San Diego State University

Chemistry and Biochemistry

Visitors | Undergraduates | Graduate Study | Faculty/Research

Chemistry 712: Chemical Kinetics

Last update: for Spring 2025

Instructor: Andrew Cooksy CSL-310

Chemical Kinetics
Syllabus

Lecture Meetings: TuTh 5:30-6:45pm, AH-3150
Office Hours: Mon/Wed 10:30-11:30am CSL-310. The Wed office hours are shared with another class.
Textbook: Steinfeld, Francisco, Hase *Chemical Kinetics and Dynamics*, 2nd ed., to be on sale in campus bookstore, and used copies ok.

Errors in Steinfeld, Francisco, and Hase, 2nd edition

Prerequisites

Students should have completed a year of undergraduate physical chemistry (SDSU's Chem 410A and 410B or equivalent). We will use some calculus at about that level. If we need other tools from math (linear algebra, transforms), they will be introduced as needed.

General Idea

This course is intended to benefit chemistry graduate students in all areas, as well as students in other departments with interests reaction chemistry. I plan to talk about chemical kinetics of enzymes, hydrocarbon combustion, interstellar gases, and organometallic catalysts. Many of these will be as specific examples of broadly applicable principles.

You're welcome to see me or email me if you want to ask about the course content or suitable preparation for the course. The emphasis should be on the principles of kinetics common to all applications of chemistry, so students are encouraged to bring issues from their own research (or other interests) to my attention for discussion (the sooner the better).

Student learning objectives:

At the conclusion of the course, the student should be able to:

- describe the fundamental properties that determine chemical reaction rates;
- carry out basic calculations on reaction rates using the rate law and numerical rate parameters;
- estimate elementary reaction rate constants based on transition state theory or collision theory models;
- evaluate the literature regarding kinetic measurements of complex reaction systems;
- calculate complex reaction rate constants and concentration dependencies using accurate computational techniques and the reasonable application of useful approximations such as the steady state, fast equilibrium, or pseudo-lower order approximations.
- use selected software packages (chem_rate_fit, RMG, ChemKin) to analyze experimental data, construct reaction mechanisms, and predict the time-dependent concentrations of a eraction mixture.
- identify and analyze chemical processes that may have a disproportionate impact on underserved populations.

These goals may be adapted to suit the needs and wishes of the students.

Course material

Chemical reaction dynamics and kinetics; primarily an examination of chemical kinetics from the microscopic perspective. I want to cover kinetics in a broad enough manner to make the course applicable to everyone involved in chemical reactions.

This year, I will partly model the course after a Chemical Engineering course in kinetics that I sat in on during my sabbatical last year at MIT. That course used this same textbook (which is the book we normally use at SDSU), but (being a chemical engineering course) there was more emphasis on practical questions than I have covered in the past, especially

1. what are the experimental challenges in getting good kinetics data?
2. what are the best options for estimating reaction rates when experimental data is not available?

Topics:

Theory
- Potential energy surfaces and reaction diagrams
- Molecular collisions and simple collision theory
- Transition state theory and the Really Scary Stuff
- Classical kinetics and obtaining the integrated rate laws

Experiment
- Reaction system design
- Probe methods: spectroscopy, mass spectrometry, classical analytical techniques
- What to do with the data

Applications
- protein folding
- interstellar chemistry
- organic synthesis
- surface chemistry
- Your Application Here

Organization

I want to deviate occasionally from the textbook, to cover the topics in an order that I find more natural. We will just lay the necessary groundwork for the microscopic picture by recapitulating the relevant results from quantum mechanics of individual molecules and a little statistical mechanics. We will not do any quantum in this course, however. The main point is that the macroscopic kinetics is more understandable when you appreciate what's happening at the molecular scale. So we start with a little about molecular collisions and potential surfaces for reactions (which are in the middle of the book), but then we pick up at chapter 1 and go through essentially the text's presentation of the material. I will probably add a few things and skip things as we go along. I hope to do lots of examples, but you'll need to keep me to my word on that.

Prerequisite Math

You should be very comfortable with algebra and the simplest derivatives and integrals (especially $e^{-x}dx$). We might cover some matrix algebra and Laplace transforms, but you need not have seen these before, and we will focus on how to use computational solutions rather than solving on paper.

