

CHEN 5390: Graduate Chemical Reaction Engineering
Chemical and Biological Engineering
Fall 2020 Syllabus

Overview:

Reaction engineering is a core component of chemical and biological engineering. Understanding the fundamentals of reaction kinetics and their implications for process design is important for research areas ranging from alternative energy to metabolic engineering to polymers to nanomaterials. A particular focus of this course will be on interpreting reaction kinetics in terms of molecular scale events. The course will begin with a review of “top-down” reaction engineering and reactor design, then shift to a discussion of the physical chemistry governing reactive processes. Examples and applications will include reactions catalyzed by surfaces and enzymes, electrochemical systems, polymerization, and other unique cases such as chemical oscillators.

Instructor: Adam Holewinski, Chemical and Biological Engineering, adam.holewinski@colorado.edu,
Primary Office: SEEC N360, Ph. 303-492-3153.

Advanced Teaching Assistant: Colleen McCollum, colleen.mccollum@colorado.edu

Emails: Please **include “CHEN 5390” in the subject line**. Instructors will attempt to be prompt but do not expect turnaround in under 24 hours.

Lectures: Tu Th , 10:05-11:20 In-person: A115 JSCBB;
Zoom: <https://cuboulder.zoom.us/j/92767264289> password: kinetics

Office Hours: Adam: Monday 4:00-5:00 on Zoom, or by appointment (same link as class)

Colleen: Sunday 4:00-5:00 on Zoom, or by appointment

Textbooks: Reading will be primarily be assigned from the following:

(1) “Chemical reactor analysis and design fundamentals” by Rawlings and Ekerdt (1st or 2nd edition both fine)

Additional resources (slides and codes for figures) at: <http://jbrwww.che.wisc.edu/home/jbraw/chemreacfun/>

(2) *Optional:* “Chemical Kinetics” by Laidler (1987). (*Necessary excerpts will be posted*)

Additional resources you may find useful, excerpts will occasionally be posted

“Fundamentals of Chemical Reaction Engineering” by Davis & Davis

(*free at <http://authors.library.caltech.edu/25070/>*).

“Reaction Kinetics” by Pilling & Seakins (1995) (More conceptual than Laidler book)

“Chemical Kinetics and Dynamics” Steinfeld (1999) (More advanced than Laidler book)

Format:

This class will not consist of 75 minutes of straight lecture, and textbook material will not be covered in its entirety during class. We will use class time to discuss key concepts, applications, and examples. We will do about half “traditional lecture” on concepts, then do conceptual (multiple choice voting) problems, work longer quantitative examples, and ask/answer questions. Active participation is expected; you must complete reading beforehand. “iClicker” polling will be used for administering many in-class problems. This is now done with a downloadable phone app (no hardware to buy) but you must register for a Clicker Reef account per instructions at:

<https://oit.colorado.edu/services/learning-spaces-technology/cuclickers>

Expectations:

- Attend all classes and be on time.
- Participate in class.
- Complete reading assignments to prepare for class

Course website:

All course materials will be posted on the CU Canvas website, including links to auxiliary sites such as Gradescope and the iClicker help site. Handouts, reading assignments, other files, announcements, HW assignments and solutions, reading quizzes, and additional useful information will be posted.

Grading:	Participation	10%
	Homework sets	25%
	Project	10 %
	Midterm	25%
	Final exam	30%

At minimum, grade cutoffs will be guaranteed at A>90%, B>80%, C>70%, D>60%, F<60%. These may be adjusted pending class averages on exams.

Participation:

The participation grade will be earned by (i) answering clicker questions in class and (ii) answering reading questions on Canvas. Thus, it will not be an attempt to quantify your role in class discussion, but it is designed to encourage engagement by staying up to date with material. The 10% of the final grade assigned to participation will be broken down as 5% preparation (reading quizzes) and 5% participation (attendance taken by clicker answers). Reading quizzes will consist of short multiple choice questions aimed to check comprehension and begin to apply concepts. Clicker questions will also be multiple choice and full credit will be received for ringing in—correct answers are not required, but you must ring in to create a record of your participation. You and you alone are responsible for making sure your iClicker account is functioning properly.

A total score of 90% of the points in each category (reading/attendance) will be scaled to the full (5%) value of the final grade. Extra credit will *not* be assigned for >90%. This threshold is to account for reading questions that you may consider ambiguous and also to permit a reasonable number of absences without penalty. Thus, reading quizzes will not be reopened or re-graded, and absences will not be factored out of your grade, unless there are extraordinary circumstances (e.g. extended illness), which will be at the discretion of the instructor.

