CHE 713: Thermodynamics I

Instructor: **Dr. Artem M. Rumyantsev** (EB1 2042), rumyantsev@ncsu.edu

In-person office hours: Tue, 4:30 – 6:00 pm, EB1 2042

Online office hours (EOL): Tue, 6:00 – 7:30 pm *by request*

or another time *by appointment only*

Classes (lectures): Tuesday & Thursday, 1:30 - 2:45 pm, EB3 2124 and online (EOL)

Teaching Assistants: **Mr. Michael Bergman**, mbergma2@ncsu.edu

In-person office hours: Tuesday, 3:00 – 4:30 pm (EB1 Atrium)

Online office hours (EOL): Wed., 6:30 – 8:00 pm *by request*

Mr. Karthik Sinha, kcsinha@ncsu.edu

In-person office hours: Thursday, 3:00 – 4:30 pm (EB1 Atrium)

Online office hours (EOL): Monday, 5:30 – 7:00 pm *by request*

Mr. Jiayi Huang, jhuang54@ncsu.edu

In-person office hours: Wed., 3:00 – 4:30 pm (EB1 Atrium)

Online office hours (EOL): Tuesday, 7:30 – 9:00 pm *by request*

Problem Sections: *Some* Thursdays (schedule below): 5:00 – 7:00 pm, EB3 2232

Recommended Texts: There is no required textbook for the course. The three two books from the list below cover almost all the content of the course. The next four books provide more in-depth coverage of some of the topics:

1. K. A. Dill and S. Bromberg. Molecular Driving Forces: Statistical Thermodynamics in Biology, Chemistry, Physics, and Nanoscience.
2. S. Shell. Thermodynamics and Statistical Mechanics: An Integrated Approach.
3. Y. A. Kaznessis. Statistical Thermodynamics and Stochastic Kinetics: An Introduction for Engineers.
4. D. Chandler. Introduction to Modern Statistical Mechanics.
5. J.J. de Pablo and J. D. Schieber. Molecular Engineering Thermodynamics.
6. L. D. Landau and E. M. Lifshitz. Statistical Physics. (Vol. 5 of the Course of Theoretical Physics).
7. J. Israelashvili. Intermolecular and Surface Forces.
8. D. Larsen at al. Physical Chemistry (LibreTexts). [link]

Course Objectives:

The course objective is to present the basic statistical mechanics concepts underlying classical chemical engineering thermodynamics and to cover the latter in more depth than that found in a typical undergraduate course. By the end of the course the attendees should be able to:

- Understand microscopic fundamentals of thermodynamics and connection to the statistical mechanics: statistical interpretation of entropy and the second law of thermodynamics; the statistical distribution laws and partition function for canonical, microcanonical, and grand canonical ensembles.
- Use the full set of thermodynamic functions for non-ideal gases, liquid, and solids systems to carry out thermodynamic calculations, including those for phase coexistence and chemical reactions.
- Understand the microscopic origin of intermolecular interactions and implications/connections to the macroscopic thermodynamic behaviors.
- Carry out thermodynamic calculations for non-ideal gases and liquids, including heat capacities of real gases and phase equilibria in liquid mixtures, using statistical thermodynamics.
- Understand the basis of molecular simulation, including Molecular Dynamics and Monte Carlo methods.

Grading:

- In-term exams: 50%
- Final Exam: 30%
- Homework: 20%

The final letter grade is assigned according to **the score itself or the quantile** in the class. The class size after the official drop/revision deadline is used for calculating the quantile. The threshold values are listed below.

Grade	A+	A	A-	B+	B	B-	C+	C	C-	D+	D	D-	F
Score	>97	93-96	90-92	87-89	83-86	80-82	77-79	73-76	70-72	67-69	63-66	60-62	<60
Quantile, %	90	75	60	55	45	35	30	25	20	10	10	10	

Example 1: If Score = 91 and Quantile = 88% then Grade = max (A-; A) = A. (Quan. criterion applies.)

Example 2: If Score = 83 and Quantile = 20% then Grade = max (B; C-) = B. (Score criterion applies.)

