CHM 7430: Chemical Kinetics
MWF 12:50–1:45 / 215 State Hall

Instructor: G. Andrés Cisneros
Office: 333 Chemistry
email: andres@chem.wayne.edu

Office Hours: WF 1:45–3:00
or by appointment

Course Description and Goals

Chemical kinetics deals with the study of rates of chemical reactions and the elementary processes (macroscopic and microscopic) that influence and determine these rates. This course is designed to provide students with the knowledge, theoretical background and modeling tools to understand experimental and theoretical aspects of chemical reaction kinetics. Familiarity with undergraduate–level physical chemistry and calculus will be necessary. Students are encouraged to bring issues from their own research (or other interest) to my attention that they would like to discuss. The emphasis should be on the principles of kinetics common to all applications of chemistry.

More specifically, at the conclusion of the course you will be able to:

- Define and describe the fundamental properties that determine chemical reaction rates
- Determine rates and time dependence of the concentration of individual components for complex reactions using computational techniques based on analytic, numerical and approximate solutions such as steady state or pseudo–lower order approximations.
- Interpret and evaluate literature involving kinetic measurements of complex reaction systems.
- Employ transition state or collision theory to estimate reaction rates.
- Identify and explain experimental and theoretical methods employed for kinetic investigations.

However, these goals may be adapted to suit the objectives of the students.

Readings

Required text: *Chemical Kinetics and Dynamics*, 2nd Ed., J.I. Steinfeld, J.S. Francisco and W.L. Hase, Prentice–Hall Inc., New Jersey, 1999.

This text is on reserve at the science library along with:

Chemical Kinetics and Reaction Dynamics, P.L. Houston

Molecular Reaction Dynamics, R.D. Levine

Unimolecular Reactions, K.A. Holbrook, M.J. Pilling and S.H. Robertson

In addition there will be occasional handouts including journal articles. These texts or links to them will be available on the course's Blackboard page.

Course Policies and Evaluation

This course will be interactive in nature; based on this, **attendance** and **participation** will be necessary for you to completely achieve the course goals. Attendance and participation will not be graded directly; however, they are important to the purposes of this course and therefore your active presence in class is expected.

Evaluation of this course will be based on a variety of in–class and take–home assignments. There will be one mid–term and one final exam. Besides these exams there will be homework assignments, **posted on Blackboard**. Homework will be due on the date specified in the schedule (below). Another course requirement is a project to be completed individually or in pairs. This project will be due on the final week of class and will involve a class presentation.

Homeworks, exams and the final project with their respective weights towards the final grade are as follows:

Homework	20%
Project	20%
Mid-term exam	25%
Final exam	35%

Although some of your evaluation will depend on how well you perform in a test–taking situation, the project will focus on learning as a process of trial–and–error, re–reading and re–thinking. Therefore, parts of the project can be submitted for comments, discussed during office hours and revised prior to the due date. The project will be decided by you and can consist of a presentation of a topic from the current literature related to kinetics and/or dynamics, or a computer simulation of a chemical reaction and subsequent kinetic analysis.

If you must miss a class, inform me ahead of time. No late assignments will be accepted and no make–up exams will be given. Deadline extensions may be given for exceptional cases or for religious observance. Excused extensions should be arranged prior to the due date. Learning is a two–way street, therefore, I will ask you for feedback throughout the course. I will take your feedback seriously, and work hard to incorporate your ideas on how to improve the course.

Course Schedule

Week 1: What is Kinetics?

Friday, September 4: Introduction, definitions, reaction order and molecularity

Week 2: Elementary Chemical Kinetics

Monday, September 7: Holiday, no class

Wednesday, September 9: Integrated reaction rate law, Arrhenius equation; *reading: chapter 1*

Friday, September 11: Exact and approximate solutions; *reading: 2.1–2.3*

Week 3: Elementary Chemical Kinetics

Monday, September 14: Transform and matrix methods; *reading: 2.4, 2.5*

Wednesday, September 16: Numerical methods; *reading: 2.6*

Friday, September 18: Experimental techniques; *reading: 3.1, 3.2*

Week 4: Experimental Methods

Monday, September 21: Experimental techniques (contd.); *reading: 3.2*, **problem set 1 due**

Wednesday, September 23: Error and data analysis; *reading: 3.3*

Friday, September 25: Simple collision theory; *reading: chapter 6*

Week 5: Reaction Rate Theory

Monday, September 28: Introduction to theoretical chemistry

Wednesday, Intermolecular interaction potentials; *reading: 7.1–7.4*

Friday, September 30, Potential Energy Surfaces (PES); *reading: 7.5, 7.6*

Week 6: Reaction Rate Theory

Monday, October 5: October 2: PES (contd.); *reading: 7.7–7.10*, **problem set 2 due**

Wednesday, October 7: *Tentative: computer lab.*

Friday, October 9: Postulates and derivation of transition state theory (TST); *reading: 10.1–10.3, 10.5*

Week 7: Transition State Theory

Monday, October 12: TST applications and quantum effects; *reading: 10.4, 10.6*

Wednesday, October 14: Corrections to TST; *reading: 10.7–10.10*

Friday, October 16: Collision models; *reading: 8.1, 8.2*

Week 8: Reaction Dynamics

Monday, October 19: **Mid-term exam**, **problem set 3 due**

Wednesday, October 21: Scattering processes; *reading: 8.2, 8.3*

Friday, October 23: Molecular beams; *reading: 9.1, 9.2*

Week 9: Reaction Dynamics

Monday, October 26: Applications; *reading: 9.3–9.5*

Wednesday, October 28: Unimolecular reactions; *reading: 11.1–11.3*

Friday, October 30: RRKM theory; *reading: 11.4–11.6*

Week 10: Reaction Dynamics

Monday, November 2: Thermal activation & energy transfer; *reading: 11.7–11.9*, **problem set 4 due**

Wednesday, November 4: non–RRKM behavior; *reading: 11.10–11.12*

Friday, November 6: Classical description; *reading: 11.13, 11.14*

Week 11: Reactions in Condensed Phase

Monday, November 9: Solution reaction rates; *reading: 4.1--4.*3

Wednesday, November 11: Slow and fast reactions; *reading: 4.4--4.7*

Friday, November 13: Solution dynamics; *reading: chap. 12*

Week 12: Catalysis

Monday, November 16: Homogeneous catalysis; *reading: 5.1, 5.2*, **problem set 5 due**

Wednesday, November 18: Heterogeneous catalysis; *reading: 5.3, 5.5*

Friday, November 20: Enzymatic catalysis; *reading: 5.4*

Week 13: Combustion Chemistry

Monday, November 23: H–O reaction; *reading: 14.1, 14.2*

Wednesday, November 25: Methane combustion; *reading: 14.2*

Friday, November 27: Thanksgiving, No Class

Week 14: Atmospheric Chemistry

Monday, November 30: Atmosphere composition; *reading: 15.1–15.3,* **problem set 6 due**

Wednesday, December 2: Stratospheric Ozone; *reading: 15.4*

Friday, December 4: Modeling and measurements; *reading: 15.5–15.8*

Week 15: Project Presentations

Monday, December 7: TBD

Wednesday, December 9: TBD

Friday, December 12: TBD

Week 16: Project Presentations

Monday, December 14: TBD

FINAL: Monday, Dec. 21, 10:40 A.M. to 1:15 P.M.