Homework:

In most weeks, homework problems will be assigned. These will be submitted through the Gradescope website (you should have received email notice if you are registered). Assignments will be fully graded, but the teaching team does not have the capacity to provide detailed feedback. Answer keys will be posted and you should plan to monitor your own progress with these. Regrade requests must be submitted in writing with one week of the graded assignment being returned to you. HW is due at the time noted on Canvas, usually 11:59pm. Credit for late assignments will be deducted in 10% increments hourly thereafter.

Exams:

The **midterm** is tentatively scheduled for **10/14**. We will discuss logistics during the first week of class and any possible conflicts (e.g. other scheduled classes) should be brought to my attention before Sept. 10. The **final** exam time is set by the registrar at **7:30pm 12/13**. The format of the exams will be specified during the course. Exams are cumulative. **NO MAKE-UP EXAMS WILL BE GIVEN.**

Prerequisites

Undergraduate course in kinetics / reaction engineering

Tentative List of Topics

Reactor Analysis and Rate Measurement ~9 weeks

- Empirical rates, Arrhenius and van't Hoff eqns.
- Mole balances and rate measurement
- Rate laws, regression and sensitivity analysis
- Energy balances
- Mass transfer effects
- Residence time distribution
- Special topics: Heterogeneous reactions, catalysis, polymerization, electrochemistry, photochemistry*

Reading

R&E Ch 1,3
“ Ch 4
“ Ch 2, 9
“ Ch 6
“ Ch 7
“ Ch 8

Ch. 5 and Handouts

Physical Chemistry of Elementary Reactions ~ 6 weeks

- Potential energy surfaces, Boltzmann distribution
- Collision theory
- Transition state theory
- Unimolecular rate theory
- Special topics: State-to-state kinetics, Reaction dynamics*

Laidler Ch 4
“
“ & Ch 11
Laidler Ch 5, P&S Ch 5
Handouts

Other important information

CLASSROOM BEHAVIOR

Both students and faculty are responsible for maintaining an appropriate learning environment in all instructional settings, whether in person, remote or online. Those who fail to adhere to such behavioral standards may be subject to discipline. Professional courtesy and sensitivity are especially important with respect to individuals and topics dealing with race, color, national origin, sex, pregnancy, age, disability, creed, religion, sexual orientation, gender identity, gender expression, veteran status, political affiliation or political philosophy. For more information, see the policies on [classroom behavior](#) and the [Student Code of Conduct](#).

REQUIREMENTS FOR COVID-19

As a matter of public health and safety due to the pandemic, all members of the CU Boulder community and all visitors to campus must follow university, department and building requirements, and public health orders in place to reduce the risk of spreading infectious disease. Required safety measures at CU Boulder relevant to the classroom setting include:

- maintain 6-foot distancing when possible,
- wear a face covering in public indoor spaces and outdoors while on campus consistent with state and county health orders,
- clean local work area,
- practice hand hygiene,
- follow public health orders, and
- if sick and you live off campus, do not come onto campus (unless instructed by a CU Healthcare professional), or if you live on-campus, please alert [CU Boulder Medical Services](#).

Students who fail to adhere to these requirements will be asked to leave class, and students who do not leave class when asked or who refuse to comply with these requirements will be referred to [Student](#)

Conduct and Conflict Resolution. For more information, see the policies on COVID-19 Health and Safety and classroom behavior and the Student Code of Conduct. If you require accommodation because a disability prevents you from fulfilling these safety measures, please see the “Accommodation for Disabilities” statement on this syllabus.

Before returning to campus, all students must complete the COVID-19 Student Health and Expectations Course. Before coming on to campus each day, all students are required to complete a Daily Health Form.

Students who have tested positive for COVID-19, have symptoms of COVID-19, or have had close contact with someone who has tested positive for or had symptoms of COVID-19 must stay home and complete the Health Questionnaire and Illness Reporting Form remotely. In this class, if you are sick or quarantined, please inform the instructor there is a medical need to miss class and estimate the period that will be missed. (Note, by student privacy laws you are *not* required to state the nature of illness).

ACCOMMODATION FOR DISABILITIES

If you qualify for accommodations because of a disability, please submit your accommodation letter from Disability Services to your faculty member in a timely manner so that your needs can be addressed. Disability Services determines accommodations based on documented disabilities in the academic environment. Information on requesting accommodations is located on the Disability Services website. Contact Disability Services at 303-492-8671 or dsinfo@colorado.edu for further assistance. If you have a temporary medical condition, see Temporary Medical Conditions on the Disability Services website.

