OUTLINE OF CHEMICAL ENGINEERING 3K4: JAN-APRIL, 2017 INTRODUCTION TO REACTOR DESIGN

Instructor: Prashant Mhaskar (JHE-345A; Ext. 23273; mhaskar@mcmaster.ca)

TAs: Abhinav Garg (JHE-361; Ext 23263; garga7@mcmaster.ca)

Madeline Simpson (JHE 256; Ext 24008; simpsomj@mcmaster.ca) Wael El-Assad (JHE 364; Ext TBA; elassaaw@mcmaster.ca)

Lectures: Mon, Wed 8:30-9:20 ITB AB102

Friday 10:30-11:20 ITB AB102

Tutorials: Fri 2:30-4:20 (T01) JHE A101

Mon 2:30-4:20 (T02) JHE A102

Tests: Schedule:

In Class Test: Feb 6

Mid Term Test 1: Feb 14, 5:30-7:20 (MCMST T13 123)

Group Submission Due Feb 17 by 8:30 AM

Mid Term Test 2: March 14, 5:30-7:20 (MCMST BSB 106, MCMST BSB

119)

Group submission Due March 17 by 8:30 AM

Notes: The test and the exam will be open book and open course

notes/solutions/handwritten notes.

Examination: Final examination, 2 hours 30 minutes.

Calculators: Any calculator may be used in the tests and final exam.

Grading: Asmts 6 % of final grade

Graded Tutorials (Group)
Graded Tutorials (Individ)
In Class Test
Mid-terms
Torm project

7 % of final grade
3 % of final grade
2 % of final grade
4 % " " "

Term project 10 % " " " Final exam 40 % " " "

For the midterms, and in class test, your final grade will be a combination of individual (20%) and group (20.%) works

of individual (80%) and group (20 %) work.

A mark of less than 50% on the final exam will lead to a grade of F in the

course.

The assignments, most of the graded workshops (except 3) and the project will be done in groups of 3. For the graded workshops, your **four** worst grades will be dropped **if you score more than 90% on the rest**.

A mark of over 95% on the final exam will result in your letter grade being moved one step higher (e.g., a B- will become a B)

Revisions to the assignments/solutions/grades/Tutorials and announcements will be posted on avenue. All assignments, graded workshops, Term project, and group submissions for the midterms are to be done in groups of three.

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/take home tests (with an official missed mark form) will be moved to the final exam.

Note: Late submissions will not be accepted.

Required Texts:

1. Lecture slides (PDF available on avenue)

Supplementary References:

- 1. H.S. Fogler, *Elements of Chemical Reaction Engineering*, Prentice-Hall, 4rd Edition, 2006, Chapters 1-6, 8, 11, parts of Chapters 13&14.
- 2. J.M. Smith, Chemical Engineering Kinetics, McGraw-Hill (1981), 3rd Edition.
- 3. O. Levenspiel, *Chemical Reaction Engineering*, 2nd Edition, Wiley (1972). 3rd Edition (1999).

Outline

Date	Material/Activity
Jan 4	Ch0;Ch1:9/79
Jan 6	Ch1; 22/79
Jan 6	Graded WS 1
Jan 9	Ch1; 40/79 (Mass Balance Done)
Jan 9	Graded WS 1
Jan 11	Species Mole balance; Ch1 66/79
Jan 13	Species Mole balance; Ch1 79/79
Jan 13	Graded WS 2
Jan 16	Ch2
Jan 16	Graded WS 2
Jan 18	

Jan 18		
Jan 19		
Jan 20	Ch2: Mole and mass balance in the presence of reactions	
Jan 22	Ch2: Batch, CSTR and PFR	
Jan 25	Ch2: Dealing with discrete events in time	
Jan 25	Graded WS4	
Jan 26	Graded WS4	
Jan 27	Ch2: Dealing with discrete events in time	
Jan 29	Discrete Repeats	
Feb 1	Discrete repeats. PFR Side Streams	
Feb 1	Graded WS5	
Feb 2	Graded WS5	
Feb 3	Ch3: Stoichiometry and net rate of formation	
Feb 5	Ch3: Simplifications for special cases Asmt 1 due back Energy balances;	
Feb 8	In-Class Test Ch4:	
Feb 8	Graded WS6	
Feb 9	Graded WS6	
Feb 10	In Class Test 1, covering upto Chapter 2	
Feb 12	Ch4: Energy balances for a mixing point In class test group submission due back	
Feb 15- 19	Break	
Feb 22	Mole mass and energy balance for a batch with discrete change	
Feb 22	Graded WS7	
Feb 23	Graded WS7	
Feb 24	Energy balance for PFR	
Feb 26	Energy balance for PFR with side streams	
Feb 29	Energy balance for a PFR with cooling jacket	
Feb 29	Graded WS8	
March 1	Graded WS8	
March 2	Chapter 4 done	
March 4	Chapter 5	
March 7	Energy balance for a CSTR with reaction	
March 7	Graded WS9	
March 8	Graded WS9	

