Polymer Reaction Engineering

An Industrial Short Course on Olefin Polymerization Processes

April 19-23, 2008

Course Coordinators

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Professor
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Invited Speakers

Mamdouh Al-Harthi
Assistant Professor
King Fahd University of Petroleum and Minerals
Dhahran, Saudi Arabia

C.P. Cheng
Chief Technology Officer
Shanghai Süd-Chemie Catalysts Co., Ltd.
Shanghai, China

Location

JW Marriott
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Course Description

This is a one-week course designed for engineers, chemists and scientist in the area of olefin polymerization with coordination catalysts, polyolefin physical properties and microstructural characterization.

The course covers olefin polymerization, polyolefin characterization techniques and physical properties, starting from fundamental concepts and expanding to the state-or-the-art technology in the field. All sessions include case studies where the concepts covered in the lectures are applied to real case situations in laboratory and industrial scales. The lectures are designed in such a way that both beginners and specialists can benefit from the course.

Full course notes describing all subjects covered in the course are provided to the participants. Lectures will be given in English, but Professor Al-Harthi speaks Arabic and will be available all the time to clarify any questions that may occur.

Instructors

Professor João B.P. Soares (*http://chentserver.uwaterloo.ca/faculty/soares.html*) is a specialist in the areas of olefin polymerization kinetics and catalysis (Ziegler-Natta, metallocene, and late transition metal catalysts), mathematical modeling of olefin polymerization processes and polyolefin microstructural characterization.

Professor Leonardo C. Simon (*http://chentserver.uwaterloo.ca/faculty/simon.html*) is a specialist in the areas of coordination catalysts for olefin polymerization, modeling polymerization mechanisms, correlation synthesis-structure-properties of polymers, polymer nanocomposites and materials.

Professor Timothy McKenna (*http://www.chemeng.queensu.ca/people/mckenna/*) is a specialist in the area of polyolefin particle morphology and experimental methods for the evaluation of particle morphology, single particle modeling, and the production of impact copolymers.

Professor Mamdouh Al-Harthi (*http://www.kfupm.edu.sa/che/facf/alharthi.htm*) is a specialist in polymer reaction engineering models using population balances, method of moments, and Monte Carlo simulation.

Dr. C.P. Cheng (*http://www.sud-chemie.com*) is a specialist in polyolefins polymerization catalysts and processes with 25 years of industrial experience in Ziegler-Natta catalyst R & D, production and applications.

Registration

Please contact Professor Soares to register in the course by e-mail (*jsoares@uwaterloo.ca*), fax (519-746-4979) or telephone (519-888-4567 x 33436). The cost per person is US$ 3,500.00 for industrial participants and US$ 1,500.00 for academic participants.

The course fee includes registration and a hardcopy of the course notes. Special discounts exist for two or more participants from the same company. Please contact Professor Soares for more information.

Location

The course will be held at the JW Marriott, Harmarain Center, Abu Baker Al Siddique Road, Deira, Dubai, United Arab Emirates, Tel. (971)(4) 262 4444, Fax. (971)(4) 262 6264, E-mail: jwdubai.reservation@marriott.com, *http://www.marriott.com/hotels/travel/dxbae-jw-marriott-hotel-dubai/*

A special room rate is available for the course participants. Please contact the hotel directly to make your reservation after October 15, 2007.

Course Contents

Saturday, April 19 (9:00 – 17:00)

1. **Introduction to Polyolefins** (JBP Soares)
   - 1.1. Polyolefin types
   - 1.2. Polymerization reactor types
   - 1.3. Catalyst types
   - 1.4. Levels of mathematical modeling for polyolefin reactors
2. **Catalyst for Olefin Polymerization** (LC Simon)
   - 2.1. Ziegler-Natta, Phillips and vanadium catalysts
   - 2.2. Metallocene and late transition metal catalysts
   - 2.3. Mechanism of Coordination Polymerization
   - 2.4. Cocatalysts
   - 2.5. Catalyst supports
   - 2.6. Catalyst characterization (FTIR, NMR, UV-Vis, XAS)
3. **Industrial Reactors** (TF McKenna)
   - 3.1. Slurry processes
   - 3.2. Gas-phase processes
   - 3.3. Solution processes
4. **Principles of Mathematical Modeling** (JBP Soares)
   - 4.1. Population balances
   - 4.2. Method of instantaneous distributions
   - 4.3. Monte Carlo simulation

