ChE 421: Advanced Chemical Reaction Engineering

Prof. Davis

Fall 2016 Syllabus

Class meeting times:

Mondays 12 – 12:50 PM in room 106
Tuesdays 4 – 5:50 PM in room 502

Prerequisites and other requirements:

The prerequisite for this class is ChE332 (Chemical Reaction Engineering). I also expect that you have already taken ChE352 (Process Simulation and Mathematical Techniques for Chemical Engineers). The course has a required textbook: <u>Chemical Reactor Design, Optimization, and Scaleup</u> by E. Bruce Nauman (2nd ed.) ISBN# 0470105259, $98 (new) @ Amazon.com on 9/2/16. It is also available electronically through the library website and there is a copy on reserve at the Cooper library. I will generally be following the textbook through the course; you should purchase it and **<u>bring your copy with you to class</u>**. You will need materials to take notes and do problems during class (paper, pencil, a calculator, and ideally two different colors of pen) and access to a computer with Matlab to do most of the homework problems.

Course overview:

In this course, you will learn the principles of chemical reaction systems and the practices of industrial reactor designers. I will emphasize heterogeneous chemical kinetics, packed bed reactors, fermentation, biochemical reaction engineering, and reactor scale-up as examples. Modeling and simulation of systems will be extensively applied. The first half of the course (before the Midterm Exam) will cover:

- Elementary Reactions in Ideal Reactors (Chapter 1)
- Multiple Reactions in Batch Reactors (Chapter 2)
- Isothermal Piston Flow Reactors (Chapter 3)
- Stirred Tanks and Reactor Combinations (Chapter 4)
- Thermal Effects and Energy Balances (Chapter 5)

The second half of the course (from the Midterm to the Final Exam) will cover:

- Packed Beds and Turbulent Tubes (Chapter 9)
- Heterogeneous Catalysis (Chapter 10)
- Biochemical Reaction Engineering (Chapter 12)
- Fermentation and bioreactor design

Course goals and objectives:

By the end of this course, you should be able to:

- Explain what an elementary reaction is and how it is relevant to reactor design
- Model an ideal, isothermal reactor from first principles
- Explain the differences and applications of batch, continuous-flow stirred tank, and tubular reactors
- Explain the effect of mixing on batch reactors and CSTRs during design scaleup
- Develop models for reactors with multiple and non-elementary reactions
- Define and implement the Quasi-Steady State Hypothesis to estimate a reaction rate
- Explain the differences between reactions in the gas or liquid phase
- Explain the design factors involved in scaleup of isothermal and non-isothermal tubular reactors
- Give equations which quantify the thermal effects of a reaction using energy balances
- Calculate the concentration profile of a given species in a packed-bed reactor or one in turbulent flow, with or without consideration of axial dispersion
- Use numerical techniques to solve for concentration, temperature, and flow profiles in reactors
- Write and use the governing equations for transport and reaction for a given reactor geometry
- Explain the concept of a rate-controlling step as it relates to pore diffusion, film mass transfer, surface kinetics, and transport between phases
- Use mass transfer coefficients to estimate the real reaction rate in a packed bed reactor
- Do elementary calculations in biochemical reaction engineering, in particular enzyme catalysis, and explain the factors in reactor design for enzyme catalysis

Homework Assignments and Exams:

You will be given five (5) homework assignments (HWs), a midterm exam, and a final project. The HWs will be due <u>before class</u> on the date listed in the course schedule and will be assigned <u>two weeks</u> prior to their due date. Homework assignments will consist of applications of concepts covered in class and will analyze a particular reactor situation. The assignments usually have a computational (Matlab) component and can take a long time; I will do as much as I can to manage this, but <u>it's up to you to keep up with the assignments, ask questions, and ask for more time if you need it</u>. This is a three credit graduate-level class; I expect that you will spend about 6 hours per week outside of class on work for this class.

The Midterm Exam will be three hours long and cover the material in chapters 1 through 5 and 9 of the textbook which I go over in class and on the homework assignments. The portion of the exam corresponding to each topic will be approximately equal to the amount of time spent in class on each topic. The Final Project will be cumulative but will focus on the material in chapters 10 and 12 which I present in class and on the homework assignments.