March 9	Mole and Energy balance for a batch; Asmt 2 Due back
March 11	Batch with discrete change with reaction
March 11	Midterm 2: Covering upto chapter 4
March 14	Energy balance for a PFR with reaction
March 14	Graded WS10
March 15	Graded WS10; Group submission for MT2 due back
March 16	Mole, Mass and Energy Balance for a PFR with reaction
March 19	Mole, Mass and Energy Balance for a PFR with side streams with reaction
March 21	Finish Chapter 5
March 21	Graded WS11
March 22	Graded WS11
March 23	Chapter 6 (Compressible fluids)
March 25	Chapter 6 (Compressible fluids)
March 28	Chapter 6 (Compressible fluids)
March 28	Graded WS12
March 29	Graded WS12
March 30	Chapter 6 (Compressible fluids)
April 1	Chapter 6 (Compressible fluids)
April 4	Chapter 6 (Compressible fluids)
April 4	Graded WS13
April 5	Graded WS13; Asmt 3 due back
April 6	Recap
April 8	Recap: Project due back

CP indicates course pack (slides available on avenue).

- 1. Dynamic mass balances and mole balances in the absence of reactions (incompressible fluids, isothermal isobaric systems)
 - 1.1 Mixing tank
 - 1.2 Handling Transitions
 - 1.3 Handling discrete events in time
 - 1.4 Plug flow tanks
 - 1.5 Handling various reactor configurations, discrete flows in space
- 2. Dynamic mass balances and mole balances in the presence of reactions (incompressible fluids, isothermal isobaric systems)
 - 2.1 The rate of formation/rate expression
 - 2.2 Applications of the mass and mole balance to
 - 2.2.1 Batch Reactor Problems
 - 2.2.2 Continuous Flow Reactors CSTR and Tubular Reactors
 - 2.3 Handling discrete points in time and space
 - 2.3.1 Handling additives (discrete points in time)
 - 2.3.2 Handling stream splitting and additions (discrete points in space)
- 3. Understanding Net Rate of Formation for a set of reactions
 - 3.1 Expressing net rate of formation using Stoichiometry
 - 3.2 Simplifying for a single reaction
 - 3.2.1 Writing mole and mass balances in terms of conversion
 - 3.2.2 Recognizing limitations
- 4. Dynamic mass, mole and energy balances in the absence of reactions (incompressible fluids, isobaric systems)
 - 4.1 Mixing tank
 - 4.2 Handling Transitions
 - 4.3 Handling discrete events in time
 - 4.4 Plug flow tanks
 - 4.5 Handling various reactor configurations, discrete flows in space
- 5. Dynamic mass balances, mole and energy balances in the presence of reactions (incompressible fluids)
 - 5.1 The heats of formations
 - 5.2 Applications of the mass, mole and energy balance to
 - 5.2.1 Batch Reactor Problems
 - 5.2.2 Continuous Flow Reactors CSTR and Tubular Reactors
 - 5.3 Handling discrete points in time and space
 - 5.3.1 Handling additives (discrete points in time)
 - 5.3.2 Handling stream splitting and additions (discrete points in space)
 - 5.4 The single reaction system:

- 5.4.1 Writing mole mass and energy balances in terms of conversion
- 5.4.2 Recognizing limitations
- 6. Dynamic mass, mole and energy balances in the presence of reactions (compressible fluids)

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 reactor type, determine 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 and kind of reactor required (design problem).
- c) Given a set of data for a reaction, establish a rate equation for that reaction.

Course outcomes	Corresponding CEAB indicator
Recognize that several reactor configurations could yield the desired product	Obtains experience with open-ended problems.
Determine a criteria for choosing a particular configuration	Obtains experience with open-ended problems.
Evaluate the options to determine the best fit to the criteria	Obtains experience with open-ended problems.
Recognize the availability of software, thus avoiding making too many simplifying assumptions in problem solving	The ability to use of modern/state of the art tools
Solve problems using software such as Polymath and Matlab	The ability to use of modern/state of the art tools

The above outcomes and indicators are for your information. Graduating from an accredited institution has many advantages. Please read more about it here: http://www.engineerscanada.ca/accreditation

POLICY REMINDER:

Academic Integrity:

You are expected to exhibit honesty and use ethical behavior 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 behavior 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.