Basic Information

- Course title and number: Chemical Kinetics and Mechanisms, Chem 578, All Sections
- Credits: 2
- Time and location of class: MW 1:10-2:00 pm
- Location: HACH 1222
- Professor's data
  - name: Wenyu Huang
  - office number: 2124 Hach Hall
  - phone number: 515-294-7084
  - e-mail address: whuang@iastate.edu
  - office hours: 4-5 pm Mondays or by appointment via email

Prerequisites

- Required: CHEM 324 (Physical chemistry: Quantum mechanics & spectroscopy) or equivalent.

Learning Objectives

- Understand different theoretical models for describing how chemical reactions occur.
- Use rate law to define a rate constant to describe the dynamics of chemical reactions.
- Determine rate law using experimental techniques.
- Derive rate law for a complex reaction from a proposed mechanism.
- Derive reaction mechanism and elementary reactions in a complex reaction.

Course Format

- Lectures, MW 1:10 pm.
- Seminars on relevant topics.
- Attendance at lectures is recommended but not required.

The textbook and notes.

The primary resource will be notes/slides posted on Canvas.
As a supplement to the notes, there are several great textbooks, and they could help you to understand the material. However, it is not required, and you can certainly do well in the course without it. Some textbooks (below) are free for ISU students.
An Introduction to Chemical Kinetics, by *Michel Soustelle*, Wiley 2011.
https://onlinelibrary.wiley.com/doi/book/10.1002/9781118604243
An Introduction to Chemical Kinetics, by *Claire Vallance*, Morgan & Claypool Publishers 2017.
https://iopscience.iop.org/book/mono/978-1-6817-4664-7.pdf
Chemical Kinetics, 3rd Edition, by *Keith J. Laidler*, Pearson, 2007.
https://www.eng.uc.edu/~beaucag/Classes/AdvancedMaterialsThermodynamics/Books/Keith%20J%20Laidler%20-%20Chemical%20Kinetics-HarperCollins%20(1987).pdf

Additional Resources*:*

1. Davis and Davis, Fundamentals of Chemical Reaction Engineering New York: McGraw-Hill, 2003. (Available here: http://resolver.caltech.edu/CaltechBOOK:2003.001)

2. Chorkendorff and Niemantsverdriet, Concepts of Modern Catalysis and Kinetics, 2nd ed. Darmstadt: Wiley, 2007.
(Available here: https://onlinelibrary.wiley.com/doi/book/10.1002/3527602658

3. Levenspiel, Chemical Reaction Engineering 3rd ed. New York: Wiley, 1999.

4. Fogler, Elements of Chemical Reaction Engineering, 5th ed. New York: Prentice Hall (Pearson), 2016.

5. Rawlings and Ekerdt, Chemical Reactor Analysis and Design Fundamentals 2nd ed. Madison WI: Nob Hill

Publishing, 2012.

6. Froment, Bischoff, and de Wilde Chemical Reactor Analysis and Design 3rd ed. New York: Wiley, 2011.

7. Constantinides and Mostaufi, Numerical Methods for Chemical Engineers with MATLAB Applications, New Jersey: Prentice Hall, 1999.

8. Douglas, McDaniel, and Alexander, Concepts and Models of Inorganic Chemistry, 3rd ed. New York: Wiley, 1994.

9. Cussler, Diffusion, Mass Transfer in Fluid Systems, 2nd ed. New York: Cambridge University Press, 1997.

10. Bartholomew and Farrauto, Fundamentals of Industrial Catalytic Processes, 2nd ed. New Jersey: Wiley, 2006.

11. Somorjai and Li, Introduction to Surface Chemistry and Catalysis, 2nd ed. New Jersey: Wiley, 2010.

12. Vannice, Kinetics of Catalytic Reactions, New Jersey: Springer, 2005.

Preliminary (and Tentative) List of Topics to be Covered:

The Kinetic Theory of Gases

The Average Translational Kinetic Energy of the Molecules in a Gas
The Distribution of the Components of Molecular Speeds
Maxwell-Boltzmann Distribution
The Frequency of Collisions and The Mean Free Path
Rate of a Gas-Phase Chemical Reaction

Chemical Kinetics: Rate Laws

The Time Dependence of a Chemical Reaction
Rate Laws Must Be Determined Experimentally
First-Order Reactions
Time-Dependent Reactant Concentration
Reversible Reactions
Rate Constants Determined by Relaxation Techniques
Rate Constants Are Temperature Dependent
Transition-State Theory

