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Course Websites:
We have arranged to administer this course online through Moodle:  
https://wolfware.ncsu.edu/courses/my-wolfware/  
Moodle will be the interface for: posting announcements; posting prepared lecture slides;  
communicating via message board (Help Forum); posting assignments; submitting assignments;  
posting solutions; posting grades.

Engineering Online (EOL) course website:  
https://www.engineeringonline.ncsu.edu/course/che-717-chemical-reaction-engineering/?display=course-home  
The EOL site will be the interface for: accessing the taped lectures; accessing handwritten content  
generated during class.

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 series of tutorial videos may be accessed here:  
https://mediasite.online.ncsu.edu/online/Catalog/catalogs/matlab-tutorial

Required Textbook:
Rawlings, James B. and Ekerdt, John G.  Chemical Reactor Analysis and Design Fundamentals,  

http://jbrwww.che.wisc.edu/home/jbraw/chemreacfun/
Supplementary References:

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

<table>
<thead>
<tr>
<th>Component</th>
<th>Weight</th>
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<tbody>
<tr>
<td>Problem sets (6)</td>
<td>15%</td>
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<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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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 (including online sources).
- The assignments will be posted and submitted via the Moodle site. Please note the due date (and time) for each posted assignment. Late assignments will be accepted, with a 50% penalty, no later than the beginning of the next class period.

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).
- Each exam will have a 2-hour time limit.
- 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.
- You provide your own materials (paper, etc.).

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 paper will cover a current research topic in the scientific literature that is related to (some of) the fundamentals learned in this course. It must be clear that chemical reaction engineering fundamentals are applicable.
- To achieve a high grade, the paper must include analysis and/or synthesis of a current research topic in the scientific literature, based on the fundamentals learned in this course. In this context, *analysis* means ‘breaking down’ and examining in detail to gain deeper insight, whereas *synthesis* means ‘putting together’ information from various sources to arrive at a novel conclusion. In contrast to those higher-level skills, reading the literature and putting the information in your own words is a summary. A paper containing summary only will not be scored highly.
- Guidelines for the scope of the paper are: 2000-3000 words, 3-4 figures, 5-10 references. These are just suggestions to give a sense of the scope.
- Any plagiarism on this assignment will result in disciplinary action via the academic integrity policy. Software may be used to analyze your document for evidence of plagiarism. In case you are not clear about what constitutes plagiarism, Wikipedia has a good entry: https://en.wikipedia.org/wiki/Plagiarism
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.

Cell Phone and Laptop Policy:
Cell phones may only be used during mid-lecture breaks and must be silenced and put away during lecture. Laptops and tablets may only be used for electronic viewing and annotating of lecture notes. This policy will be modified if it is found that laptops or tablets are being used frivolously.

Academic Integrity:
Students are required to comply with the university policy on academic integrity found in the Code of Student Conduct (https://policies.ncsu.edu/policy/pol-11-35-01). It is the instructor's understanding and expectation that the student's name on any assignment means that the student completed the assignment in question and neither gave nor received unauthorized aid. Authorized aid on an individual assignment includes discussing the interpretation of the problem statement, sharing ideas or approaches for solving the problem, and explaining concepts involved in the problem. Any other aid would be unauthorized and a violation of the academic integrity policy. All cases of academic misconduct, including plagiarism, will be submitted to the Office of Student Conduct. Students found guilty of academic misconduct will be subject to, at a minimum, a zero on the assignment in question, up to failing grade in the course, depending on the nature of the violation. In addition, if you are found guilty of academic misconduct in the course, you will be on academic integrity probation for the remainder of your years at NCSU and may be required to report your violation on future professional school applications. It's not worth it!

Students with Disabilities:
North Carolina State is subject to the Department of Health, Education, and Welfare regulations implementing Section 504 of the Rehabilitation Act of 1973. Section 504 provides that: "No otherwise qualified handicapped individual in the United States. . . shall, solely by reason of his handicap be excluded from participation in, be denied the benefits of, or be subjected to discrimination under any program or activity receiving Federal financial assistance." This regulation includes students with hearing, visual, motor, or learning disabilities and states that colleges and universities must make "reasonable adjustments" to ensure that academic requirements are not discriminatory. Modifications may require rescheduling classes from inaccessible to accessible buildings, providing access to auxiliary aids such as tape recorders, special lab equipment, or other services such as readers, note takers, or interpreters. It further requires that exams actually evaluate students' progress and achievement rather than reflect their impaired skills. This may require oral or taped tests, readers, scribes, separate testing rooms, or extension of time limits. Reasonable accommodations will be made for students with verifiable disabilities. In order to take advantage of available accommodations, students must register with the Disability Services Office at Suite 2221, Student Health Center, Campus Box 7509, 919-515-7653. For more information on NC State's policy on working with students with disabilities, please see the Academic Accommodations for Students with Disabilities Regulation (REG02.20.01 https://policies.ncsu.edu/regulation/reg-02-20-01)

