CHEN E4330 Advanced Chemical Kinetics

Time: TBD

Location: TBD

Course Description: Reaction kinetics, molecular view of reaction kinetics, reactions in liquid, reactions at surfaces, diffusion-reaction systems. Applications to the design of batch and continuous reactors. Special topics in kinetics and reactor design.

Prerequisites: Undergraduate Chemical Kinetics, Mass transport, or Kinetics S2E Module.

Course Objectives:
1. Understand kinetic rate expressions and how to design experiments to determine them.
2. Develop computer skills for mathematical modeling of reactive systems, with the understanding that these skills can be broadly applied to a wide range of real-world problems.
3. Develop problem-solving methodologies and creative thinking skills for the design and optimization of continuous and batch reactors.
4. Gain exposure to advanced topics in kinetics and reactor design relevant to graduate-level research and industry, with an emphasis on opportunities to engineer more sustainable chemical and energy conversion systems.

Required Textbook:
S. Fogler, Elements of Chemical Reaction Engineering, **5th Ed.**, Prentice Hall, 2016.
****Unless you are very strong in programming (Matlab, Python, etc) or another package with numerical solvers (e.g. Mathematica) you are strongly encouraged to purchase a version of Fogler that includes Polymath software. Polymath contains simple-to-learn ODE and non-linear equation solvers, and educational versions of Polymath are available $20 (4 mo. license), $30 (12 mo. license), or $39 (perpetual-use license. You can purchase and download this software from: http://www.polymath-software.com/fogler/ (Note: unfortunately Polymath is only available for Windows, and not Mac)

Fogler's 5th Ed. website: http://umich.edu/~elements/5e/ (additional resources found here)

Highly recommended Textbook:
P.L. Houston, Chemical Kinetics and Reaction Dynamics, 2nd Ed., Dover Publishing, 2006.
Note: the paperback and e-book versions of Houston are available online for around $20.

Other potentially helpful references:

- Sandler, S. Chemical, Biochemical, and Engineering Thermodynamics, Wiley, 2006. (for chemical equilibrium)
- Atkins and de Paula, Physical Chemistry (for molecular kinetics)
- Steinfeld, Francisco, and Hase, Chemical Kinetics and Dynamics, Prentice Hall, 1998.

- Rawlings and Ekerdt, Chemical Reactor Analysis and Design Fundamentals, Nob Hill Publishing, 2002.
- Matlab Guide, Higham and Higham, SIAM: Philadelphia, 2005, ISBN 0-89871-578-4.

Exams: These dates are tentative and subject to change

Midterm 1: TBD Midterm 2: TBD

Final: TBD.

Course Grades (*may be adjusted slightly depending on attendance app)

Final grade will be determined by: Attendance (3%), Class participation (5%), Homework assignments (20%), Midterm #1 (17%), Midterm #2 (25%), Final exam (30%). Class participation is based on active participation in discussions, Q&A, and Canvas discussion board.

Other Information:

- **Course Website:** Canvas will be used for course maintenance and information dissemination: https://courseworks2.columbia.edu/
- **Computational software:** Certain homework problems will require Matlab, Polymath, Python, Mathematica, or other comparable software to be used. If you do not know how to program (i.e. for Matlab or Python), then students are recommended to learn Polymath, which contains canned solvers and is relatively easy to learn. Videos of tutorials of Polymath and Matlab solvers that will be useful for this course can be found in the "Video Library" tab on the course page on Canvas. The demo files used in those videos are located under Files → Helpful Resources & Handouts → Matlab_Polymath Session Materials
- Matlab and Mathematica are available for free download by Columbia students here.
- See information on the previous page for downloading Polymath at this website.

SYLLABUS *(Schedule subject to change)*

Week 1 (1/21, 1/23)	Course overview, review of undergrad concepts.	Notes, Fogler 1
Week 2 (1/28, 1/30)	Chemical equilibrium	Notes
Week 3 (2/4, 2/6)	Rate laws / classical kinetics	Fogler Ch. 3.1-3.3, Houston Ch 2
Week 4 (2/11, 2/13)	Analyzing rate data, multiple reactions	Fogler Ch. 7.1-7.4, 8.1-8.4
Week 5 (2/18, 2/20)	Surface reactions	notes, Fogler 10.1-10.3
Week 6 (2/25, 2/27)	**2/25: Midterm 1** 2/27: Surface reactions and catalysis	notes, Fogler 10.1-10.3
Week 7 (3/3, 3/5)	Molecular kinetics: collision theory, potential energy surfaces (PES)	notes, Fogler Prof. Ref. R3.1, R3.2, Houston Ch 1, 3
Week 8 (3/10, 3/12)	Molecular kinetics: Activated complex theory (ACT)	notes, Fogler Prof. Ref. R3.1, R3.2, Houston Ch 1, 3
Week 9	**Spring Break - No Class**	
Week 10 (3/24, 3/26)	3/26: ACT	Houston Ch. 3
Week 11 (3/31, 4/2)	3/31: ACT / partition functions 4/2: Introduction to reactor design	Notes, Fogler Ch. 1,2
Week 12 (4/7, 4/9)	4/2: Introduction to reactor design 4/9: pressure drop / PBRs 4/10: **Midterm 2**	Fogler Ch. 2,4
Week 13 (4/14, 4/16)	non-isothermal reactors	Fogler Ch. 11, 12.1-12.5
Week 14 (4/21, 4/23)	Kinetics and mass transport	Fogler Ch. 14, 15
Week 15 (4/28, 4/30)	Advanced reactor design concepts.	Notes, parts of Fogler Ch. 6, 12, 16
May 8th -15th	Final Exam. Location TBD.^	

Homework Policy

- Homework is due at the ***beginning*** of class (8:40 am) on the due date specified. No exceptions. **Include a cover page on your HW, and clearly list your collaborators** at the top of this cover page. **Starting with HW4, HWs must be turned in electronically via Canvas -> Assignments before the day/time listed on the top of the assignment sheet.

- Late homework will be accepted with a ***50% penalty*** up until the date the graded assignment is returned to the class. Each student will be allowed no more than ***two*** late assignments in the semester.

- Select homework problems will be graded for correctness, while the remainder will be graded for completeness / effort.

- You must **show your work** in order to receive full credit. For problems solved using software such as Matlab or Python, include your code at the end of the hw set. If excel was used to generate solution plots, be sure to write up (in Microsoft Word or similar software) key equations that were used to generate those plots and fully describe the methodology used to solve the problem.

- **Collaboration** with classmates on homework is encouraged, within acceptable limits.

  - Acceptable collaboration includes discussing the problem statement, sharing ideas or approaches to solving the problem, and explaining concepts to one another.

  - **"Copying" answers from ANY source is unacceptable.** Turning in anything that does not represent your own work and thought process is considered plagiarism and is subject to the Columbia Policy on Academic Integrity: http://www.studentaffairs.columbia.edu/fysaac/forms/acadinteg.pdf

- For the report sections of the final project, plagiarism or "copying" of written sections is also strictly prohibited. Cite all references for information used within your report.

Exam Policy

- No cell phones, computers, i-pads, or similar items may be used during exams.
- Graphing calculators are not necessary and not allowed. **Bring a scientific calculator with you to the exam**.
- Communication with classmates during the exam is strictly prohibited
- At the top of your exam, write down the names of your classmates sitting directly to your left and right.