ASEN 5251 – Molecular Thermo & Kinetics – Fall 2025
TuTh 4:00-5:15 pm – Aero N240
& Recorded Lectures

Instructor: Prof. Timothy K. Minton
Office: AERO 371
Phone: (303) 492-5826
E-mail: tminton@colorado.edu
Office Hours: Aero 371 or by appointment; time TBD

TA: Henri Doucet, Henri.Doucet@colorado.edu
TA Office Hrs. Mondays, 1:00 pm – 2:00 pm, Aero N353
Thursdays, 2:00 pm – 3:00 pm, Aero N353
https://cuboulder.zoom.us/j/6225952484
or by appointment

Web Page: This course uses CANVAS.

Overview: The objective of this course is to provide an entry point into the microscopic manifestations of chemistry and chemical change for engineering graduate students with limited knowledge of molecular-level processes. This course is an introduction to chemical kinetics and theories of chemical reactions. The focus is on gas-phase and gas-surface interactions, so kinetic theory of gases will be covered at a basic level. There is an introduction to quantum mechanics and statistical mechanics, and the course draws on these descriptions of matter to help understand the magnitudes of chemical reaction rates and how they vary with macroscopic parameters, such as temperature, and with microscopic parameters, such as molecular size, structure, and energy spacing of quantum states.

Adopted Textbooks: *Molecular Physical Chemistry for Engineers*, John T. Yates, Jr. and J. Karl Johnson, University Science Books, Sausalito, CA, 2007. [*Note: Print books can be ordered from the publisher and a variety of on-line sites. Students can also direct-order eBooks (to own or to lease) by browsing to RedShelf.com. This book is also available on Perusall.com.*]

Chemical Kinetics and Reaction Dynamics, Paul L. Houston, McGraw Hill, 2001. [Re-published by Dover in 2006]

Recommended Textbooks: *Chemical Kinetics and Dynamics: Second Edition*, Jeffrey I. Steinfeld, Joseph S. Francisco, and William L. Hase, Prentice Hall, Upper Saddle River, NJ, 1999.
Known errors in this book:
- 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 $k_1-k_1e^{-(k1+k2)t}$, not $k_1+k_1e^{-(k1+k2)t}$.
- 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.

Physical Chemistry: A Molecular Approach, Donald A. McQuarrie and John D. Simon, University Science Books, Sausalito, CA, 1999.

Additional Texts: Numerous texts on physical chemistry, quantum mechanics, statistical mechanics, chemical kinetics.

Approximate Course Outline:

I. Overview of Quantum Mechanics
- The dawn of quantum theory
- Schrödinger equation
- Solutions to Schrodinger equation in the context of the “particle in a box”
- Postulates and general principles of quantum mechanics
- Harmonic oscillator and rigid rotor
- Hydrogen atom
- Electronic structure of atoms and molecules
- Electronic spectroscopy of diatomic molecules

II. Overview of Statistical Mechanics
- The Boltzmann factor and canonical partition functions
- Molecular partition functions for ideal gases

III. Chemical Kinetics
- Basic concepts of kinetics
- Kinetics of complex reactions
- Temperature dependence of the rate coefficient
- Catalysis
- Kinetics at the gas-surface interface

IV. Microscopic Theories of Chemical Reactions
- Collision theory
- Intermolecular potentials and potential energy surfaces
- Dynamics of bimolecular reactions
- Dynamics of gas-surface interactions
- Transition state theory
- Unimolecular reaction dynamics
- Photochemistry?

Grading:
24% 7 Problem Sets
38% Exam 1 (take home)
38% Exam 2 (take home)
Grades will be assigned to indicate a student's level of competency in the course material. Accordingly, adjustments may be made in the assignment of final grades to reflect students' performance with respect to the class average and Prof. Minton's experience with student achievement in related courses. It is anticipated, though not guaranteed, that the average grade (regardless of the absolute score) will be on the A-/B+ borderline.

Office Hours:
- Office hours shall be used as a time for students to ask the TA or each other questions about problem sets, exams, concepts presented in the lecture, etc. **Students are expected to come to office hours with targeted questions.**
- The office-hour periods shall not be used as a time/place for students simply to study or work on their homework when they are not actively using the time to ask questions, participate in discussions, or listen to explanations provided by the TAs or student peers.

