polymerization Reactions (ACOMP) and its Applications*
Wayne Reed, Tulane University, USA

15:50 – 16:40 *Simultaneous Process and Control System Design*
Claudia Sarmoria, Universidad Nacional del Sur, Argentina

16:40 – 17:00 Coffee Break

17:00 – 17:20 *Monitoring Industrial Polymerization Reactors for Early Detection of Agglomeration*
Ruud van Ommen, Technical University of Delft, Netherlands

17:20 – 18:10 *Model Based Control in the Polymer Industry*
Magne Hillestad, Cybernetica, Norway

18:10 – 18:30 *Open Loop Industrial Polymerization Reactors: How long does it take to reach steady state after disturbances?*
Zhang Min, Dow Chemical Company, USA

19:00 – 20:30 Dinner

20:30 – 21:30 Social Hour

Wednesday, May 24, 2006

07:00 – 08:30 Breakfast

Session IV: New Polymerization Systems

Chair: **W.H. Ray** and **M. Morbidelli**

08:30 – 09:20 *Polymer Synthesis: Towards Controlled 2D and 3D Structures*
Dieter Schlüter, ETH Zurich, Switzerland

09:20 – 09:45 *Phase Inversion in Free-Radical Bulk Graft Polymerization: Experimental Study and Monte Carlo Simulation*
Bo-Geng Li, Zheziang University, China

09:45 – 10:10 *Polymerization Compounding on the Surface of Nanoparticles*
Babak Esmaeili, Poly Montreal, Canada

10:10 – 10:40 Coffee Break

10:40 – 11:30 *Reaction Engineered Polymer Nanocomposites*
Leonardo Simon, University of Waterloo, Canada

11:30 – 11:55 *Reaction of Microbial Polysaccharide and Blocked Polyisocyanate to Produce Polyurethane Networks*
Natali Kozak, NAS of Ukraine

12:15 – 17:00 Lunch on your own and free afternoon

17:00 – 19:00 **Poster Session II** with social hour

19:00 Banquet

20:30 **Plenary Lecture**
Innovation Chain at BASF – An Example for the Process of Innovation in the Chemical Industry
Thomas Bott, BASF

Thursday, May 25, 2006

07:00 – 08:30 Breakfast

Session V: PRE and Industrial Process Innovation

Chairs: **K-D Hungenberg** and **A. Penlidis**

08:30 – 09:10 *Research Parks, Incubators, and Technology Transfer: The Expanding Role of the University in Industrial Innovation*
Ken Malone, University of Southern Mississippi, USA

09:10 – 09:50 *The Advanced Polymerization Technology Platform, an Example of the Interdisciplinary R&D in Degussa Project Houses*
Rüdiger Carloff, Degussa, Germany

09:50 – 10:20 *Competition and Cooperation between Start-ups and Established Firms in Commercializing Emerging Technologies*
Fred Pries, University of Waterloo, Canada

10:20 – 10:50 Coffee Break

10:50 – 11:30 *Innovative Polymer Product and Process Development at DuPont*
Ken Leffew, DuPont, USA

11:30 – 12:10 *From Emulsion Polymerization to Disease Detection: A Path of Innovation*
Luis Garcia-Rubio, University of Southern Florida, USA

12:15 – 13:30 Lunch followed by Halifax Harbour Cruise on the Tall Ship *Silva*. Go to the Queen's Wharf, at the foot of Prince Street. Board at 1:30 pm and return to pier at 3:30 pm

Dinner on your own

Friday, May 26, 2006

07:00 – 08:30 Breakfast

Session VI: Industrial Applications

Chairs: **M. Grady** and **M. Bartke**

08:30 – 09:20 *Dispersion Polymerization in Supercritical Fluids*
Giuseppe Storti, ETH Zurich, Switzerland

09:20 – 09:45 *Continuous Reactor Concepts with Superimposed Secondary Flow:
Polymerization Process Intensification*
Werner Pauer, University of Hamburg, Germany

09:45 – 10:10 *Polymers: Properties and Polymerization Processes (P4): An Integrated Model-
Based Framework for Rapid Scale-up and Efficient Identification of Novel
Polymers*
Charles Immanuel, Imperial College, UK

10:10 – 10:40 Coffee Break

10:40 – 11:30 *Bulk (Co)Polymerization in a Continuous Kneader Reactor*
Pierre-Alain Fleury, List AG, Switzerland

11:30 – 12:10 *A Straightforward and Unified Modeling Approach for Mixing of Non-Newtonian
Fluids in the Laminar, Transition and Turbulent Regions*
Karl-Heinz Wassmer, BASF

12:10 – 12:30 Conference Wrap-up

Departure