Sunday, April 20 (9:00 – 17:00)

5. **Polymerization with Single-Site Catalysts** (JBP Soares)
   - 5.1. Molecular weight distribution
   - 5.2. Chemical composition distribution
   - 5.3. Long chain branch distribution
6. **Single Particle Models: Transport Phenomena and Particle Growth I** (TF McKenna)
   - 6.1. Mass and heat transfer in growing polymer particles
   - 6.2. Polymeric flow and multigrain models
   - 6.3. New trends in single-particle modeling: particle morphology
7. **Polyolefin Microstructural Characterization I** (JBP Soares)
   - 7.1. Gel permeation chromatography
   - 7.2. Batch fractionation
   - 7.3. Extraction or solution fractionation
   - 7.4. Crystallization analysis fractionation
   - 7.5. Temperature rising elution fractionation
   - 7.6. Solution calorimetry
   - 7.7. Field flow fractionation
   - 7.8. Mass spectrometry
   - 7.9. Cross-fractionation
8. **Polyolefin Microstructural Characterization II** (LC Simon)
   - 8.1. Nuclear magnetic resonance (^{1}H and ^{13}C)
   - 8.2. Fourier transform infrared

Monday, April 21 (9:00 – 17:00)

9. Applications of mathematical modeling techniques (JBP Soares)
- 9.1. Chain walking and late transition metal catalysts
- 9.2. Production of thermoplastic elastomers via heterogeneous long chain branching
- 9.3. Production of linear-block olefin copolymers

10. Polyolefin Properties (LC Simon)
- 10.1. Crystallinity and morphology
  - 10.1.1. X-ray diffraction
- 10.2. Thermal analyses
  - 10.2.1. Differential scanning calorimetry
  - 10.2.2. Thermal gravimetric analysis
- 10.3. Thermal properties
  - 10.3.1. Melting point
  - 10.3.2. Glass transition
  - 10.3.3. Heat distortion temperature

11. Population Balances and the Method of Moments (JBP Soares)
- 11.1. Homopolymerization
- 11.2. Copolymerization and the method of pseudo-kinetic constants

12. Parameter Estimation for Polymerization Kinetic Models (JBP Soares)
- 12.1. Homopolymerization models
- 12.2. Copolymerization models
- 12.3. Effect of impurities on productivity and molecular weight

Tuesday, April 22 (9:00 – 17:00)

13. Single Particle Models: Transport Phenomena and Particle Growth II (TF McKenna)

14. Dynamic Monte Carlo Polymerization Modeling (M Al-Harthi and JBP Soares)
- 14.1. Stopped-flow reactors
- 14.2. Living and controlled polymerizations

15. Multiple-Site Catalysts (JBP Soares)
- 15.1. Characteristics of Ziegler-Natta and Phillips polymers
- 15.2. MWD deconvolution for Ziegler-Natta polymers
- 15.3. CCD deconvolution for Ziegler-Natta polymers
- 15.4. Mathematical models for TREF and CRYSTAF

16. Polyolefin Mechanical Properties and Testing (LC Simon)
- 16.1. Stress-strain curves
- 16.2. Dynamic mechanical properties
- 16.3. Impact testing
- 16.4. Creep

Wednesday, April 23 (9:00 – 17:00)

17. Industrial Catalysis and Polymerization Processes (CP Cheng)
- 17.1. Industrial reactor design considerations
- 17.2. Industrial catalyst manufacturing and testing
- 17.3. What are the requirements for a successful industrial catalyst?

18. Steady-State and Dynamic Simulation of Industrial Reactors in Series (JBP Soares)

19. Functional Polyolefins (LC Simon)
- 19.1. Catalysts for polar comonomer
- 19.2. Post-polymerization reactions
- 19.3. Properties of functional polyolefins

20. Polyolefin/Clay Nanocomposites (LC Simon)
- 20.1. Catalyst supports
- *20.2.* Properties of nanocomposites