Chemical Engineering 3K4, Winter 2013
Introduction to Reactor Design

Instructor

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Class time and location

- Class time: T13, room 127. Monday, Wednesday, Thursday, 17:30 to 18:30 (1 hour, not 50 minutes)
- Tutorial A, T13, room 107, Monday, 11:30 to 13:20
- Tutorial B, T13, room 107, Tuesday, 08:30 to 10:20

Disclaimer

This outline **may be modified**, as circumstances change.

1 About the course

Official description

Stoichiometry of multiple reactions, kinetics of homogeneous reactions, interpretation of batch data, design of ideal and non-ideal CSTR and plug flow reactors.

What you must be able to demonstrate by the end of the course

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

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

Prerequisites

MATH 2M06 (or 2M03 and 2MM3), or both MATH 2P04 and 2Q04, or both MATH 2Z03 and 2ZZ3, and registration or credit in CHEM ENG 2F04 and 3D03; or a grade of at least B+ in CHEM ENG 2B03 and permission of the Department.

The math prerequisites in this course are important. This course can be seen as an applied mathematics course where differential and integral equations play an important role. Also, your 3E04 (Process Model Formulation and Solution, a.k.a. Numerical Methods) course is important when solving systems of equations which cannot be integrated analytically; especially nearer the end of the course.

Course materials

The course website will be permanently available: http://learnche.mcmaster.ca/3K4. You may use this as a resource even after you graduate.

Course materials, tutorials, assignments and solutions will be available from the website. Course announcements will only be posted to the main page of the website - students are expected to check the website **at least 3 times per week, or more frequently**. No other form of communication will be used.

Required textbook

The official course textbook is the book by Fogler. There are two options available:

- *F2006*: H.S. Fogler, "*Elements of Chemical Reaction Engineering*", Prentice-Hall, 4rd edition, 2006.
- *F2011*: H.S. Fogler, "*Essentials of Chemical Reaction Engineering*", Pearson Education, 1st edition, 2011.

F2011 is a revised version of F2006, however some of the later chapters from F2006 do not appear in F2011 anymore. However, the coverage of F2011 is the same, perhaps better, than in F2006, so feel free to purchase either one. Reference to both will be given in the course, so you will not be at a disadvantage.

F2011 contains a greater emphasis on safety, alternative energy sources such as solar and bioreactions, and unsteady state reactor design, so it may be a better option if you are the type of student that retains your textbooks for future use. *Also see the course outline below*.

Recommended textbooks and readings

Materials to supplement the course material are:

1. Smith, "*Chemical Engineering Kinetics*", McGraw-Hill (1981), 3rd edition.
2. Levenspiel, "*Chemical Reaction Engineering*", 2nd edition, Wiley (1972). 3rd edition (1998).

Other reference texts are listed on the course website and are generally available in Thode Library.

Course outline

The course is divided into 8 main sections, taught over 12 weeks. Chapter numbers refer to the F2006 Fogler textbook numbering.

1. Mole balances (also chapter 1 in F2011)
2. Conversion and reactor sizing (also chapter 2 in F2011)
3. Rate laws and stoichiometry (chapter 3 and 4 in F2011)
4. Isothermal reactor design (chapter 5 and 6 in F2011)
5. Collection and analysis of rate data (chapter 7 in F2011)
6. Multiple reactions (chapter 8 in F2011)
8. Steady-state nonisothermal reactor design (spread across chapters 11 and 12 in F2011)
13. Distributions of residence times for chemical reactors (not in F2011, but notes and other references will be provided)

Several enrichment topics may also be covered throughout the course.

2 Grading

To assess your understanding of the course materials, the grading for the course will be assessed in the following way.

Component	Fraction	Notes
Tutorials/Assignments	15%	Expect around 5 assignments; may be completed in groups of 2, or by yourself.
Midterm exam	20%	A written exam covering the material in the course up to the day before the exam.
Project	15%	The design and rating of a reaction system.
Final exam	50%	A written exam, lasting 3 hours.