Grading criteria

Grading Scheme

- in-class assignments: 15%
- writing assignment: 5%
- papers/project: 30%
- exam 1: 25%
- exam 2: 25%

There is no final exam.

grade	range
A	85-100%
B	70-85%
C	55-70%

Exam Dates for Spring 2025

- exam 1: Tue Mar 15
- exam 2: Thu May 8

There is no final exam.

Papers/projects

Students choose one of the following:

- present a 20-minute lecture to the class, illustrating a textbook topic or a study from a recently published research paper;
- investigate a two- or three-step reaction system using a quantum chemistry program, and present results to the class;
- carry out a computational analysis of a small-molecule reaction system using RMG and ChemKin;
- carry out an analysis of experimental data from a complex reaction mechanism using Igor, chem_rate_fit, or other software, including a thorough error analysis.

Writing assignment

Students will write a 1-2 page report on the impact of a chemical process which may have disproportionate impacts on underserved populations. Examples could include chemical synthesis in manufacturing, green chemistry applications, chemical approaches to study or treatment of diseases, enivronmental impacts of pollution or chemically-induced climate change.

Exams

Both exams are in-class. No communication with other naturally or artifically intelligent entities regarding any aspect of the exam is permitted during the exam period. For these purposes, the instructor is not to be considered an intelligent entity, so you may ask me to clarify a question (or point out a mistake) during the exam. (Also for these purposes, assistance via the Internet *is* considered communication with intelligent beings, in case you were wondering.) Exams that the instructor finds to be not entirely the student's own work, or which have been shared with others, will be courteously declined.

Errors in the text

In my experience, Steinfeld, Francisco, and Hase is widely considered to be the best text available on this topic. I hope you find it readable and informative. It does, however, have a few proofreading errors which you should correct in your copy:

- p. 7, Eq. 1-27. the denominator on the left side should be [A], not dt.
- p. 9, after Eq. 1-45. Solve the right side of 1-45 and equate it to the right side (not left) of Eq. 1-44.
- p. 23, Eq. 2-7. The first line should end $-[A_1]$, not $+[A_1]$. The next two lines are then correct.
- p. 29, Eq. 2-43. The second "=" sign should be removed, so that $[A_1]_0$ multiplies the whole expression.
- p. 32, Eq. 2-70. The second equation is the solution for $[A_2]$, not $[A_1]$.
- p. 33, Eq. 2-76. Remove the "-" from the right side.
- p. 40, after Eq. 2-133. The concentration of $[A_1]$, not $[A_2]$, remains nearly constant.
- p. 54, Eq. 2-209. The bottom term in the last vector should be $k_1-k_1e^{-(k_1+k_2)t}$, not $k_1+k_1e^{-(k_1+k_2)t}$.
- p. 118, Eq. 3-77. The denominator on the left should be K_2, not K_1.
- p. 151, bottom of page. The second "=" should be "-".
- p. 467, Table 14-1. Columns 3 and 4 are missing the powers of ten (available from the original paper, *Combust. Sci. Tech.* 15, 99 (1976)) and the products for reaction 12 should be $CO + H_2O$, not $CO + OH$.

Land Acknowledgment

For millennia, the Kumeyaay people have been a part of this land. This land has nourished, healed, protected, and embraced them for many generations in a relationship of balance and harmony. As members of the San Diego State University community, we acknowledge this legacy. We promote this balance and harmony. We find inspiration from this land, the land of the Kumeyaay.

Essential Student Information

For essential information about student academic success, please see the SDSU Student Academic Success Handbook.

SDSU provides disability-related accommodations via Student Disability Services (sds@sdsu.edu |https://sds.sdsu.edu/). Please allow 10-14 business days for this process.

Class rosters are provided to the instructor with the student's legal name. Please let me know if you would prefer an alternate name and/or gender pronoun.

Students should not use generative AI applications in this course except as approved by the instructor. Any use of generative AI outside of instructor-approved guidelines constitutes misuse. Misuse of generative AI is a violation of the course policy on academic honesty and will be reported to the Center for Student Rights and Responsibilities.