Chemical Kinetics: Reaction Mechanisms

Elementary Reactions
Principle of Detailed Balance States
Consecutive and Single-Step Reactions
The Steady-State Approximation
The Rate Law and Reaction Mechanism
Lindemann Mechanism
Reaction Mechanisms Involve Chain Reactions
Catalyst Affects the Mechanism and Activation Energy
Michaelis-Menten Mechanism for Enzyme Catalysis

Gas-Phase Reaction Dynamics

Hard-Sphere Collision Theory and
Energy-Dependent Reaction Cross Section
Rate Constant and the Orientations of the Colliding Molecules
Internal Energy of the Reactants
Reactive Collision and Crossed Molecular Beam Machines
Vibrationally Excited Molecules by Reaction
Molecular Picture of the Chemical Reaction

Surface Chemistry and Catalysis

Crystal Structure Factor and the Electron Density
Physisorb or Chemisorb to a Solid Surface
Sorption Isotherms
Langmuir Isotherm and Rate Laws for Surface-Catalyzed Gas-Phase Reactions
Catalytic Ammonia Synthesis

Possible Special Topics

Isotope Effect
Surface Reaction Mechanisms
Modern Computational Kinetics
Microkinetics Modeling

Grades, homework, and exams:

- There will be 4 exams, each of which counts for 22.5% of the total grade. One of these 4 is the final exam. The final is cumulative.
- Homework counts for 10% of the final grade. Homework will not be graded on the validity of the answers, only on the evidence that reasonable effort was expended to solve the problems. Each homework set is worth 10 points. Each homework due date will be announced about 1 week in advance. Students are encouraged to work on the homework in groups, but each student must hand in his/her own copy. Homework is always due at the beginning of class on the due date via electronic submission on Canvas.
- The grade cutoffs are semi-fixed. Based on total points, letter grades will be:
  A to A-: Grades above (85 %)
  B+ to B-: Grades above (70 %)
  C+ to C-: Grades above (55 %)
- Equations to be memorized will be marked by asterisks (***) in the lecture notes. There are only a few.
- Exams will have cover sheets with equations and constants that may be useful. These will be published in advance of each exam date.

COURSE POLICIES

Academic Dishonesty. The class will follow Iowa State University's policy on academic dishonesty. Anyone suspected of academic dishonesty will be reported to the Dean of Students Office (https://www.studentconduct.dso.iastate.edu/academic-misconduct).

Accessibility Statement. Iowa State University is committed to assuring that all educational activities are free from discrimination and harassment based on disability status. Students requesting accommodations for a documented disability are required to work directly with staff in Student Accessibility Services (SAS) to establish eligibility and learn about related processes before accommodations will be identified. After eligibility is established, SAS staff will create and issue a Notification Letter for each course listing approved reasonable accommodations. This document will be made available to the student and instructor either electronically or in hard-copy every semester. Students and instructors are encouraged to review contents of the Notification Letters as early in the semester as possible to identify a specific, timely plan to deliver/receive the indicated accommodations. Reasonable accommodations are not retroactive in nature and are not intended to be an unfair advantage. Additional information or assistance is available online at www.sas.dso.iastate.edu, by contacting SAS staff by email at accessibility@iastate.edu, or by calling 515-294-7220. Student Accessibility Services is a unit in the Dean of Students Office located at 1076 Student Services Building.

Disclaimer about Freedom of Speech and Academic Freedom
Iowa State University supports and upholds the First Amendment protection of freedom of speech and the principle of academic freedom in order to foster a learning environment where open inquiry and the vigorous debate of a diversity of ideas are encouraged. Students will not be penalized for the content or viewpoints of their speech as long as student expression in a class context is germane to the subject matter of the class and conveyed in an appropriate manner.

Discrimination and Harassment. Iowa State University does not discriminate on the basis of race, color, age, ethnicity, religion, national origin, pregnancy, sexual orientation, gender identity, genetic information, sex,

marital status, disability, or status as a U.S. Veteran. Inquiries regarding non-discrimination policies may be directed to Office of Equal Opportunity, 3410 Beardshear Hall, 515 Morrill Road, Ames, Iowa 50011, Tel. 515-294-7612, Hotline 515-294-1222, email eooffice@iastate.edu

Religious Accommodation. Iowa State University welcomes diversity of religious beliefs and practices, recognizing the contributions differing experiences and viewpoints can bring to the community. There may be times when an academic requirement conflicts with religious observances and practices. If that happens, students may request the reasonable accommodation for religious practices. In all cases, you must put your request in writing. The instructor will review the situation in an effort to provide a reasonable accommodation when possible to do so without fundamentally altering a course. For students, you should first discuss the conflict and your requested accommodation with your professor at the earliest possible time. You or your instructor may also seek assistance from the Dean of Students Office (https://www.studentassistance.dso.iastate.edu/) at 515-294-1020 or the Office of Equal Opportunity, (https://www.eoc.iastate.edu/) at 515-294-7612.