Groups:

You may be assigned groups at two points in this class (depending on enrollment). You will work together on all HWs and be graded together on those assignments. Groups will be assigned by me on the second day of class for HW1, HW2, and HW3. After HW3 has been submitted, you may choose your own group to work with (subject to my approval of your group) for HW4 and HW5. I reserve the right to reassign groups at any time without consent of any members of that group based on the following criteria: performance on the assignments or the Midterm Exam (either too low or too high), well-founded complaints by one or both of the members of the group, or the need to split up another group (and thus break up two groups to form two new groups).

The HWs will be done in groups of 2-3 but each group member must submit THEIR OWN work. Only one of the 2-3 assignments (chosen randomly by me) may be graded and handed back. The grade on that submission AND ONLY THAT SUBMISSION will be given to all group members. It is the responsibility of each group member to ensure that all assignments are of similar quality.

You are REQUIRED to put the names of ALL members of your group on your submissions. If one or both names do not appear on any submission, I reserve the right to give a zero grade to the person whose name does not appear at my discretion. You are also REQUIRED to submit a group member evaluation form for each group member you work with during the semester. The evaluation form will be available to print out on Moodle.

Attendance and Grading Policy:

Attendance in class is mandatory. <u>Please E-mail me before class if you cannot attend for whatever reason.</u> If you miss class, please come to my office hours to find out what you missed. There will be no make-up or extra credit work associated with this class. Please ensure that you hand in your assignments on time and that you can attend both exams. All assignments and exams must be completed for a passing grade in the class.

Students will be graded as follows:

	Homework	**Midterm Exam**	**Final Project**
% of grade	30	40	30

Letter grades will be determined at the end of the semester using each student's raw score from above, the average raw score for the class, and my discretion (in that order). My discretion will be based on class attendance / participation, effort on homework assignments, and improvement over the course of the semester.

Office hours:

Tuesdays	2 – 3 PM in room 419
Wednesdays	4 – 5 PM in room 419
Thursdays	1 – 2 PM in room 419

Please do your best to bring questions to me during those times only. My E-mail address is bdavis@cooper.edu if you have a question which is brief or if you need to let me know you're going to be absent, late, etc. If you send me an E-mail, please put "ChE 421" as the start of the subject, e.g. "ChE 421: HW1 Question".

Group Work and Academic Integrity Policy:

I believe group work is important to learning; I may be requiring you to work in groups on your homework assignments. However, each student MUST submit their own work product for each HW. I will choose randomly each week which group member's homework submission I will grade. This means that you must work closely with your group members to ensure that you are all doing the work and that you are doing it correctly.

Plagiarism is the presentation of another person's "work product" (ideas, words, equations, computer code, etc.) as one's own. Whether done intentionally or unintentionally, plagiarism will not be tolerated in this class. You are plagiarizing if:

1. You present as your own work product (code, written answers, etc.) a submission that includes the work product of your other group members
2. You present as your own work product a submission that contains the efforts or work product of other individuals aside from your other group members
3. The help and contributions of other individuals are not acknowledged in writing on your submission (by writing their names)
4. You copy the work of other students on an in-class examination or communicate with other individuals in any fashion during an exam
5. You submit as part of a homework assignment material that has been copied from any source (including, but not limited to, a textbook, a periodical, an encyclopedia, the internet) without properly citing the source, and/or without using quotation marks. It is also prohibited to submit such materials in a minimally altered form without proper attribution. Improperly copied material might include text, graphics (computer or otherwise), computer source code, etc.

If I have a strong suspicion that you have plagiarized your submission for an assignment (homework or project,) you will receive a zero on that assignment. If you commit another act of plagiarism during the course after this first act, I will refer the matter to the Dean's office. Other prohibited acts of academic dishonesty include (but are not limited to):

6. Attempting to obtain a copy of an examination before it is administered
7. Dishonesty in dealing with me or another professor, such as misrepresenting the statements of another professor

8. Bringing a text or study materials of any kind (including electronically) into an exam when forbidden to do so
9. Bringing any device, electronic or otherwise, into class at any time when not expressly permitted by me
10. Bringing any device into an examination that allows communication with other individuals or computers or computer databases (i.e. no cell phones or laptops during exams)

If I have a strong suspicion that you have cheated on an examination, you will receive a zero on that examination and likely receive a D or F in the course. The above was modified from the course catalog from the 2009-10 academic year.

