CHE 372: Chemical Reactor Analysis and Design

Unique Number: 14710 and 14715

Instructor:
Dr. Hal Alper
CPE 5.408; P: 471-4417
Office Hrs:
W 2 - 4 PM
F 1 - 2 PM
halper@che.utexas.edu

Teaching Assistant:
Eric Young
CPE 5.128
Office Hrs:
T 4:30 – 6 PM (CPE 4.446)
Th 11 AM - Noon (CPE 5.128)
young@che.utexas.edu

Grader:
Ben Reed
reedbc@gmail.com

Lectures:
M, W, F 10:00 – 11:00 AM (CPE 2.218)
Please be punctual. Attendance is strongly suggested as there will be unannounced quizzes (see quizzes section below). Most lectures (and some quizzes) will be based on reading assignments that you should complete prior to coming to class.

Recitation:
M 11 – 12 noon (CPE 2.206), Unique #14710 and M 12 – 1 PM (CPE 2.220), Unique #14715
Please be punctual. Attendance is not compulsory but is strongly encouraged as there will be unannounced quizzes (see quizzes section below). Your TA will be going over practice problems and answering questions at these sessions.

Course Goals and Overview:
Chemical Reactor Analysis and Design is a unique, capstone course in the chemical engineering curriculum that distinguishes this field from other engineering disciplines. In this regard, this course can be seen as a culmination of your undergraduate education in chemistry, material and energy balances, transport phenomena, numerical methods, and thermodynamics. Overall, this course will provide an introduction to the principles and calculation techniques used to analyze and design chemical reactors for the production of petrochemicals, advanced materials, polymers, and biochemicals. This course is designed to:

- Provide you with the fundamentals of material and energy balances as applied to chemical reactor design for ideal reactors
- Offer practice in defining problems, analyzing data, and designing chemical processes
- Provide you with an understanding of rate laws and their derivation.
- Provide you with an appreciation for the topics of heterogeneous catalysis, biological catalysis and non-ideal reactor schemes.

Course Prerequisites:

- A grade of at least a C in ChE 322, 348, and 354.
- A comprehensive knowledge of transport phenomena is essential. This course relies on shell balances and the constituent equations to develop the material and energy balances

for various reactors, and to develop the balances in heterogeneous catalysts that account for diffusion with reaction. Transport phenomena concepts are used to appreciate the consequences of turbulent flow on velocity, temperature and concentration profiles that form the basis of the one-dimensional models. (ChE 353)

- Knowledge of heat transfer processes. (ChE 353 and ChE 354)
- Understanding of reaction equilibria and heat of reaction. (ChE 322)
- Ability to solve linear differential equations. (M427K)
- Familiarity with matrix multiplication. (ChE 348)
- Ability to solve ODEs using explicit numerical methods and to have a working knowledge of how these methods work. (ChE 348)
- Ability to solve sets of linear and nonlinear algebraic equations numerically (ChE 348).
- Familiarity with numerical optimization procedures. (ChE 348)
- Working knowledge of MATLAB numerical software that operates on the Department Learning Resource Center computers. (ChE 210 and ChE 348)

Course Textbook:
J.B. Rawlings and J.G. Ekerdt, *Chemical Reactor Analysis and Design Fundamentals*, Second Printing, Nob Hill Publishing, 2004.
(see http://jbrwww.che.wisc.edu/home/jbraw/chemreacfun/ for an Errata and other resources)

Additional Textbooks on Reserve:
Additional textbooks of interest have been placed on reserve at the Engineering Library. These include *Elements of Chemical Reaction Engineering* by Fogler, *Chemical Reaction Engineering* by Levenspiel, and *Chemical Reactor Analysis and Design* by Froment and Bischoff.

Computational Resources: Polymath and Matlab are available in the ChemE computer labs.

Course Website: A course page will be maintained on Blackboard—Please check it regularly!

Course Structure:
Lectures will be structured around defining the key concepts of reactor design and engineering. Emphasis will be placed on defining key concepts and conceptual understanding. Some example problems will be worked out in class. Recitation sections will be dedicated to problem solving (both analytical and numerical techniques).

Grading:
You may select one of two grading schemes [choice should be indicated in writing on the last day of class]:

	Scheme A		Scheme B
Homework	10	Homework	10
Best of 5 Quizzes	20	Best of 5 Quizzes	20
Comprehensive Project	10	Comprehensive Project	10
Exams	60	Exams (Best of 2)	40
Final Exam	0	Final Exam	20

Note that grades will be curved as necessary and letter grades assigned based on natural breaks in the distribution. Plus/Minus grading will be used in this course.

Homework: Homework will be generally be assigned at the end of the lecture period on Wednesdays; they are due at the beginning of the specified lecture period (usually a week from assigned date). Your homework must be neatly presented in the standard chemical engineering format. Homework must be handed in individually, but you are encouraged to work in groups to discuss how to solve the problems. Homework problems are graded with an emphasis on effort and setting up the problem, and only selected problems within each assignment will be graded. Homework handed in late will be deducted 25% less for each weekday it is turned in late, unless a prior arrangement has been made with the instructor.

Reading Assignments: At the end of each lecture, you will also be given a reading assignment. Read the sections prior to the next lecture. Work the example problems in your textbook as a guide to whether you have fully understood the material.

