ChE421: Advanced Chemical Reaction Engineering

Prof. Davis

Fall 2022 Syllabus

Class meeting times:

Tuesdays 5 – 5:50 PM in room 503
Wednesdays 5 – 6:50 PM in room LL210

Prerequisites and other requirements:

The prerequisite for this class is ChE332 (Chemical Reaction Engineering), but I expect you have all taken ChE352 (Process Simulation and Mathematical Techniques for Chemical Engineers) as well. The course has a required textbook: <u>Chemical Reactor Design, Optimization, and Scaleup</u> by E. Bruce Nauman (2^{nd} ed.) ISBN# 0470105259. It is 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>be ready to access it during class</u>**. You will need to be prepared to take notes and do problems during class and you will need access to a computer with Python to do HWs.

Course overview:

In this course, you will learn the principles of chemical reaction systems and the practices of industrial reactor designers. The course will emphasize heterogeneous chemical kinetics, biochemical reaction engineering, polymerization reactions, and reactor scale-up. Modeling and simulation of systems will be extensively applied. The first part 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)
- Packed Beds and Turbulent Tubes (Chapter 9)

The second half of the course will cover:

- Heterogeneous Catalysis (Chapter 10)
- Biochemical Reaction Engineering (Chapter 12)
- Fermentation and bioreactor design
- Polymer Reaction Engineering (Chapter 13)
- Molecular weight distributions in polymers

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 between and applications of batch, continuous-flow stirred tank (CSTR), 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 design factors involved in scaleup of isothermal/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 find concentration, temperature, and flow profiles in reactors
- Write and use 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 and explain the factors in reactor design for fermentation
- Do elementary calculations in polymer reaction engineering, in particular determining the kinetics of step-growth and free-radical polymerizations
- Explain what a molecular weight distribution is and why it is so important to polymerization reactors

Homework Assignments and Exams:

You will be given six (6) homework assignments (HWs), one 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 (Python) 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.

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 first day of class for HW1 and HW2. After HW2 has been submitted, I will reassign groups for HW3 and HW4. You may choose your own group to work with (subject to my approval of your group) for HW5, HW6, and the final project. 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 (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 on Teams to print out or submit electronically.

Attendance and Grading Policy:

Attendance in class is mandatory. Please E-mail me before class if you cannot attend for whatever reason. 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; all assignments must be completed for a passing grade in the class.

Students will be graded as follows:

	Homework	**Midterm Exam**	**Final Project**
% of grade	48	30	22

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:

Mondays 3 – 4 PM in room 409, room 419, or on MS Teams
Tuesdays 3 – 4 PM in room 409, room 419, or on MS Teams
Thursdays 11 AM – 12 PM in room 409, room 419, or on MS Teams

Please do your best to bring questions to me during those times only. My E-mail address is ben.davis@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 "ChE421" as the start of the subject, e.g. "ChE421: 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.

The engineering school policy on academic integrity is linked here. 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)

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.

Non-bolded rows are in-person weeks – class will be in our normal room
Rows in **BOLD** are remote weeks – class will be via MS Teams

Week	Hour #	Day	Date	Topic	Due
1	1	Tue	8/30	Introduction to the class / Syllabus	
1	2,3	Wed	8/31	Chapter 1: Elementary reactions and ideal reactors	
2	4	Tue	9/6	Chapter 1: Isothermal reactors, nomenclature	
2	5,6	Wed	9/7	Chapter 2: Multiple reactions in batch reactors	
3	7	Tue	9/13	Chapter 2: Variable volume batches	HW1
3	8,9	Wed	9/14	Chapter 3: Variable density tubular reactors	
4	**10**	**Tue**	**9/20**	**Chapter 3: Scaleup of tubular reactors**	
4	**11,12**	**Wed**	**9/21**	**Chapter 4: CSTRs**	
5	13	Tue	9/27	Chapter 4 / Chapter 5: T effects and E balances in non-isothermal reactors	HW2
5	14,15	Wed	9/28	Chapter 5: T^*, E balances	
6	16	Tue	10/4	Chapter 5: HT models for tubes and tanks	
6	17,18	Wed	10/5	Chapter 5: Reactor safety, Adiabatic T rise	
7	**19**	**Tue**	**10/11**	**Chapter 5: HT for scaleup**	HW3
7	**20,21**	**Wed**	**10/12**	**Chapter 9: Packed bed reactors**	
8	22	Tue	10/18	Chapter 9: Differential MT Equation, turbulent tubes	
8	23,24	Wed	10/19	Chapter 9: 2D reactor models / Method of Lines	
9	--	Tue	10/25	Midterm Exam Review Session	
9	--	Wed	10/26	Midterm Exam (3 HOURS – IN CLASS)	Exam
10	**25**	**Tue**	**11/1**	**Chapter 10: Heterogeneous catalysis**	HW4
10	**26,27**	**Wed**	**11/2**	**Chapter 10: Heterogeneous catalytic reactors**	
11	28	Tue	11/8	Chapter 12: Biochemical reaction engineering	
11	29,30	Wed	11/9	Chapter 12: Fermentation / Yields	
12	--	Tue	11/15	**NO CLASS** (AIChE Annual Meeting)	
12	--	Wed	11/16	**NO CLASS** (AIChE Annual Meeting)	HW5
13	--	Tue	11/22	**NO CLASS** (Friday schedule)	
13	--	Wed	11/23	**NO CLASS** (Thanksgiving)	
14	31	Tue	11/29	Chapter 12: Bioreactor design – batch/chemostat	
14	32,33	Wed	11/30	Chapter 12: Bioreactor design and scaleup	
14	34,35	Fri	12/2	**MAKEUP CLASS** (Ch. 13: Step growth, living polymers)	Proj
15	36	Tue	12/6	Chapter 13: Step growth MWD, Flory distribution	
15	--	Wed	12/7	**NO CLASS** (Friday schedule)	
16	**37**	**Tue**	**12/13**	**Chapter 13: Chain growth polymerization kinetics**	
16	**38,39**	**Wed**	**12/14**	**Chapter 13: Free radical polymerization**	HW6