**CHM 7430: Chemical Kinetics**
TTh 6:00–7:20 PM/327 State Hall

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Office Hours: Tue 1:00–2:30
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

Suggested 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

*Concepts of Modern Catalysis and Kinetics*, I. Chorkendorff and J.W. Niemanstvertdriet

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% (20 pts.) |
| **Project** | 20% (20 pts.) |
| **Mid-term exam** | 25% (25 pts.) |
| **Final exam** | 35% (35 pts.) |

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.

It is expected that you will abide by the academic integrity requirements as stated in the graduate program requirements document for the department of chemistry. Turn your cell phone, ipod, etc. off during class time. Use of these devices during class is disrespectful to your classmates and myself. Any person using these devices during class will have points deducted off her/his final grade. The dealine to withdraw from the course is the end of the 10th week of classes. Thus, the deadline for this semester will be Sunday, November 15th.

If you have a documented disability that requires accommodations, you will need to register with Student Disability Services (SDS) for coordination of your academic accommodations. The SDS office is located at 1600 David Adamany Undergraduate Library in the Student Academic Success Services department. SDS telephone number is 313-577-1851 or 313-577-3365 (TTY: telecommunication device for the deaf; phone for hearing impaired students only). Once you have your accommodations in place, I will be glad to meet with you privately during my office hours to discuss your special needs. Student Disability Services' mission is to assist the university in creating an accessible community where students with disabilities have an equal opportunity to fully participate in their educational experience at Wayne State University.

**Social Media Policies:** please see the document on Blackboard (under "content")

Course Schedule

*Week 1:* What is Kinetics*?*

Thursday, Sept. 3: Introduction, definitions, reaction order and molecularity

*Week 2:* Elementary Chemical Kinetics

Tuesday, September 8: Integrated reaction rate law, Arrhenius equation;
*reading: chapter 1*

Thursday, September 10: Exact and approximate solutions;
*reading: 2.1–2.3*

*Week 3:* Elementary Chemical Kinetics

Tuesday, September 15: Transform, matrix and numerical methods;
*reading: 2.4–2.6*

Thursday, September 17: Experimental techniques;
*reading: 3.1, 3.2* **problem set 1 due**

*Week 4:* Experimental Methods

Tuesday, September 22: Yom Kippur, No Class:

Thursday, September 24: Simple collision theory;
*reading: chapter 6*

*Week 5:* Reaction Rate Theory

Tuesday, September 29: Introduction to theoretical chemistry, intermolecular interaction potentials;
*reading: 7.1–7.4*

Thursday, October 1, Potential Energy Surfaces (PES);
*reading: 7.5, 7.10 (GAC: handout from Piella 6.4–6.12)* **problem set 2 due**

*Week 6:* Reaction Rate Theory

Tuesday, October 6: Postulates and derivation of transition state theory (TST);
*reading: 10.1–10.3, 10.5*

Thursday, October 8: Postulates and derivation of transition state theory (TST) (contd.);
*reading: 10.1–10.3, 10.5*

*Week 7:* Transition State Theory

Tuesday, October 13: TST applications, corrections and quantum effects;
*reading: 10.4–10.10 (GAC handout from KIE, Jenks, cap. 4)*

Thursday, October 15: **Mid-term exam**, **problem set 3 due**

*Week 8:* Reaction Dynamics

Tuesday, October 20: Collision models and scattering processes;
*reading: 8.1–8.3*

Thursday, October 22: Molecular beams;
*reading: 9.1, 9.2*

*Week 9:* Reaction Dynamics

Tuesday, October 27: Applications;
*reading: 9.3–9.5*, unimolecular reactions;

*reading: 11.1–11.3*

Thursday, October 29: RRKM theory;
*reading: 11.4–11.6*

*Week 10:* Reaction Dynamics

Tuesday, November 3: Thermal activation, energy transfer and non–RRKM behavior;
*reading: 11.7–11.12*, **problem set 4 due**

Thursday, November 5: Classical description;
*reading: 11.13, 11.14*

*Week 11:* Reactions in Condensed Phase

Tuesday, November 10: Solution reaction rates;
*reading: 4.1–4.7*

Thursday, November 12: Solution dynamics;
*reading: chap. 12*

*Week 12:* Catalysis

Tuesday, November 17: Homogeneous and Heterogeneous catalysis;
*reading: 5.1– 5.3*, **problem set 5 due**

Thursday, November 19: Enzymatic catalysis;
*reading: 5.4 (GAC:Warshel & Hammes-Schiffer papers on enzyme movement)*

*Week 13:* Combustion Chemistry

Tuesday, November 24: H–O reaction and methane combustion;
*reading: 14.1, 14.2*

Thursday, November 26: Thanksgiving, No Class

*Week 14:* Atmospheric Chemistry

Thursday, December 1: Atmosphere composition;
*reading: 15.1–15.3,* **problem set 6 due**

Tuesday, December 3: Stratospheric Ozone, Modeling and measurements;
*reading: 15.4–15.8*

*Week 15:* Project Presentations

Tuesday, December 8: TBD

Thursday, December 10: TBD

*Week 16:* Final Exam Week

FINAL: 12/17