Instructor: Prof. Jason Haugh  
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Lectures: Tue/Thur, 10:15-11:30 am/EB3 2232  

Course objectives:  
The intent of this course is to help the student master several advanced concepts in chemical reaction engineering, notably:  
1) advanced reactor design, including consideration of the energy balance;  
2) chemical reaction mechanisms and rate theories;  
3) transport effects in reactive systems;  
4) biomolecular applications of chemical kinetics.  

On completion of the course, the student should be able to design/analyze a variety of complex reacting systems in both traditional and non-traditional areas of chemical engineering.  

Prerequisites:  
1) An undergraduate course in chemical kinetics/reactor design that covered, in detail: ideal reactors (batch, plug flow, perfectly mixed), application of these three reactors to single and multiple reactions for isothermal operation, analysis of kinetic data, and derivation of rate equations from sequences of elementary reactions.  
2) Ability to solve coupled ordinary differential equations (ODEs), either analytically or numerically. A guide for using MATLAB to solve nonlinear ODEs may be accessed here:  
http://www.che.ncsu.edu/academics/documents/matlab_che.pdf  
A serious of tutorial videos may be accessed here:  
https://mediasite.online.ncsu.edu/online/Catalog/catalogs/matlab-tutorial  

Required textbook:  
http://jbrwww.che.wisc.edu/home/jbraw/chemreacfun/  

Supplementary references:  
Grading basis:
The overall course grade will be determined as follows.
- Problem sets (6) 15%
- Midterm exams (3) 70%
- Final paper (1) 15%

Problem sets:
All problem sets are to be completed individually; i.e., without the use of other students’ solutions and without consulting solutions that may be available via other sources. Failure to adhere to this policy will result in disciplinary action via the NCSU academic integrity policy.

Problem sets are due on the specified due date and are to be submitted to me and to the TAs by email. Here are the other particulars.
1) Saved in PDF format, < 5 MB (if scanning a hard copy, don’t use high resolution).
2) Sent by email to me and copy both TAs.
3) Sent by 5 pm EST on the due date.

Midterm exams:
All midterm exams will be open book, open notes and cumulative; that is, all material covered up to that point in the course is fair game (this provision obviates the need for a final exam). Standard calculators are allowed, but electronic devices with an active data connection are not allowed. A laptop or tablet may be used to view stored files (e.g., lecture notes), provided that the wireless data connection is disabled.

Policy on posting solutions:
Solutions to problem set and exam problems will be distributed, on the condition that all students sign the Restriction on Sharing Course Content form. The form should be submitted no later than the due date of the first problem set.

Final paper:
The final paper must include analysis and/or synthesis (i.e., more than a summary) of a current research topic in the scientific literature, based on the fundamentals learned in this course. Guidelines for the scope of the paper are: 2000-3000 words, 3-4 figures, 5-10 references. Any plagiarism on this assignment will result in disciplinary action via the academic integrity policy.

Assignment of grades:
Course grades will be determined based on overall average, with letter grade cut-offs set based on the distribution of scores. No problem set or exam grades will be dropped or weighted disproportionally. Typically, the top half of the class earns B+ or better.

Academic Integrity:
Campus-wide definitions and policies related to academic integrity are outlined in the NCSU Code of Student Conduct:
https://policies.ncsu.edu/policy/pol-11-35-01

NCSU Policy on Working with Students with Disabilities:
https://policies.ncsu.edu/regulation/reg-02-20-01
Captured Lectures:
This on-campus course will be captured and distributed via the Internet and/or electronic media as part of the Engineering Online (EOL) program for the distance students. These video recordings may contain an image of you entering the classroom, asking questions or being a part of the studio class. Please notify Dr. Linda Krute, Director of EOL, in writing at ldkrute@ncsu.edu if you DO NOT want your image to be included in the lecture presentation. If we do not hear from you after the first week of the class, we will assume that you are in agreement with this procedure.

Instructions and Guidelines for Engineering Online (EOL) Students

1. Communication: I will be corresponding with you mostly if not exclusively by email. Messages addressed to the online section will be sent through a mailing list (CHE717-601@wolfware.ncsu.edu). Only I and the TAs can send messages to the list. IMPORTANT: At least to my knowledge, the mailing lists established through the Wolfware system use your NCSU email address. I understand that for many of you, this is not your preferred address; if so you will want to set up email forwarding immediately: https://oit.ncsu.edu/my-it/email-calendaring/email-forwarding/

2. Submitting Problem Sets: Refer to the instructions above. Do not submit to EOL.

3. Taking Exams: Here are the particulars.
   1) All exams will be proctored. Your proctor will submit your exams to EOL.
   2) Refer to the details under Grading basis on the previous page.
   3) Each exam will have a time limit; you should tentatively plan for 2 hours for each.
   4) You may take each exam anytime during the 3-day window comprised of the scheduled exam date and the two following business days (e.g., Fri/Mon/Tue for a Friday exam).

