ChBE 4300B: Kinetics and Reactor Design
Syllabus
Fall 2012

Instructor: Prof. Carsten Sievers
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Office Hours: Monday 8:30-9:30
Wednesday 2:00-3:30

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Office Hours: Thursday 12:00-1:00
Upon request by email

Class Times: Monday, Wednesday, Friday 1:05-1:55 pm
Class Location: ES&T L1125

Recitation time: Thursday 11:05-11:55, starting August 28
Recitation location: ES&T L1125

Textbook: Chemical Reaction Engineering, O. Levenspiel, John Wiley, 3rd edition, 1999.

Additional reading (optional): Fundamentals of Chemical Reaction Engineering, M. Davis and R. Davis. This textbook can be downloaded for free at:
http://faculty.virginia.edu/davislab/textbook.htm

Course Prerequisites: ChBE 3110 and ChBE 3200

Course Objectives:
This course introduces two basic concepts: (i) reaction mechanisms and kinetic rate expressions for homogeneous and heterogeneous reaction systems, including enzyme catalyzed reactions and cell growth kinetics, and (ii) reactor design for the homogeneous reaction systems. The design principles for ideal homogeneous reactors are introduced, followed by the concept of RTD (residence time distribution) to diagnose and account for the non-idealities in flow patterns. For heterogeneous reactions, the role of transport (diffusion) effects, Thiele modulus, and catalyst effectiveness factor are introduced.

Learning Outcomes: By the end of this course, a student should be able to:
1. Analyze reaction mechanisms for homogeneous & heterogeneous reactions and develop kinetic rate expressions for the reactions.

2. Develop microscopic and macroscopic mass and energy balances for various reactor types and identify the initial and boundary conditions
3. Discern reaction kinetics by analyzing data from a variety of reactor types
4. Design ideal isothermal reactors
5. Design non-isothermal reactors by accounting for the heat effects (endothermic or exothermic reactions) as well as non-adiabatic reactor configurations
6. Analyze RTD (residence time distribution) data to identify non-idealities in reactor configurations and utilize this information to predict reactor performance
7. Analyze for the role of transport effects in isothermal heterogeneous reactions.

Grading:	Quiz I (September 24, 2012)	20%
	Quiz II (October 29, 2012)	25%
	Final exam (December 10, 2012)	40%
	Tests	15%
	Total	100%*

* A bonus of 2 points is awarded to the entire class if the CIOS response rate is 90% or higher by the beginning of the last class (i.e. 1:05 p.m. on December 7).

Regrades have to be requested in writing within one week from when the exam/test was returned. This period is extended if you miss the lecture, in which the exam/test is returned, with a valid excuse. After this time, no regrades will be considered.

Dr. Sievers will grade the exams.

Exams:
We will try to find an acceptable solution for scheduling the quizzes, so that you can work on the problems for 90 minutes. Alternatively, the quizzes will be held during class periods (i.e. 50 minutes). The quizzes and final will start with a closed-book part consisting of ten short questions that can be answered in one sentence or less. The closed-book part will be weighted as 25% of the total exam score. Once you hand in this part you will receive the problems for the open-book part. All data required for solving the problems will be provided. All exams must be completed independently. No wireless and/or internet enabled devices (including cell phones and laptops) are allowed during exams. Make-up exams are only provided for acceptable, well documented reasons (e.g. documented illness). Absence at the exam date must be discussed ahead of time if at all possible. All make-up exams are oral and closed-book. All exams are cumulative.

Rules for Homework:
1. Homework assignments are intended as an exercise that helps you learn how to apply the concepts taught in class.
2. Solutions will be posted on T-Square.
3. Homework will not be graded.
4. There will be unannounced short tests after the due date of the homework assignment. The tests are closed book – closed notes. All required equations will be provided.

Honor Code:
Students are expected to abide the Georgia Tech Honor Code at all times and avoid all instances of academic misconduct including, but not limited to:

1. Possessing, using, or exchanging improperly acquired written or oral information in preparation for quizzes, exams and the final.
2. Copying homework solutions from classmates, previous students, solution manuals, or otherwise representing the work of others as your own.
3. Using prohibited materials or means to complete exams or the final.

For reference please consult: **http://www.honor.gatech.edu/plugins/content/index.php?id=9**

Expectations:
You can expect that your instructor and TA:

1. Are prepared for classes, review sessions, office hours.
2. Notify you in advance if we have to cancel office hours (e.g. sickness, travel).
3. Are available to discuss your questions after most classes or during office hours.
4. Grade your tests and exams fairly using the same standards as for all other students.
5. Will give you one week to work on a homework assignment.
6. Treat you respectfully.

We expect that you:

1. Take responsibility for your own learning. Instructors and TAs will help if you ask for it, but you will have to initiate the contact.
2. Attend classes regularly.
3. Read the textbook. Preferably before class.
4. Ask questions when you do not understand something.
5. Keep track of your grades. We will not continuously calculate your average grade during the semester; you can do this easily if you are picking up your graded assignments.
6. Think about homework problems before you come to an office hour to discuss it.
7. Abide the honor code.
8. Treat us respectfully.

Tentative Schedule for ChBE 4300

This schedule is intended as a rough orientation and recommendation complementary reading. The time line may vary.

Week	Topic	Chapter*
1	Reaction Thermodynamics - Heat of reaction effects - Reaction free energy and equilibrium constant - Effect of pressure and temperature on equilibrium conversion	**9**
2,3	Theories and Mechanisms of Homogeneous Reactions - Bimolecular collision theory and Transition state theory - Reaction intermediates and Bodenstein steady-state approximation - Chain and non-chain reactions - Kinetic rate expressions derived from reaction mechanisms - Michaelis-Menten kinetics	**2**
4-7	Definitions of Rate and Design Equations in Different Reactor Types - Mass balances around ideal homogeneous reactors - Fractional conversion as a design variable in single reactions - Integration of kinetics into the reactor design equation - Graphical interpretation of reactor design equations - Analysis of Reactor Data	**3-7**
8,9	Multiple Reactions in Homogeneous Reactors - Series vs. parallel reactions - Yield and selectivity in multiple reactions - Reactor design considerations	**7 and 8**
10,11	Non-isothermal Homogeneous Reactor Design - Energy balances around non-adiabatic reactors - Numerical vs. graphical approach to reactor design - Multiple reactions in a non-isothermal reactor	**9**

12,13	Non-idealities in Homogeneous Reactors
	- Residence time distribution (RTD)
	- Non ideal reactor models
	  - Segregated flow model
	  - Axial dispersion model
	  - CSTR's in series model
		11 and 13

14-16	Heterogeneous Reactions - Reaction mechanisms - Langmuir-Hinshelwood kinetics - Catalyst structure and transport - Single pore diffusion model - Thiele modulus and catalyst effectiveness factor	**17 and 18**

* Chemical Reaction Engineering, O. Levenspiel, John Wiley, 3rd edition, 1999.