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Course hours/classroom: See viewing schedule


Course objectives:  
The intent of this course is to help the student master several advanced concepts in chemical reaction engineering. On completion of the course, the student should be able to design/analyze a variety of complex reacting systems in both traditional and nontraditional areas of chemical engineering. Specifically, the student will be able to:

1. Use matrix algebra to analyze large systems of reactions;
2. Use knowledge of reaction rate theories and/or reaction mechanisms to derive expressions for rate of reaction
3. Design and analyze the stability of reactor systems, including consideration of the energy balance
4. Analyze the effect of transport in reactive systems
5. Apply chemical kinetics analysis to biological systems, and
6. Relate concepts in chemical reaction engineering to current research in chemical and biomolecular 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, either analytically or numerically using MATLAB
3. Basic understanding of matrix algebra
Grading:
Problem Sets (7) 15%
Midterm Exams (3) 60%
Final Exam (1) 25%
All tests will be open book, open notes. Exams will be “take-home” and students will have 24 hrs to work on the exam.

Course Notes:
All course material provided by the instructor will be posted on http://vista.ncsu.edu

Expected workload
It is expected that an average student will spend a total of approximately 13-16 hours per week on this course (~ 4 hrs viewing lectures and ~9-12 hrs outside of class)

Student code of conduct
The instructor implicitly assumes the highest level of integrity and honesty in the students taking this course. The student must be familiar with and comply with the NCSU Student Code of Conduct. http://www.ncsu.edu/policies/student_services/student_discipline/POL11.35.1.php

Supplementary References:


COURSE SCHEDULE (This is a basic outline of how course material is covered over every lecture. Some deviations from this outline may occur)

Topics (Rawlings & Ekerdt chapters)

**PART I: BASIC PRINCIPLES OF REACTOR DESIGN AND CHEMICAL KINETICS**

1. Course introduction, reaction stoichiometry (1, 2)
2. Rate equations; ideal, isothermal reactors: design equations (4)
3. Ideal, isothermal reactors (4)
4. Ideal, isothermal reactors (4)
5. Ideal, isothermal reactors (4)
6. Ideal, isothermal reactors: reactors in series (4)
7. Chemical kinetics: elementary reactions, laws of mass action (5)
8. Chemical kinetics: elementary reactions, laws of mass action (5)
9. Chemical kinetics: rate laws from reaction mechanism (5)
10. Chemical kinetics: Biological systems
11. Chemical kinetics: Biological systems
12. Chemical kinetics: stochastic modeling (4)
13. Chemical kinetics: transition state theory (5)
14. Chemical kinetics: transition state theory (5)

**PART II: ADVANCED REACTOR DESIGN AND NONLINEAR DYNAMICS**

15. Ideal reactor design with energy balance (6)
16. Ideal reactor design with energy balance (6)
17. Ideal reactor design with energy balance (6)
18. Stability of nonisothermal reactors; nonlinear dynamics (6)
19. Stability of nonisothermal reactors; nonlinear dynamics (6)
20. Stability of nonisothermal reactors; nonlinear dynamics (6)
21. Stability of nonisothermal reactors; nonlinear dynamics (6)
22. Stability of nonisothermal reactors; nonlinear dynamics (6)
23. Nonideal reactors: residence-time distribution (8)
24. Nonideal reactors: residence-time distribution (8)
25. Nonideal reactors: residence-time distribution (8)

**PART III. INTERACTION OF REACTION AND TRANSPORT**

26 Oct 26  Heterogeneous catalysis: isothermal reactions in porous catalysts (7)
27 Oct 28  Heterogeneous catalysis: isothermal reactions in porous catalysts (7)
28 Oct 30  Heterogeneous catalysis: isothermal reactions in porous catalysts (7)
29 Nov 2   Heterogeneous catalysis: isothermal reactions in porous catalysts (7)
30 Nov 4   Heterogeneous catalysis: external mass transfer (7)
31 Nov 6   Heterogeneous catalysis: heat transfer effects (7)
32 Nov 11  Heterogeneous catalysis: heat transfer effects (7)
33 Nov 13  Heterogeneous catalysis: multiple reactions in porous catalysts (7)
34 Nov 16  Diffusion-controlled reactions
35 Nov 18  Special topics – application of concepts to problems in literature/outside ChemE
36 Nov 20  Special topics – application of concepts to problems in literature/outside ChemE
37 Nov 30  Special topics – application of concepts to problems in literature/outside ChemE
38 Dec 2  Course review
39 Dec 4  Course review

*Additional notes will be provided*