Problem Sets:
- The purpose of the problem sets is to aid the student in learning by working on problems related to the course material.
- Students must submit electronic versions of their worked problem sets through Canvas by **5:00 pm on their due dates. Late problem sets will not be accepted – no exceptions.** It is expected that students will upload their problem sets with sufficient time to overcome any problems with the upload, including potential problems with Internet access. Furthermore, it is expected that students will verify that their problem sets have been successfully uploaded. Insufficiently legible work, including corrupted files, will not be graded. Partially completed problem sets will be graded; therefore, if a student is not able to fully complete the problem set by the deadline, then submitting a partially completed problem set is better than submitting no problem set at all. Questions about the problem sets may be directed to the TA or Prof. Minton, although the TA should generally be consulted first.
- Problem set solutions will be posted on Canvas. For questions regarding the grading of a problem set, students should first discuss the issue with the TA, who will then decide whether the issue needs to be escalated to Prof. Minton.
- Collaboration is permitted on problem sets, but efforts are individual. **Every student is expected to turn in his/her/their own individual problem set for grading.** This means

that students may discuss the means and methods for solving problems and even compare answers, but they are **not permitted to copy someone's work, find solutions on the Internet, or copy from in a solutions manual.** Copying material from any resource and submitting it as one's own work may be considered plagiarism and an Honor Code violation.

- Use of MATLAB or other computer codes is permitted, but not always desirable. With the exception of making graphs, it is anticipated that a software tool will ***not*** be required to solve problems. Thus, it is not sufficient to set up a problem and then use a software tool to solve the remainder of the problem, unless the only thing that remains is to make a graph. Work shall be written in legible format, and sufficient work must be shown to indicate to a grader that the student understands how the problem is solved. If the student prefers to submit typed solutions, that is acceptable, but all steps in the process of arriving at the solution, without the use of software tools, must be shown. All graphs must be legible and have meaningful axes and legends. If any fitting parameters from a graph are needed for the solution of a problem, then these may come from the graphing tool used.
- **The use of generative artificial intelligence software** (e.g., ChatGPT) to assist in solving problems for problem sets **is not permitted**, and its use will be considered a violation of the Honor Code.
- Students should bear in mind that thinking independently about problems will enhance both learning and success on exams.

Exams:

The two exams will be take-home, with 4 days allotted for the completion of each exam, possibly including weekdays. Each exam will focus on new material presented since the start of the course or since the previous exam. Principles, concepts, results, terminology learned at any time since the start of the course may be expected knowledge when solving problems pertaining to the new material. Exams will be distributed on Canvas at an announced time, and a due date and time will be given when the exam is distributed. Completed exams shall be turned in on Canvas before the deadline, in a similar manner as the problem sets. Similar to the problem sets, software tools may not be used to work any solutions to exam questions, except when necessary to make graphs or obtain fitting parameters from graphs. No communication with other intelligent beings **regarding any aspect of the exam** is permitted during the exam period (i.e., from receipt of the exam until it is due). Intelligent beings are defined as the Internet, AI, and any other on-line resources, fellow students, professors, and any other people, with the exception of Prof. Minton. You may ask Prof. Minton questions about the exam if you wish, and he will respond only insofar as necessary to help make the problem clearer. It is acceptable to use physical books and notes. The assistance of a computer or tablet, for example, to write solutions, to read ***stored*** journal articles or notes, to function as a scientific calculator, or to make graphs as appropriate, is permissible.

