Chem Eng 4B03/6B03 – Fall 2017 Polymer Reaction Engineering

Course Objective: To study polymerization kinetics (condensation, free radical, controlled radical, anionic, cationic, Ziegler-Natta, and metallocene), polymerization processes (bulk, solution, precipitation, suspension, emulsion, gas-phase, and slurry), polymerization reactor design and control (batch, semi-batch, and continuous). To study various polymer characterization methods, polymer chain structure and material property relationships, and some recent developments in the field.

Instructor: Dr. Darko Ljubic (JHE A105/C, ext. 27200, ljubicd@mcmaster.ca)

TA: Ms. Ilinka Mirkovic (JHE A105/B, ext. 27323, mirkoi1@mcmaster.ca)

Lecture Hours: Monday 2:30-3:20 pm; Wednesday 2:30-4:20 pm

Lecture Room: JHE-A102

Assessment: 4 assignments 20 %

2 hours midterm examination30 %2.5 hours final examination50 %

6B03 (Grad students only): 20% Extra work is required.

- There might be a grade adjustment recurving
- The final percentage grades will be converted to letter grades using the Registrar's recommended procedure.
- If you miss midterm with good reason, your midterm mark will be calculated from the class average midterm x your final / class average final; If you miss an assignment with a good reason, you are still required to do late submission and the mark is calculated from the same equation with respect to other assignments. This makeup policy does not apply if more than 50% assignments are missed.

Recommended textbooks:

- (1) Chem Eng 4B03/6B03 Course Notes (provided by the instructor).
- (2) S. Zhu, A.E. Hamielec "Polymerization Kinetic Modeling and Macromolecular Reaction Engineering" In: Matyjaszewski K and Möller M (eds.) Polymer Science: A Comprehensive Reference, Vol 4, pp. 779–831. Amsterdam: Elsevier BV (provided by the instructor).

- (3) Paul Hiemenz, Timothy Lodge, "Polymer Chemistry, The Basic Concepts", 2nd edition, Marcel Dekker, 2007
- (4) George Odian, "Principles of Polymerization", 4th edition, Wiley-Interscience, 2004

References:

- (1) J.A. Biesenberger, D.H. Sebastian, "Principles of Polymerization Engineering", John Wiley & Sons, 1983
- (2) A. Rudin, "The Elements of Polymer Science and Engineering", 2nd edition, Academic Press, 1998
- (3) H.R. Allcock, F.W. Lampe, J.E. Mark, "Contemporary Polymer Chemistry", 3rd edition, Prentice Hall, 2003
- (4) P.J. Flory, "Principles of Polymer Chemistry", Cornell University Press, 1953
- (5) J.M.G. Cowie, "Polymers: Chemistry and Physics of Modern Materials" 2nd Edition, Blackie A&P, 1994
- (6) R.J. Young, P.A. Lovel "Introduction to Polymers" 2nd edition, CRC, 2000
- (7) T.L. Richardson, "Industrial Plastics: Theory and Application", 2nd ed., Delmar Publishers, 1989

The Faculty of Engineering is concerned with ensuring an environment that is free of all discrimination. If there is a problem, individuals are reminded that they should contact the Department Chair, the Sexual Harassment Officer or the Human Rights Consultant, as the problem occurs.

University Policy: Academic dishonesty consists of misrepresentation by deception or by other fraudulent means and can result in serious consequences, e.g. the grade of zero on an assignment, loss of credit with a notation on the transcript (notation reads: "Grade of F assigned for academic dishonesty"), and/or suspension or expulsion from the university. It is your responsibility to understand what constitutes academic dishonesty. For information on the various kinds of academic dishonesty please refer to the Academic Integrity Policy, specifically Appendix 3.

"The instructor and university reserve the right to modify elements of the course during the term. The university may change the dates and deadlines for any or all courses in extreme circumstances. If either type of modification becomes necessary, reasonable notice and communication with the students will be given with explanation and the opportunity to comment on changes. It is the responsibility of the student to check their McMaster email and course websites weekly during the term and to note any changes."

Course Content

- 1. What is chemical engineering? What does a chemical engineer do? What is chemical reaction engineering? What is advanced/polymer reaction engineering?
- 2. What is polymer? From polymer to macromolecule. Polymer classification. Polymer properties. Polymer history
- 3. Polymerization mechanisms and kinetics: condensation polymerization, free radical polymerization, Ziegler-Natta polymerization.
- 4. Polymerization rate and polymer molecular weight distribution
- 5. Copolymerization. Copolymer composition. Penultimate model. Branching and crosslinking. Flory's theory of gelation
- 6. Batch, semi-batch and continuous reactors. Mass balance and reactor feeding policies. Heat balance and reactor cooling. Semi-batch control over polymer composition.
- 7. Bulk, solution and precipitation polymerizations. Suspension and emulsion polymerization
- 8. Influence of reactor type on polymer properties. RTD. Denbigh rules. Reactor dynamics and stability.
- 9. (Optional) Basic concepts and principles related to polymer processing: shear-thinning, viscoelasticity, relaxation and creeping, Boltzmann superposition principle, elastic modulus, storage modulus, shear modulus and dynamic viscosity, rheometry and dynamic mechanical analysis, temperature-time shifting factor.

10. (Optional) Basic concepts and principles related to polymer materials: glassy, rubbery and viscous states, semi-crystalline polymer Tg and Tm, crystallinity, elasticity, materials selection.