Equal Opportunity:
NC State University provides equality of opportunity in education and employment for all students and employees. Accordingly, NC State affirms its commitment to maintain a work environment for all employees and an academic environment for all students that is free from all forms of discrimination. Discrimination based on race, color, religion, creed, sex, national origin, age,
disability, veteran status, or sexual orientation is a violation of state and federal law and/or NC State University policy and will not be tolerated. Harassment of any person (either in the form of quid pro quo or creation of a hostile environment) based on race, color, religion, creed, sex, national origin, age, disability, veteran status, or sexual orientation also is a violation of state and federal law and/or NC State University policy and will not be tolerated. Retaliation against any person who complains about discrimination is also prohibited. NC State’s policies and regulations covering discrimination, harassment, and retaliation may be accessed at https://policies.ncsu.edu/policy/pol-04-25-05 or https://www.ncsu.edu/equal_op/. Any person who feels that he or she has been the subject of prohibited discrimination, harassment, or retaliation should contact the Office for Equal Opportunity (OEO) at 919-515-3148.

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.

Additional Information and Guidelines for EOL Students

1. Communication: Announcements will be distributed by email. At least to my knowledge, the mailing lists established in Moodle 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: In addition to the parameters specified under Midterm Exams,
   • All exams will be proctored. Your proctor will submit your exams to EOL.
   • 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. 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 all three TAs on all email correspondence. Regarding help on homework, we advise you to scan/take a picture of your work, i.e., to show us 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). We also encourage use of the Help Forum on the Moodle site. If these routes prove to be insufficient to address a particular question or issue, an alternative mode of communication (e.g., Skype) will be sought.

5. 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 23       Course introduction, reaction stoichiometry, rate equations (1,2)
2. T Aug 28       Ideal, isothermal reactors: design equations (4)
3. Th Aug 30       Ideal, isothermal reactors: design equations (4)
4. T Sep 4         Ideal reactors: multiple reactors, multiple reactions (4)
5. Th Sep 6        Ideal reactors: multiple reactors, multiple reactions (4)
Problem Set #1 due Friday, Sept. 7
6. T Sept 11       Chemical kinetics: rate laws from reaction mechanism (5)
7. Th Sept 13      Chemical kinetics: rate laws from reaction mechanism (5)
8. T Sept 18       Chemical kinetics: rate laws from reaction mechanism (5)
9. Th Sept 20      Special topic
Problem Set #2 due Friday, Sept. 21
10. T Sept 25      Special topic
   Th Sept 27         No class
Midterm exam #1: Friday, Sept. 28

PART II. ADVANCED REACTOR DESIGN AND NONLINEAR DYNAMICS
11. T Oct 2        Ideal reactor design with energy balance (6)
   Th Oct 4         No class (Fall Break)
12. T Oct 9        Stability of nonisothermal reactors; nonlinear dynamics (6)
13. Th Oct 11      Stability of nonisothermal reactors; nonlinear dynamics (6)
Problem Set #3 due Friday, Oct. 12
14. T Oct 16       Stability of nonisothermal reactors; nonlinear dynamics (6)
15. Th Oct 18      Stability of nonisothermal reactors; nonlinear dynamics (6)
16. T Oct 23       Nonideal reactors: residence-time distribution (8)
17. Th Oct 25      Nonideal reactors: residence-time distribution (8)
Problem Set #4 due Friday, Oct. 26
18. T Oct 30       Special topic
   Th Nov 1         No class
Midterm exam #2: Friday, Nov. 2
PART III. INTERACTION OF REACTION AND TRANSPORT

19. T Nov 6  Heterogeneous catalysis: reactions in porous catalysts (7)
20. Th Nov 8  Heterogeneous catalysis: reactions in porous catalysts (7)

21. T Nov 13  Heterogeneous catalysis: reactions in porous catalysts (7)
22. Th Nov 15  Heterogeneous catalysis: reactions in porous catalysts (7)

Problem Set #5 due Friday, Nov. 16

23. T Nov 20  Heterogeneous catalysis: reactions in porous catalysts (7)
Th Nov 22  No class (Thanksgiving)

24. T Nov 27  Heterogeneous catalysis: reactions in porous catalysts (7)
25. Th Nov 29  Special topic

Problem Set #6 due Friday, Nov. 30

26. T Dec 4  Special topic
Th Dec 6  No class

Midterm exam #3: Friday, December 7

Final paper due Friday, December 14