Student learning objectives:

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

- understand, at least in part, the motivation behind the development of quantum mechanics;
- have an understanding of the postulates of quantum mechanics and be proficient with the conceptual tools required to use those postulates;
- to describe four model systems of quantum chemistry, explain the solutions of their

Schrödinger equations, and use the results to explain chemical phenomena;
- have a basic understanding of the electronic structure of atoms and molecules;
- have a basic understanding of transitions between quantum states and the relationship between these transitions and spectroscopic signatures;
- achieve a basic understanding of ensembles, the Boltzmann factor, and partition functions;
- appreciate the relationship between thermodynamic functions and the molecular properties of a system;
- have a basic knowledge of molecular partition functions and how to calculate them;
- 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 analytical methods as well as the reasonable application of useful approximations such as the steady state, fast equilibrium, or pseudo-lower order approximations;
- understand the basics of potential energy surfaces and their use in describing atomic and molecular collisions;
- comprehend scientific talks or seminars that describe modern research in gas-phase (including unimolecular and bimolecular) and gas-surface reaction kinetics and dynamics;
- achieve foundational knowledge in quantum mechanics, statistical mechanics, chemical kinetics, and reaction dynamics in preparation for more advanced courses and/or further independent learning/research in one or more of these areas.

Evaluated Outcomes:

The Department of Aerospace Engineering Sciences has adopted a policy of assigning grades according to "evaluated outcomes" in each course:

O1 Professional context and expectations (ethics, economics, business environment, etc.)
O2 Current and historical perspective
O3 Multidisciplinary, systems perspective
O4 Written, oral, graphical communication ability
O5 Knowledge of key scientific/engineering concepts
O6 Ability to define and conduct experiments, use instrumentation
O7 Ability to learn independently, find information
O8 Ability to work in teams
O9 Ability to design
O10 Ability to formulate and solve problems
O11 Ability to use and program computers

Evaluation of these outcomes allows an assessment of the student's performance and provides a major portion of the process that the faculty use for continuous assessment and improvement of

the entire AES curriculum. The model for these outcomes derives from several sources including the "Desired Attributes of an Engineer" as defined by The Boeing Company, and "curriculum reviews" from major aerospace corporations including The Boeing Co., Lockheed Martin Corp., and Ball Aerospace Corp. These inputs were combined with the AES faculty vision of the desired attributes of an aerospace engineer and the requirements of the Accreditation Board for Engineering and Technology (ABET) to produce this list of evaluated outcomes. Each assignment is designed and graded to assess some combination of several or a few of the outcomes.

Behavioral Expectations:

- Both students and faculty are responsible for maintaining an appropriate learning environment in all instructional settings, whether in-person, remote, or online. This includes respectful and courteous behavior, as well as ensuring a quiet work atmosphere without noise distractions (e.g., talking and audible sounds from electronic devices). Professional courtesy and sensitivity are especially important with respect to individuals and topics dealing with race, color, national origin, sex, pregnancy, age, disability, creed, religion, sexual orientation, gender identity, gender expression, veteran status, political affiliation, or political philosophy. Those who fail to adhere to behavioral standards may be subject to discipline. For more information, see the classroom behavior policy, the Student Code of Conduct, and the Office of Institutional Equity and Compliance.
- Students are requested to use both title and name (i.e., **"Professor Minton", "Prof. Minton", or "Dr. Minton"**) when addressing Prof. Minton in electronic correspondence or during in-person conversations. **The use of "Professor" without a following name, "Hello" without a following title and name, the word, "Hey," and no name or salutation at all, are considered by Prof. Minton to be impolite and disrespectful.**

Accommodation for Disabilities:

If a student qualifies for accommodations because of a disability, the student must submit his/her accommodation letter from Disability Services to the instructor in a timely manner (**minimum of two weeks before any accommodation must be met**) so that the student's needs can be addressed. Furthermore, **that student shall contact Prof. Minton and receive verification that the request has been received and shall work with Prof. Minton in good faith in any scheduling required to meet the accommodation**. Disability Services determines accommodations based on documented disabilities in the academic environment. Information on requesting accommodations is located on the Disability Services website. For assistance, Disability Services may be contacted at 303-492-8671 or dsinfo@colorado.edu. A student with a temporary medical condition should see Temporary Medical Conditions on the Disability Services website. If a student has a temporary illness, injury, or required medical isolation, then the student shall contact Prof. Minton and discuss whether a special accommodation is needed.

Preferred Student Names and Pronouns:

CU Boulder recognizes that students' legal information doesn't always align with how they identify. Students may update their preferred names and pronouns via the student portal; those preferred names and pronouns are listed on instructors' class rosters. Students may also choose to notify Prof. Minton directly of their preferred pronouns. In the absence of such updates, the name that appears on the class roster is the student's legal name.