PREFERRED STUDENT NAMES AND PRONOUNS

CU Boulder recognizes that students' legal information doesn't always align with how they identify. Students may update their preferred names and pronouns via the student portal; those preferred names and pronouns are listed on instructors' class rosters. In the absence of such updates, the name that appears on the class roster is the student's legal name.

HONOR CODE

All students enrolled in a University of Colorado Boulder course are responsible for knowing and adhering to the Honor Code. Violations of the policy may include: plagiarism, cheating, fabrication, lying, bribery, threat, unauthorized access to academic materials, clicker fraud, submitting the same or similar work in more than one course without permission from all course instructors involved, and aiding academic dishonesty. All incidents of academic misconduct will be reported to the Honor Code (honor@colorado.edu); 303-492-5550). Students found responsible for violating the academic integrity policy will be subject to nonacademic sanctions from the Honor Code as well as academic sanctions from the faculty member. Additional information regarding the Honor Code academic integrity policy can be found at the Honor Code Office website.

SEXUAL MISCONDUCT, DISCRIMINATION, HARASSMENT AND/OR RELATED RETALIATION

The University of Colorado Boulder (CU Boulder) is committed to fostering an inclusive and welcoming learning, working, and living environment. CU Boulder will not tolerate acts of sexual misconduct (harassment, exploitation, and assault), intimate partner violence (dating or domestic violence), stalking, or protected-class discrimination or harassment by members of our community. Individuals who believe they have been subject to misconduct or retaliatory actions for reporting a concern should contact the Office of Institutional Equity and Compliance (OIEC) at 303-492-2127 or cureport@colorado.edu. Information about the OIEC, university policies, anonymous reporting, and the campus resources can be found on the OIEC website.

Please know that faculty and instructors have a responsibility to inform OIEC when made aware of incidents of sexual misconduct, dating and domestic violence, stalking, discrimination, harassment and/or related retaliation, to ensure that individuals impacted receive information about options for reporting and support resources.

RELIGIOUS HOLIDAYS

Campus policy regarding religious observances requires that faculty make every effort to deal reasonably and fairly with all students who, because of religious obligations, have conflicts with scheduled exams, assignments or required attendance. In this class, please contact the instructor to make arrangements. Requests will be accommodated insofar as possible but must be made at least 3 weeks in advance of any course event to be impacted. See the [campus policy regarding religious observances](#) for full details.

Tentative reading schedule

An approximate schedule with reading timeline is posted below. This is tentative and subject to change.

Please be understanding that with COVID 19 pandemic protocols, the format (remote/in-person) will be subject to change, possibly on short notice. Updates will be communicated through Canvas.

Reading quizzes will be due each week THURSDAY.

Homeworks will be due TUESDAY of each week they are assigned. HW 1 will be due Sept 8.

* Instructor “traveling”. Schedules for those days are not final but if there is a conflict lectures will be pre-recorded or class taught by TA

Week	Dates	Reading	Comment
1	Aug. 25, 27	R&E Ch 1; 4.1-4.4	
2	Sep. 1, 3	R&E Ch. 4.5-4.7	<i>In 4.5 will only do ideal gases</i>
3	Sep. 8,10*	R&E Ch 2.1-2.6; 9.2 (p509-34); 4.8	<i>In 9.2 nonlinear cases just FYI for now</i>
4	Sep. 15,17	Ch. 5.5-5.7	<i>Catch up time</i>
5	Sep. 22, 24	Handouts	
6	Sep. 29, Oct. 1	Handouts, R&E Ch 6.1-6.3 (to p299)	
7	Oct. 6,8	R&E Ch 6.3-6.6	
8	Oct. 13, 15 <i>Midterm 10/14</i>		<i>Midterm will cover what we have done by 10/8. Some review on 10/13</i>
9	Oct. 20,22	R&E Ch 7.1-7.4	<i>Only will do isothermal but finish Ch7</i>
10	Oct. 27, 29	R&E Ch. 8.1-8.3	
11	Nov. 5*, 7	<i>Catch up space</i>	
12	Nov. 10*,12	Laidler Ch 4	<i>All non R&E readings will be posted</i>
13	Nov. 17, 19	Laidler Ch 4 and Ch11	
	Nov 24.		
	Nov 26: Break	ALL CLASS REMOTE AFTER THANKSGIVING (if not sooner...)	
14	Dec. 1, 3	Laidler Ch 5 / P&S Ch 5	
15	Dec. 8,10		
<i>Final Exam</i>	Sun. Dec. 13 7:30-10:00pm		