Resources which may (or may not) be helpful:

http://site.ebrary.com/lib/cooper/detail.action?docID=10296771 – Website for Nauman book

Chemical Reactor Analysis and Design by G. Froment and K. Bischoff (2nd ed.) ISBN# 0471510440

The Engineering of Chemical Reactions by L. Schmidt (1st ed.) ISBN# 0195105885

Elements of Chemical Reaction Engineering by H. Fogler (4th ed.) ISBN# 0130473944

http://www.umich.edu/~essen/indexweb.htm – Website for Fogler textbook

Chemical Reaction Engineering by O. Levenspiel (3rd ed.) ISBN# 047125424X

Principles of Polymer Systems by Rodriguez et al. (5th ed.) ISBN# 1560329394

Bioprocess Engineering: Basic Concepts by Shuler and Kargi (2nd ed.) ISBN# 0130819085

Biochemical Engineering by Blanch and Clark (2nd ed.) ISBN# 0824700996

http://www.youtube.com/user/LearnChemE/ - Videos on selected ChE topics (there's a whole section of videos on Reaction Engineering)

Sequence of topics and class schedule:

Below is a rough outline of the order of topics I plan to cover in class. Homework assignment due dates are indicated in the right-most column.

Week	Hour #	Day	Date	Topic	Due
1	1,2	Tue	9/6	Introduction to the class, Chapter 1	
1	3	Mon	9/12	Chapter 1: Elementary reactions and ideal reactors	
2	4,5	Tue	9/13	Chapter 2: Multiple reactions in batch reactors	
2	6	Mon	9/19	Chapter 2: Variable volume batches	
3	7,8	Tue	9/20	Chapter 3: Variable density tubular reactors	HW1
3	9	Mon	9/26	Chapter 3: Scaleup of tubular reactors	
4	10,11	Tue	9/27	Chapter 4: CSTRs	
4	12	Mon	10/3	Chapter 4 / Chapter 5: T effects and energy balances in non-isothermal reactors	
5	13,14	Tue	10/4	Chapter 5: Energy balances and scaleup	HW2
5	15	Mon	10/10	Chapter 5: Adiabatic T rise	
6	16,17	Tue	10/11	Chapter 9: Packed bed reactors	
6	18	Mon	10/17	Chapter 9: Modeling packed beds	
7	19,20	Tue	10/18	Chapter 9: Turbulent tubular reactors	HW3
8	--	Mon	10/24	Review for midterm exam	
8	--	Tue	10/25	Midterm Exam	
9	21	Mon	10/31	Chapter 10: Heterogeneous catalysis	
9	22,23	Tue	11/1	Chapter 10: Heterogeneous catalytic reactors	
9	24	Mon	11/7	Chapter 12: Biochemical reaction engineering	
10	25,26	Tue	11/8	Chapter 12: Enzyme kinetics	
10	--	Mon	11/14	NO CLASS – AIChE Annual Meeting	
11	--	Tue	11/15	NO CLASS – AIChE Annual Meeting	HW4
12	27	Mon	11/21	Chapter 12: Fermentation	
12	--	Tue	11/22	NO CLASS – Thanksgiving	
13	28	Mon	11/28	Chapter 12: Yields for bioreactors	
14	29,30	Tue	11/29	Chapter 12: Bioreactor design	HW5
14	31	Mon	12/5	Chapter 12: Modeling bioreactors	
15	32,33	Tue	12/6	Chapter 12: Modeling bioreactors	
15	34	Mon	12/12	Chapter 12: Modeling bioreactors	
16	35,36	Tue	12/13	Chapter 12: Modeling bioreactors	
16	--	Tue	12/20	Final Project Due	Proj