OUTLINE OF CHEMICAL ENGINEERING 3K4: JAN-APRIL, 2012
INTRODUCTION TO REACTOR DESIGN

Instructor:	Dr. P. Mhaskar (JHE-345A; Ext. 23273; email: mhaskar@mcmaster.ca)
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Lectures:	M, Th 12:30-1:20, T 1:30-2:20 ITB/AB102
Tutorials:	Th 15:30-17:20 (T01) T13/106 Fr 14:30-16:20 (T02) T13/106
Tests:	Schedule: Mid Term Test 1: Feb 2, 6-8 PM (Venue: TBA) Mid Term Test 2: March 14, 6-8 PM (Venue: TBA)
Notes:	The test and the exam will be open book and open course notes (slides).
Examination:	Final examination, 3 hours.
Calculators:	Any calculator may be used in the tests and final exam.

Grading:

Assignments	1 %	of final grade
In-class participation	1 %	" " "
Mid-terms	28%	" " "
Term project	10 %	" " "
Final exam	60 %	" " "

Revisions to the assignments/solutions/grades/Tutorials and announcements will be posted on avenue. The final percentage grades will be converted to letter grades using the Registrar's recommended procedure. Adjustments to final grades may be done at the discretion of the instructor. No make-up midterms will be given. Marks of missed midterm (with an official missed mark form) will be moved to the final exam.

Note: Late assignments will not be accepted. In class participation marks will be awarded on the basis of reasonable (even if incorrect) answers to questions asked in the class. Every reasonable response will earn 0.25% (By the next working day after the lecture day, email your question and answer to corbeb@mcmaster.ca with a copy to mhaskar@mcmaster.ca). Late emails will not be accepted.

Required Text: H.S. Fogler, *Elements of Chemical Reaction Engineering*, Prentice-Hall, 4rd Edition, 2006, Chapters 1-6, 8, 11, parts of Chapters 13&14.

Supplementary References:

1. J.M. Smith, *Chemical Engineering Kinetics*, McGraw-Hill (1981), 3rd Edition.
2. O. Levenspiel, *Chemical Reaction Engineering*, 2nd Edition, Wiley (1972). 3rd Edition (1999).

Outline (as in Fogler)

1. Mole Balances
   - 1.1 Definition of the Rate of Reaction
   - 1.2 The General Mole Balance Equation
   - 1.3 Batch Reactors
   - 1.4 Continuous Flow Reactors – CSTR and Tubular Reactors
   - 1.5 Industrial Reactors

2. Conversion and Reactor Sizing
   - 2.1 Definition of Conversion
   - 2.2 Batch Reactor Design Equations
   - 2.3 Design Equations for Flow Reactors
   - 2.4 Applications of the Design Equations
   - 2.5 Reactors in Series
   - 2.6 Some Further Definitions

3. Rate Laws and Stoichiometry
   - 3.1 Basic Definitions
   - 3.2 Reaction Order and Rate Law
   - 3.3 Reaction Rate Constant
   - 3.5 Batch Systems
   - 3.6 Flow Systems

4. Isothermal Reactor Design
   - 4.1 Design Structure for Isothermal Reactors
   - 4.2 Scale-Up of Liquid-Phase Batch Reactor Data to the Design of a CSTR
   - 4.3 Design of Continuous Stirred Tank Reactors (CSTRs)
   - 4.4 Tubular Reactors
   - 4.5 Pressure Drop in Reactors
   - 4.6 Synthesizing a Chemical Plant
   - 4.7 Mole Balances on CSTRs, PFRs, PBRs, and Batch Reactors
   - 4.9 Membrane Reactors
   - 4.10 Unsteady-State Operation of Stirred Reactors
   - 4.11 The Practical Side

5. Collection and Analysis of Rate Data
   - 5.1 Algorithm for Data Analysis
   - 5.2 Batch Reactor Data
   - 5.3 Method of Initial Rates
   - 5.4 Method of Half-Lives
   - 5.5 Differential Reactors
   - 5.6 Experimental Planning
   - 5.7 Evaluation of Laboratory Reactors

6. Multiple Reactions

- 6.1 Definitions
- 6.2 Parallel Reactions
- 6.3 Maximizing the Desired Product in Series Reactions
- 6.4 Algorithm for Solution to Complex Reactions
- 6.5 Multiple Reactions in a PFR/PBR
- 6.6 Multiple Reactions in a CSTR
- 6.7 Membrane Reactors to Improve Selectivity
- 6.9 Sorting it All Out
- 6.10 The Fun Part

8. Steady-State Nonisothermal Reactor Design

- 8.1 Rationale
- 8.2 The Energy Balance
- 8.3 Adiabatic Operation
- 8.4 Steady-State Tubular Reactor with Heat Exchange
- 8.5 Equilibrium Conversion
- 8.6 CSTR with Heat Effects
- 8.7 Multiple Steady States
- 8.8 Nonisothermal Multiple Chemical Reactions
- 8.10 The Practical Side

13. Distributions of Residence Times for Chemical Reactors

- 13.1 General Characteristics
- 13.2 Measurement of the RTD
- 13.3 Characteristics of the RTD
- 13.4 RTD in Ideal Reactors

Objectives

To develop a fundamental understanding of the application of principles of chemical kinetics, material balances, heat transfer and mass transfer to the modeling and design of chemical reactor systems. Students should be able to apply this knowledge to the formulation and solution of the following problem types:

a) Given the starting or inlet conditions and the specifications of a batch, stirred tank or tubular reactor, calculate the output concentrations and temperature of that reactor (rating problem).

b) Given the starting or inlet conditions and the desired output conditions, calculate the size of a batch, stirred tank or tubular reactor required (design problem).

c) Given a set of data for a reaction, establish a rate equation for that reaction.

POLICY REMINDER:

Academic Integrity:
You are expected to exhibit honesty and use ethical behaviour in all aspects of the learning process. Academic credentials you earn are rooted in principles of honesty and academic integrity.

Academic dishonesty is to knowingly act or fail to act in a way that results or could result in unearned academic credit or advantage. This behaviour 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 the various types of academic dishonesty please refer to the Academic Integrity Policy, located at **http://www.mcmaster.ca/academicintegrity**

The following illustrates only three forms of academic dishonesty:
1. Plagiarism, e.g. the submission of work that is not one's own or for which other credit has been obtained.
2. Improper collaboration in group work.
3. Copying or using unauthorized aids in tests and examinations.