CHE 717, Chemical Reaction Engineering, Fall 2013

COURSE SYLLABUS

http://engineeringonline.ncsu.edu/onlinecourses/coursehomepages/FALL-2013/CHE717.html

Instructor: Prof. Jason Haugh
3100 Partners II, Centennial Campus
E-mail: jason_haugh@ncsu.edu

TAs: Anisur Rahman Tim Shay
E-mail: arahman3@ncsu.edu E-mail: twshay@ncsu.edu

Lectures: Tue/Thur, 9:35-10:50 am/MRC 313

Required Textbook:

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

Grading basis:
The overall course grade will be determined as follows.

<table>
<thead>
<tr>
<th>Component</th>
<th>Percentage</th>
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<tbody>
<tr>
<td>Problem sets (6)</td>
<td>15%</td>
</tr>
<tr>
<td>Midterm exams (3)</td>
<td>70%</td>
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<tr>
<td>Final paper (1)</td>
<td>15%</td>
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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 (see below).

For the live section, problem sets are due at the beginning of class on the due date (online students, refer to the next page)

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 other electronic devices (i.e., those with a data connection) are not.

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.

Course grades will be determined based on overall average, with letter grade cut-offs set at the instructor’s discretion. No problem set or exam grades will be dropped or weighted disproportionately. 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:
http://policies.ncsu.edu/policy/pol-11-35-01

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 (you may be submit it together with your problem set).

**NCSU Policy on Working with Students with Disabilities:**
http://policies.ncsu.edu/regulation/reg-02-20-01

**Supplementary References:**
Bailey, James E. and Ollis, D.F. *Biochemical Engineering Fundamentals*, 2nd Ed.
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, as instructed here: http://oit.ncsu.edu/email/email-forwarding

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

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 might 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 (i.e., Tue/Wed/Thur for a Tuesday exam or Thur/Fri/Mon for a Thursday exam).

4. **Returning Graded Problem Sets and Exams:** Will be done through EOL.

5. **Getting Help:** In my experience, this is by far the biggest source of consternation for online students. We are here to help, but it is a challenge. Usually, email works best. For questions about grading, always contact the TA who graded the assignment or exam first. For all other questions, it is best to email me. Only if a question is not easily resolved by email, we might then offer to schedule a more in-depth conversation over the phone or by Skype. 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 an advantage on that front.
COURSE SCHEDULE (Tentative)

Topics (Rawlings & Ekerdt chapters)

PART I. BASIC PRINCIPLES OF REACTOR DESIGN AND CHEMICAL KINETICS

1. Th Aug 22  Course introduction, reaction stoichiometry, rate equations (1,2)
2. T Aug 27  Ideal, isothermal reactors: design equations (4)
3. Th Aug 29  Ideal, isothermal reactors: design equations (4)
4. T Sep 3  Ideal reactors: multiple reactors, multiple reactions (4)
5. Th Sep 5  Chemical kinetics: elementary reactions (5)  PS #1 due
6. T Sept 10  Chemical kinetics: rate laws from reaction mechanism (5)
7. Th Sept 12  Chemical kinetics: transition state theory (5)
8. T Sept 17  Special topic: stochastic modeling  PS #2 due
9. Th Sept 19  Special topic: biological kinetics

T Sept 24  Midterm exam #1

PART II. ADVANCED REACTOR DESIGN AND NONLINEAR DYNAMICS

10. Th Sept 26  Ideal reactor design with energy balance (6)
11. T Oct 1  Ideal reactor design with energy balance (6)
12. Th Oct 3  Stability of nonisothermal reactors; nonlinear dynamics (6)
13. T Oct 8  Stability of nonisothermal reactors; nonlinear dynamics (6)  PS #3 due
  Th Oct 10  No class (Fall Break)
14. T Oct 15  Stability of nonisothermal reactors; nonlinear dynamics (6)
  Th Oct 17  No class (JMH out of town)
15. T Oct 22  Nonideal reactors: residence-time distribution (8)
16. Th Oct 24  Nonideal reactors: residence-time distribution (8)  PS #4 due
17. T Oct 29  Nonideal reactors: residence-time distribution (8)
  Th Oct 31  Midterm exam #2
PART III. INTERACTION OF REACTION AND TRANSPORT

18. T Nov 5  Heterogeneous catalysis: reactions in porous catalysts (7)
19. Th Nov 7  Heterogeneous catalysis: reactions in porous catalysts (7)

20. T Nov 12 Heterogeneous catalysis: reactions in porous catalysts (7)
21. Th Nov 14 Heterogeneous catalysis: reactions in porous catalysts (7)  PS #5 due

22. T Nov 19 Heterogeneous catalysis: non-isothermal effects (7)
23. Th Nov 21 Heterogeneous catalysis: non-isothermal effects (7)

24. T Nov 26 Special topic: reaction/transport coupling in biology  PS #6 due
Th Nov 28  No class (Thanksgiving)

25. T Dec 3 Special topic or/and exam review
Th Dec 5  Midterm exam #3

Th Dec 12  Final paper due