Syllabus for Chemistry 111

Chemical Kinetics

Class meets: Tue, Thu **12:30 – 1:45** PM **Girvetz Hall 1112**

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Office Hours: Tue, Thu (5:30-6:30 PM) or by appointment
Course website: http://www.chem.ucsb.edu/~kalju/chem111

Lecture Textbooks:

Recommended: "Principles of Chemical Kinetics" by J. E. House, 2007
Recommended: "Physical Chemistry: Kinetics" by Horia Metiu, Taylor & Francis, 2006

***The Course*:**

The main goal of Chem 111 is to teach principles of reaction kinetics and catalysis. Topics covered include the laws and theories governing rates of chemical reactions and reaction mechanisms in the gas phase, in solution, and at the solid-liquid interface. Emphasis is placed on modern experimental approaches to study kinetics in complex chemical and biochemical systems. Analysis of experimental data is introduced. Computational approaches to estimate rates of chemical reactions and study the mechanism of catalysis are discussed

Expectations of Students:

1) Attendance and taking good lecture notes is expected. Supplementing the lecture notes with study notes based on the textbook(s) is a good way to improve your chances to be successful in this course.

2) The House textbook has many excellent worked-out problems. The practice problems in the book are quantitative and require a good understanding of the math. I will suggest which ones are good to solve but you are free to tackle more difficult problems on your own.

3) Two mid-terms (each 80 points) and a final exam (200 points) will be given. The two mid-terms test your *knowledge* of topics covered prior to exam. The final will cover all the topics that were taught in this course and also test your ability to *understand* the material. There are two 20-point homeworks.

4) Honesty and academic integrity must be always preserved. While working with others is encouraged outside the classroom, you must answer the homework and exam questions individually. No supplemental material should be used during an exam.

5) No student shall give, sell, or otherwise distribute to others or publish any electronically available course materials or recordings made during any course presentation without the written consent of the instructor.

6) There are no excuses for class absence, especially on the exam days. There are no make-up exams. If you must miss a test, contact the lecturer in advance and provide a verifiable doctors excuse.

7) The grade is based on the number of points out of 400 points total. The last time I taught, there were 5 As, 6 Bs, 1 C, 1D, and 1 F in the course.

Study tips:

- Read the relevant material before the class meets. I like to interact with students during our meetings and you enjoy the lectures more if you can think along
- Review (or rewrite) your class notes the same day and supplement them with material from the textbook and other resources (books, Internet). Ask for help if something remains unclear.
- Do not even hope that you can be successful by trying to memorize all the material few days before the exam. The final exam expects that you understand, not only remember the material.

Proposed Topics for Fall 2013

The CHEM 111 course rests on three pillars:

- **how to collect kinetic data,**
- **how to analyze kinetic data**
- **how to interpret kinetic data**

The course is taught in a highly non-linear fashion: instead of covering each of the pillars in one month, we will start climbing up all three pillars roughly simultaneously. The course starts by discussing (i) how to study simple reactions with methods that you are well familiar with, and how to interpret the results with quite simple models. We then proceed to more difficult reactions that will be studied with more complex methods, require more advanced calculus, and rely on more advanced theory for interpretation. I am open to suggestions from students, so if you have some special interests, please let me know.

1) Experimental techniques to study reaction kinetics
- Principles of signal detection; separation methods vs. continuous monitoring
- Optical Spectroscopies: UV-Vis, Fluorescence, Circular Dichroism
- Rapid mixing techniques
- Pressure and temperature jump methods
- Flash photolysis, Pulse radiolysis, Discharge flow
- Monitoring of protein folding and unfolding
- NMR as a tool to study both slow and fast reactions

2) Analysis of experimental kinetic data
- Simple irreversible reactions
- Reversible reactions and relaxation kinetics
- Parallel reactions
- Consecutive reactions
- Autocatalysis

3) Theories of chemical reactions
- Potential energy surfaces
- Transition state theory: Fundamental assumptions
- Thermodynamic formulation: Rate constants and activation barriers
- Isotope effects and transition state theory

4) Analysis and modeling of chemical reactions with Mathematica®

Lecture and Lab Schedule:

Apr 2	Introduction to Chemical Kinetics.
Apr 4	Measurements of Reaction Rates
Apr 9	Rate laws: differential and integrated forms, determination of reaction order
Apr 11	First-order irreversible reactions: principles and data analysis
Apr 14	First homework due. Determination of reaction order and mechanism
Apr 15	First-order reversible reactions. Relaxation methods for fast reactions
Apr 18	Parallel reactions. Temperature- and pressure dependence of equilibrium and rate constants
Apr 23	Discussion of Jacob paper. Second- and higher order A + nA →P type reactions
Apr 25	Midterm I
Apr 26	Last day to drop classes
Apr 30	Second-order A + B →P type reactions; flow tube reactions and fluorescence detection methods
May 2	Introduction to *Mathematica* (Computer Lab, Chem 1153)
May 7	Reversible mixed and second order reaction s; pseudo-first-order approximation
May 9	Consecutive reactions. Study of fast reactions: stopped flow, continuous flow, quenched flow
May 12	Second homework due. Study of reversible reactions
May 14	Review of linear algebra. Discussion of Egawa paper.
May 16	Mathematical analysis of A →B→C kinetics (Computer Lab, Chem 1153)
May 21	Pharmacokinetics.
May 23	Collision theory. Transition state theory. Kinetic isotope effect
May 28	Midterm II
May 30	Computational modeling of transition states and reaction rates (Computer Lab, Chem 1153)
June 4	NMR for study of rapid reaction kinetics
June 6	NMR in kinetics: data collection (NMR room, PSB-N 3614) followed by analysis in Chem 1153)
June ?	**Final Examination**

Good luck! — Kalju