Chemistry 712: Chemical Kinetics — Course Syllabus

Fall 2016, Tues & Thurs 5:00 – 6:15, SSW-2512

Instructor Dr. David Pullman, CSL–301, 619–594–5573, dpullman@mail.sdsu.edu

Office Hours Tues, Wed, Thurs 1:00–2:00

Textbook *Chemical Kinetics and Dynamics*, 2nd Ed., J.I. Steinfeld, J.S. Francisco, and W.L Hase

Prerequisites Chemistry 410B or equivalent

Catalog Description Theory of rate processes; applications of kinetics to the study of reaction mechanisms.

Course Overview After an initial treatment of the basic phenomenological view of kinetics, we will cover classical analyses of reaction mechanisms (steady-state approximation, pre-equilibria, etc), transition-state theory, classical and quantum estimation of rate constants, and various modern experimental methods of determining reaction rates and mechanisms. Reactions taking place in the gas phase, liquid phase, and on surfaces (including nanoparticles) will be discussed, and as much as possible, examples will be taken from all areas of chemistry, including interdisciplinary areas such as atmospheric chemistry, combustion, and catalysis. The course will be largely based on the textbook by Steinfeld, Francisco, and Hase, but will also be augmented by additional material as needed. Chemical kinetics simulation software as well as general purpose software, such as Excel, Maple, and Igor will be used when appropriate to help solve problems. We will also use the electronic structure program, Gaussian, to calculate a reaction profile for a simple reaction.

Course Structure The lectures will roughly follow the text, with additional examples drawn from the chemical literature as well as from research in SDSU's Chem&Biochem Department. Some lectures will be devoted to tutorials in the use of computer software; these lectures will be held in the departmental computer lab, GMCS-245 (Note: you do *not* need to purchase any software since it will be available on the departmental computers). During the last few weeks of the semester, each student will give a ~20 minute presentation discussing a literature article they have selected.

Grading

Exam I	22% (tentatively the week of September 26)
Exam II	22% (tentatively the week of October 31)
Final Exam	31% (Thursday December 15, 2013, 3:30 – 5:30)
Final Project	25% (presented in weeks of Nov. 21, Nov. 28, Dec. 5, and Dec. 12)

- No makeup exams will be given.
- The grading scale is:

A	80-100%
B	65-80%
C	50%-65%

+/– grading will be used

- The final project consists of selecting (in consultation with the instructor) a kinetics paper from the research literature and preparing and presenting a ~20 minute talk to the class in which you discuss and critically evaluate the article. 80% of your grade for the project will be based on your presentation, while 20% will be based on your participation in asking questions during the other student presentations.

Topics

We will cover topics from all or parts of the following chapters in the text:

Chap 1 Basic Concepts of Kinetics
Chap 2 Complex Reactions
Chap 3 Kinetic Measurements
Chap 4 Reactions in Solutions
Chap 5 Catalysis (including enzyme catalysis)
Chap 6 The Transition from the Macroscopic to the Microscopic Level
Chap 7 Potential Energy Surfaces
Chap 10 Statistical Approach to Reaction Dynamics: Transition State Theory
Chap 11 Unimolecular Reaction Dynamics
Chap 12 Dynamics Beyond the Gas Phase
Chap 14 Kinetics of Multicomponent Systems: Combustion Chemistry
Chap 15 Kinetics of Multicomponent Systems: AtmosphericChemistry

Student Learning Outcomes

Upon completing Chem 712, students will be able to:

1. Understand and articulate the basic principles of Chemical Kinetics
2. Describe the fundamental chemical and physical properties that determine chemical reaction rates
3. Carry out calculations on reaction rates using the rate law
4. Estimate elementary reaction rate constants based on collision theory, statistical theories, and transition state theory
5. Perform kinetics calculations and simulations using Excel, Maple, Gaussian, and dedicated kinetics simulation software
6. Evaluate the literature regarding kinetic measurements of complex reaction systems

Problem Sets

There will usually be one problem set per chapter. Problem sets will ***not*** be graded; you do not need to hand them in. You can download them from the web (http://www-rohan.sdsu.edu/~dpullman/group/classes.htm). **As in any technical class, doing the problem sets is of the utmost importance to learning the material and doing well on exams**.

Add/Drop Procedure

The add/drop deadline is Sept. 12, 2016. For details, see http://arweb.sdsu.edu/es/registrar/schedule_adjustment.html

Students with Disabilities

If you are a student with a disability and believe you will need accommodations for this class, it is your responsibility to contact Student Disability Services at (619) 594-6473. To avoid any delay in the receipt of your accommodations, you should contact Student Disability Services as soon as possible. Please note that accommodations are not retroactive, and that accommodations based upon disability cannot be provided until you have presented your instructor with an accommodation letter from Student Disability Services. Your cooperation is appreciated.