Policies regarding the course and regarding grading

- *Very important note*: **Achieving a grade of below 50% in the final exam will automatically imply failure in the course, with a grade of F, no matter what your other grades for the project, tests, and assignments are.**
- *Another important note*: portions of the midterm exam may be converted to several smaller, electronic tests that you complete outside class time, on an internet-enabled device. If this occurs you will be informed about it ahead of time, and be given some practice problems that you can attempt to get comfortable with electronic testing.
- Tutorial times are an opportunity to see questions that are the same/similar to those that will be handed in for the assignments. No solutions will be given to tutorial problems, since the TA and instructor will be on hand in the tutorial time slot to provide guidance on the questions.

  Tutorials will be done in groups of 2 (the same groups as for the assignments). The instructor and TA's will randomly call on groups to present their line of thinking (and potential answers) to the class. Attendance at tutorials is strongly encouraged: you will probably learn more during this time than any other time during the course.
- We encourage you to complete the assignments in groups of no more than 2 members.
- You, and your group, will receive the greatest benefit if you each do **all** the questions yourselves. Arrange to meet and review your solutions, discussing various approaches.
- Assemble a **single submission** for the group - the TA's will not grade loose sheets handed in after the first submission. All group submissions must clearly show the names of the group members.
- You are defeating the purpose of the group-based assignment if you simply divide the assignment into sections, one for each group member. This is definitely not recommended, because you are losing out on the learning opportunity of seeing your mistakes and the group member's mistakes, and learning from them.
- No sharing of any work may be done between groups for assignments. This includes handwritten documents and electronic files of any type. This will be strictly enforced. Please ensure that you have read the University's academic integrity policy (part of which is reproduced below).
- This is a large class of about 90 students, so late hand-ins interfere with the TA's ability to efficiently grade your assignments. Late assignments will be penalized by deducting **30%** per day for every late day. A grade of zero will be given for submissions handed in after the solutions are posted (usually within 2 days of assignment hand-in).
- Emergencies and such arise, so each person has 2 "late day" credits for assignments. So you can hand in one assignment 2 days late, or 2 assignments each one day late, without penalty.
- Grading of all work submitted in the course will include contributions for clarity and organization of presentation.
- No make-ups will be given for assignments, tutorials or midterms.
- Any paper-based materials (textbooks, notes, *etc*) are allowed during tests and exams. Electronic textbooks are, unfortunately, not permitted.
- The *mid-term test is optional* and there is no make-up for it. If you choose not to write the midterm, or cannot write it due to illness or other reasons, then the usual approach will be followed: the contribution from the midterm will be added to the final examination weighting. This is obviously a tremendous risk, since you will be placing a large balance of your grade on a single examination.
- All assignments will be graded and you should expect 5 assignments evenly spaced throughout the course.
- Any calculator may be used during the tests and exams.
- The final percentage grades will be converted to letter grades using the Registrar's recommended procedure.
- Adjustment to the final grades may be done at the discretion of the instructor.
- The final exam will be cumulative, based on the entire semester's material.

3 Important notes

Class participation: Please bring a calculator to every class.

Course software

Use of a computer is occasionally required in the course and will be required to complete the project. Software tools that you wrote in 3E04 (Numerical Methods) to integrate equations will be useful.

Out-of-class access

The instructor has office hours posted on his website, or other times may be arranged by email.

The TA's for this course can be contacted by email - please see their addresses above. Try to send email from your McMaster account - email from personal accounts are sometimes discarded by spam filters.

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4 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 on 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: this point is particularly important and will be strongly penalized in this course.
3. Copying or using unauthorized aids in tests and examinations.

5 Important dates

A list of *tentative* dates:

Date	**Description**
09 January 2013	Overview class: review of course content and administrative issues
16 January	Assignment 1 due
30 January	Assignment 2 due
13 February	**Written midterm**
20-24 February	*Midterm break*
27 February	Assignment 3 due
13 March	Assignment 4 due
27 March	**Project due**
03 April	Assignment 5 due
08 April	Optional review class
12 April	Exams start