Honor Code:
All students enrolled in a University of Colorado Boulder course are responsible for knowing and adhering to the Honor Code. Violations of the policy may include, but are not limited to: plagiarism (including use of paper writing services or technology [such as essay bots]), cheating, fabrication, lying, bribery, threat, unauthorized access to academic materials, clicker fraud, submitting the same or similar work in more than one course without permission from all course instructors involved, and aiding academic dishonesty. All incidents of academic misconduct will be reported to Student Conduct & Conflict Resolution (StudentConduct@colorado.edu). Students who are found responsible for violating the Honor Code will be assigned resolution outcomes from the Student Conduct & Conflict Resolution as well as be subject to academic sanctions from the faculty member. Additional information regarding the Honor Code academic integrity policy can be found on the Honor Code website.

Sexual Misconduct, Discrimination, Harassment and/or Related Retaliation:

- CU Boulder is committed to fostering a positive and welcoming learning, working, and living environment. University policy prohibits protected-class discrimination and harassment, sexual misconduct (harassment, exploitation, and assault), intimate partner violence (dating or domestic violence), stalking, and related retaliation by or against members of our community on- and off-campus. These behaviors harm individuals and our community. The Office of Institutional Equity and Compliance (OIEC) addresses these concerns, and individuals who believe they have been subjected to misconduct can contact OIEC at 303-492-2127 or email cureport@colorado.edu. Information about university policies, reporting options, and support resources can be found on the OIEC website.
- Faculty and graduate instructors must inform OIEC when made aware of any issues related to these policies regardless of when or where they occurred to ensure that individuals impacted receive outreach from OIEC about resolution options and support resources. To learn more about reporting and support options for a variety of concerns, students should visit Don't Ignore It.

Religious Holidays:
Campus policy regarding religious observances requires that faculty make every effort to deal reasonably and fairly with all students who, because of religious obligations, have conflicts with scheduled exams, assignments, or required attendance. Prof. Minton will make every effort to accommodate a student's religious obligations provided that the student gives notification well in advance of the scheduled conflict **(minimum of two week's advance notice)**. See the campus policy regarding religious observances for full details.

Mental Health and Wellness:
The University of Colorado Boulder is committed to the well-being of all students. If a student who is struggling with personal stressors, mental health or substance use concerns that are impacting academic or daily life should contact Counseling and Psychiatric Services (CAPS) located in C4C or call (303) 492-2277, 24/7. Free and unlimited telehealth is also available through Academic Live Care. The Academic Live Care site also provides information about additional wellness services on campus that are available to students.

ASEN 5251 – FALL 2025 SCHEDULE (to be updated as appropriate)

TUESDAY	THURSDAY
	Aug. 21
Aug. 26	Aug. 28
Sept. 2 **Prob. Set 1 due, 11:59 pm**	Sept. 4
Sept. 9	Sept. 11
Sept. 16	Sept. 18 **Prob. Set 2 due, Fri., Sept. 19, 11:59 pm**
Sept. 23	Sept. 25
Sept. 30	Oct. 2 **Prob. Set 3 due, Fri., Oct. 3, 11:59 pm**
Exam 1: Oct. 4, 8:00 am Oct. 7, 11:59 pm	
Oct. 7	Oct. 9
Oct. 14	Oct. 16 **Prob. Set 4 due, Fri., Oct. 17, 11:59 pm**
Oct. 21	Oct. 23
Oct. 28	Oct. 30 **Prob. Set 5 due, Fri., Oct. 31, 11:59 pm**
Nov. 4	Nov. 6
Nov. 11	Nov. 13 **Prob. Set 6 due, Fri., Nov. 14, 11:59 pm**
Nov. 18	Nov. 20
Nov. 25 FALL BREAK no class	Nov. 27 FALL BREAK no class
Dec. 2	Dec. 4 **Prob. Set 7 due, Fri., Dec. 5, 11:59 pm**
Exam 2: Dec. 6, 8:00 am Dec. 9, 11:59	