CHEMICAL KINETICS and DYNAMICS - CHEM 633 – Spring 2012

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Class meets Tues 7:20-10pm – Robinson A105

TEXTS – There will not be a specific assigned text. Several texts and assigned readings will be in the JC library reserve, including- Chemical Kinetics by Keith Laidler - third edition - Harper and Row Publishers, Chemical Kinetics and Reaction Mechanisms by Espenson - McGraw Hill, Chemical Kineticcs & Dynamics – 2nd ed., Prentice Hall – J. I. Steinfeld, J. S Francisco and W. L. Hase, others as needed. Lecture slides will be relatively comprehensive. Use these slides and your lecture notes to identify what is important and to locate additional information in various texts. This is a graduate level course and the student is expected to hone their skills in identifying and researching important information from various sources.

The general course outline follows. There may be slight changes in order. Some subjects will be covered to a greater or lesser depth than others. Attend class. Most lecture slides will be on web page. Everything is not on slides so take lecture notes and valuable information and concepts are through class discussion. Class discussion is encouraged.

1. Introduction - basic concepts
   - What is Rate
   - Historical Perspectives
   - How is Rate Measured
   - Rate Equations - order, rate constants
   - Elementary Reactions vs. Net Reactions

2. Analysis of Kinetic Data
   - Differential Method
   - Integral Method
   - Graphical Techniques
   - Half-Life and Method of Half-Lives
   - Experimental Techniques for Fast Reactions
     - Flow Methods, Flash Photolysis, Shock-Tubes, etc.
   - Temperature Dependence and Arrhenius Equation

3. Activation Energy and Chemical Dynamics
   - Statistical Distribution of Energies – Statistical Mechanics
   - Partition Functions (we will probably spend a week or so here)
   - Potential Energy Surfaces
   - Quantum Mechanical Approaches

4. Reaction Rate Theory
   - Collision Theory
   - Statistical Approaches
   - Thermodynamic Approaches
   - Transition State Theory
   - Microscopic Reversibility

5. Gas Phase Reactions
   - Bimolecular
   - Trimolecular
   - Unimolecular
   - Disproportionation and Radical Recombination

6. Reactions in Solution
    - Solvent Effects
    - Collision in Solution
    - Transition State Theory
    - Solvation and Internal Pressure
    - Ionic Reactions
    - Substituent Effects
    - Diffusion and Diffusion Controlled Reactions

7. Reactions on Surfaces - Heterogeneous Reactions and Catalysis
    - Adsorption Isotherms - Langmuir
    - Mechanisms of Reactions on Solid Surfaces
    - Unimolecular
    - Bimolecular
    - Catalysis

8. Analysis of Complex Reactions
    - Multiple Differential Equations
    - Confirmation of a Proposed Mechanism
    - Steady State Approximation
    - Pseudo-First Order

9. Miscellaneous Topics of Interest
    - Photochemistry
    - Laser Spectroscopy
    - Others that come up during class discussion

10. Student Special Topic Paper

    Pick a topic in conjunction with the instructor on some aspect of Kinetics or Dynamics. Ideally, select a published paper(s) in a journal or a current review. Select something of personal interest, perhaps related to what you may do at your place of employment or related to your thesis research. Specific examples will be discussed as the semester progresses. Your written paper should be a comprehensive review of the subject with references, written in a professional "journal-like" format, with pictures, graphs, tables as needed to make it clear and user-friendly. Papers will be due at the last class (May 1). Quality PowerPoint slides should be attached to the paper. Due to class size, it is very likely that actual student presentations will not be give, only slides that would have been uses handed in with paper.

Course grading is based on a mid-term test (20% in class, 80% take home), paper, a few graded homework sets and a final exam (20% in class, 80% take home). Homework =10%, Mid-term =35%, Final =35%, Paper & Presentation = 20%. Final Exam covers the entire semester. George Mason University has a Honor Code. It is strongly recommended that you review now related parts of your General Chemistry Text and Physical Chemistry Text to get up-to-speed. In-class part of final exam is Tues May 15 7:20-10. Take-home part of final is also due at that time. Mid-term in-class and take-home due date is Tues April 3 (subject to change). Take-home tests are generally given out a week before they are due.

The goal of the course is to develop a broad understanding of those molecular and atomic forces and energy relationships that drive chemical reactions and determine their rate and equilibrium. Emphasis will be on Kinetics more than Thermodynamics. Numeric data analysis techniques will be used to develop and better understand the theories regarding these molecular forces. Math is a working tool in kinetics. The development of useful, user-friendly Excel spreadsheet "models" will be necessary. We will discuss laboratory techniques and their implication as applied to the study of the kinetics and dynamics. Although the course is taught in lecture format, discussion and questions are encouraged.