4. Returning Graded Problem Sets and Exams: Graded problem sets will be returned to you by email (from the TA who graded the assignment). Graded exams will be returned by EOL.

5. Questions/Getting Help: In my experience, this is by far the biggest source of consternation for online students, because email is the only reliable conduit that we have. Please know that we are here to help, and expect your emails! To achieve the fastest response, we recommend that you copy me and both TAs on all email correspondence. Regarding help on homework, we advise you to scan/take a picture of your work, i.e., where you are stuck. Because of potential lags in email communication, sending questions sooner rather than later is recommended (i.e., don’t wait until the night before a problem set due date).

6. Assigning Grades: CHE 717 is a core course in our graduate curriculum, and therefore the assignment of grades cannot be affected by the offering of an online section. For this reason, grading statistics (means and standard deviations) that I distribute will be for the live section only. At the end of the semester, course grades for the live section will be determined first, and then that distribution will be used to assign grades for the online section. The only adjustment to the online section grades will be to normalize the averages of the problem set grades, recognizing that the live cohort has the advantage of communicating with each other about solution approaches.
COURSE SCHEDULE (Tentative)

Topics (Rawlings & Ekerdt chapters)

PART I. BASIC PRINCIPLES OF REACTOR DESIGN AND CHEMICAL KINETICS

1. Th Aug 18  
   Course introduction, reaction stoichiometry, rate equations (1,2)

2. T Aug 23  
   Ideal, isothermal reactors: design equations (4)

3. Th Aug 25  
   Ideal, isothermal reactors: design equations (4)

4. T Aug 30  
   Ideal reactors: multiple reactors, multiple reactions (4)

5. Th Sep 1  
   Ideal reactors: multiple reactors, multiple reactions (4)

   Problem Set #1 due Friday, Sept. 2

6. T Sept 6  
   Chemical kinetics: rate laws from reaction mechanism (5)

7. Th Sept 8  
   Chemical kinetics: rate laws from reaction mechanism (5)

8. T Sept 13  
   Chemical kinetics: rate laws from reaction mechanism (5)

9. Th Sept 15  
   Special topic: biological kinetics

   Problem Set #2 due Friday, Sept. 16

10. T Sept 20  
    Special topic: stochastic modeling

    Th Sept 22  
    No class

    Midterm exam #1: Friday, Sept. 23

PART II. ADVANCED REACTOR DESIGN AND NONLINEAR DYNAMICS

11. T Sept 27  
    Ideal reactor design with energy balance (6)

12. Th Sept 29  
    Stability of nonisothermal reactors; nonlinear dynamics (6)

13. T Oct 4  
    Stability of nonisothermal reactors; nonlinear dynamics (6)

    Th Oct 6  
    No class (Fall Break)

    Problem Set #3 due Friday, Oct. 7

14. T Oct 11  
    Stability of nonisothermal reactors; nonlinear dynamics (6)

15. Th Oct 13  
    Stability of nonisothermal reactors; nonlinear dynamics (6)

16. T Oct 18  
    Nonideal reactors: residence-time distribution (8)

17. Th Oct 20  
    Nonideal reactors: residence-time distribution (8)

   Problem Set #4 due Friday, Oct. 21

18. T Oct 25  
    Special topic: nonlinear dynamics in biology

    Th Oct 27  
    No class

    Midterm exam #2: Friday, Oct. 28
PART III. INTERACTION OF REACTION AND TRANSPORT

19. T Nov 1  Heterogeneous catalysis: reactions in porous catalysts (7)
20. Th Nov 3  Heterogeneous catalysis: reactions in porous catalysts (7)

21. T Nov 8  Heterogeneous catalysis: reactions in porous catalysts (7)
22. Th Nov 10  Heterogeneous catalysis: reactions in porous catalysts (7)

Problem Set #5 due Friday, Nov. 11

23. T Nov 15  Heterogeneous catalysis: reactions in porous catalysts (7)
24. Th Nov 17  Heterogeneous catalysis: reactions in porous catalysts (7)

25. T Nov 22  Special topic: diffusion-controlled reactions
Th Nov 24  No class (Thanksgiving)

Problem Set #6 due Friday, Nov. 25

26. T Nov 29  Special topic: reaction/transport coupling in biology
Th Dec 1  No class

Midterm exam #3: Friday, December 2

Final paper due Friday, December 9