Contact Information for Academic Issues. If you are experiencing, or have experienced, a problem with any of the above issues, email academicissues@iastate.edu

ADDRESS STUDENTS WITH SPECIAL NEEDS
Iowa State University is committed to assuring that all educational activities are free from discrimination and harassment based on disability status. All students requesting accommodations are required to meet with staff in Student Disability Resources (SDR) to establish eligibility. A Student Academic Accommodation Request (SAAR) form will be provided to eligible students. The provision of reasonable accommodations in this course will be arranged after timely delivery of the SAAR form to the instructor. Students are encouraged to deliver completed SAAR forms as early in the semester as possible. SDR, a unit in the Dean of Students Office, is located in room 1076, Student Services Building or online at www.dso.iastate.edu/dr/. Contact SDR by e-mail at disabilityresources@iastate.edu or by phone at 515-294-7220 for additional information.

RELATED TO ISU'S PRINCIPLES OF COMMUNITY: Students are responsible for living the tenets established in ISU's Principles of Community: Respect, Purpose, Cooperation, Richness of Diversity, Freedom from discrimination, and the Honest and respectful expression of ideas. Visit ISU's Principles of Community website (http://www.diversity.iastate.edu/principles-of-community)

REGARDING A STUDENT'S NAME, GENDER IDENTITY AND/OR GENDER EXPRESSION: Class rosters are provided to the instructor with the student's legal name. I will gladly honor your request to address you by an alternate name or gender pronoun. Please advise me accordingly early in the semester so that I may make appropriate changes to my records.

SUPPORTING STUDENT HEALTH AND WELLNESS: Iowa State University is committed to proactively facilitating all students' well-being. We welcome and encourage students to contact the following on-campus services for their physical, intellectual, occupational, spiritual, environmental, financial, social, and/or emotional needs:

- Student Wellness call 515-294-1099 or via website (http://studentwellness.iastate.edu);
- Thielen Student Health Center call 515-294-5801 (24/7 Medical Advice) or via website (http://www.cyclonehealth.org);
- Student Counseling Services call 515-294-5056 or via website (https://counseling.iastate.edu);
- Recreation Services call 515-294-4980 or via website (http://recservices.iastate.edu).
- Students dealing with heightened feelings of sadness or hopelessness, thoughts of harm or suicide, or increased anxiety may contact the ISU Crisis Text Line (Text ISU to 741-741) or contact ISU Police Department 515-294-4428.

FOSTERING A SAFE COMMUNITY:

Green Dot Project: A green dot is any choice, behavior, word or attitude that promotes safety for everyone and communicates utter intolerance for power-based personal violence in our Iowa State University community. A green dot is anything you do to make our community safer. What is your Green Dot? Visit the Green Dot – Student Wellness website (http://www.studentwellness.iastate.edu/greendot/).

Title IX Reporting Responsibilities: Download Equal Opportunity's Sample Syllabi Language for Title IX Regarding Reporting Responsibilities (PDF), (https://www.eoc.iastate.edu/sites/default/files/uploads/Sample%20TIX%20Syllabi%20Language.pdf)

ABOUT MUTUAL RESPECT AND PROFESSIONALISM: You are expected to treat your instructor and all other participants in the course with courtesy and respect. Your comments to others should be factual, constructive, and free from harassing statements. You are encouraged to disagree with other students, but such disagreements need to be based upon facts and documentation (rather than prejudices and personalities). It is the instructor's goal to promote an atmosphere of mutual respect in the classroom. Please contact the instructor if you have suggestions for improving the classroom environment. It is preferable if students discuss issues directly with the instructor, however, students may also leave a note in the instructor's mailbox.

RELEVANT TO THE ISU INCLUSIVE LANGUAGE POLICY: All university publications and communication, whether oral or written, shall use inclusive language and illustrations. Inclusive language refers to language that makes every attempt to include comprehensively all groups in the community. Whenever possible, selection of academic materials will also reflect efforts to uphold this university policy." Visit the Policy Library's Inclusive Language website.

RELATED TO USABILITY, DISABILITY AND DESIGN: I am committed to creating a course that is inclusive in its design. If you encounter barriers, please let me know immediately so that we can determine if there is a design adjustment that can be made or if an accommodation might be needed to overcome the limitations of the design. I am always happy to consider creative solutions as long as they do not compromise the intent of the assessment or learning activity. You are also welcome to contact the Student Accessibility Services (515-294-7220) to begin this conversation or to establish accommodations for this or other courses. I welcome feedback that will assist me in improving the usability and experience for all students.