Quizzes: There will be a total of six unannounced quizzes of one or two questions held during the lecture period or recitation period. You will be allowed to drop one and only one quiz grade, which may be a missed quiz or the lowest quiz grade. These quizzes are based on materials covered in reading assignments, classroom discussions, and homework. A bonus of 5 points will be added to your final grade if you score perfect tens on the five quizzes counted towards the grade. You have one week after the quiz is returned to you to request for re-grading. Re-grading requests should be submitted in writing at the end of that lecture period.

Comprehensive Project: There will be one comprehensive project assigned during the class due **Monday, November 29**. This project will be worked in groups to prepare a short report and solutions (Groups to be assigned in class when project is announced). This set of problems will be assigned near the end of the semester and will require you to use a collection of different concepts from 372 along with major concepts from previous ChE courses. This exercise will help you appreciate reactor design as an integral part of designing chemical engineering systems.

Exams: Three exams are scheduled for **6:30-9:30 pm** on Wednesday evenings: **September 29, October 20, and November 23**. *Exam rooms and details of room assignments will be provided 1 week prior to the exams.* **There will be no make-up exams offered!** In exchange for evening examinations, classes will not meet on September 10, November 8 and November 10, and one additional day to be announced. You have one week after the exam is returned to you to request for re-grading. Re-grading requests should be submitted in writing at the end of that lecture period. Re-grade requests should consist of a few sentences on a separate page that describe your rationale for why a re-grade is necessary. Nothing is to be marked on the original exam paper. Optional review sessions (outside of class time) will be held before each of the exams. These dates/times are tentatively: Sunday 9/26, Sunday 10/17, and Sunday 11/21 at 2 PM in CPE 2.218.

Final Exam: The final exam (for those who select Grading Scheme B) is currently scheduled for **Wednesday, December 8, 2:00-5:00 PM**.

The University of Austin provides upon request appropriate academic accommodations for qualified students with disabilities. For more information, contact the Office of the Dean of Students at 471-6259, 471-6441 TTY.

Absence: No excuses for missed tests, exams, or quizzes will be accepted other than written certified medical excuses or written letters on university letterhead for UT-related school activities. By UT Austin policy, you must notify me of your pending absence at least fourteen days prior to the date of observance of a religious holy day. If you must miss a class, an examination, a work assignment, or a project in order to observe a religious holy day, you will be given an opportunity to complete the missed work within a reasonable time after the absence.

Knowledge, Abilities, and Skills Students Should Gain From this Course:

1. Ability to derive and apply the energy and material balances that are required to design isothermal and nonisothermal batch, plug flow, fixed-bed and continuous stirred tank reactors.
2. Ability to solve problems of variable density and multiple independent reactions.
3. Ability to solve problems of mass transfer with reaction in heterogeneous catalysts.
4. Ability to solve problems incorporating simple, one-parameter nonideal reactor modeling.
5. Knowledge of chemical reaction analysis concepts and chemical kinetics concepts.

Chemical Engineering ABET Program Outcomes Achieved:

c. An ability to design a system, component, or process to meet desired needs within realistic constraints such as economic, environmental, social, political, ethical, health an safety, manufacturability, and sustainability

e. An ability to identify, formulate, and solve engineering problems.

k. An ability to use the techniques, skills, and modern engineering tools necessary for engineering practice.

Academic Integrity:

The University has a strict policy on academic integrity. Any form of plagiarism or academic dishonesty will NOT be tolerated in ChE 372. Forms of academic dishonesty include copying homework assignments, systematic cheating on exams, use of unauthorized materials for exams, and changing solutions to returned assignments and exams. If you have any questions, please consult the websites below:

http://deanofstudents.utexas.edu/sjs/acint_student.php
http://www.utexas.edu/courses/clubmed/plgrism_cit.html

Failure to comply with the University's policy will result in a "zero" in the assignment and an "F" for CHE 372.

Course content outline (as of August 25)

Part 1: Isothermal Reactor Design and Analysis		
	Introduction to Chemical Reactors and Material Balances	Chapter 1,2,4.1
	Batch Reactors	Chapter 4.2
	Continuous Stirred Tank Reactors (CSTRs)	Chapter 4.3
	Semi-Batch Reactors	Chapter 4.4-4.5
	Plug Flow Reactors	Chapter 4.6
	Multiple Reactions and Reactor Selection	Chapter 4.7, Handout
	Defining Rate Laws	Chapter 5.4-5.5
Part 2:Ideal Reactor Energy Balances		
	Overall Energy Balance for Reactors	Chapter 6.1
	Batch Reactors	Chapter 6.2
	CSTRs	Chapter 6.3
	PFRs	Chapter 6.5
Part 3: Heterogeneous Catalysis		
	Overview of heterogeneous catalysis	Chapter 7.1-7.2
	Defining Catalysis Rate Laws	Chapter 5.6
	External Diffusion Considerations	Chapter 7.3-7.5
	Internal Diffusion Considerations	Chapter 7.3-7.5
	Packed Bed Reactor Design	Chapter 7.7
	Energy Balance Considerations	Chapter 7.7
Part 4: Other Topics in Chemical Reactor Engineering and Kinetics		
	Enzyme Reactions	In Class
	Bioreactors	In Class
	Pharmacokinetics	In Class
	Residence Time Distributions and Real Reactors	Chapter 8.1-8.2
	Data Analysis	Chapter 9