Classes Schedule and Preliminary Content

T=Thermodynamics   SF = Fundamentals of Stat. Mech.   SA = Applications of Stat. Mech.

	Tuesday	Thursday	Pr. S.	HW Set #
Week 1 Aug 19 – 23; (2 classes)	T0. Course Policy. TD & Stat. Phys.	T1. Laws of TD.		HW Set 0 (Bio + Form)
Week 2 Aug 26 – Aug 30; (2 classes)	T2. Entropy and Internal Energy.	T3. Extrem. Princl. TD Potentials.		
Week 3 Sep 2 – Sep 6; (2 classes)	T4. Maxwell Rel-s. Stability.	T5. Phase Equil. Gibbs Phase Rule.	Kin. T. of Gas	HW Set 1 (TD)
Week 4 Sep 9 – Sep 13; (2 classes)	SF1. Binomial & Gaussian Distr.	SF2. Analytical Mech, Equipart.		
Week 5 Sep 16 – Sep 20; (1 class) **Sep 17 = No Class (Well-s Day)**	**No Class**	SF3. Quantum Mechanics	Diffus. Rand Walks	HW Set 2 (Stat. Distr.)
Week 6 Sep 23 – Sep 27; (2 classes)	SF4. Microcanon. Ensemble	SF5. Canonical Ensemble	Shroed Eqn	HW Set 3 (AM + QM)
Week 7 Sep 30 – Oct 4; (2 classes)	SA1. Sackur-Tetrode Eqn.	SA2. Virial Expansion		
Week 8 Oct 7 – Oct 11; (2 classes)	Midterm Exam #1	SA3. Intermol Interactions 1.	CS EOS	HW Set 4 (IG, Vir.)
Week 9 Oct 14 – Oct 18; (1 class) **Oct 15 = No Class (Fall Break)**	**No Class**	SA4. Intermol Interactions 2.		
Week 10 Oct 21 – Oct 25; (2 classes)	SA5. Lattice Theor. Flory-Huggins.	SA6. Einstein Solid.	e- gas, FD stat	HW Set 5 (Intmol. Int.)
Week 11 Oct 28 – Nov 1; (2 classes)	AIChE Week: Exam Review	AIChE Week: Midterm Exam #2		
Week 12 Nov 4 – Nov 8; (2 classes)	SA7. Debye Solid.	SA8. Dipolar Gas. Langevin Func.	C_v dip. Gas	HW Set 6 (LJ + FH)
Week 13 Nov 11 – Nov 16; (2 classes)	SA9. Molecular Part Functions.	SA10. Chemical Reactions.		
Week 14 Nov 18 – Nov 22; (2 classes)	SF6. G Can Part F. Fluctuations	SA11. Langmuir Adsorption.	Phys. Assoc.	HW Set 7 (Ext, MPF)
Week 15 Nov 25 – Nov 29; (1 class) **Nov 28 = No Class (TG-ing)**	SA12. Interfaces. Wetting. Nucleation.	**No Class**		
Week 16 Dec 2 – Dec 6; (1 class) **Dec 3 = The Last Class**	SA13. Simulations	**No Class**		HW Set 8 (Flucts. & React. Syst.)
Week 17 Dec 9 – Dec 13; (0 class + exam) **Dec 10 = Final Exam** **Grades due by Dec 13**	**Final Exam** 12:00 - 2:30 pm in the usual room (EB3 2124)	**No Class**		

The most up to date schedule will be posted on Moodle and updated during the Semester.

POLICIES AND PROCEDURES

- **Communication:** Dr. Rumyantsev and the TAs will use e-mail to communicate with the class. You should read your email and check the course website at least daily.

- **In-class questions:** We will use Top Hat for in-class questions. Information on Top Hat can be found in at *delta.ncsu.edu/learning-technology/instructional-tools/top-hat/*

- **Homework:** There will be a homework assignment *approximately* every second week. Homework assignments are to be completed individually. It is strongly recommended to start working on the homework once it is available because some problems may be time-consuming. The due dates for the submission will be posted on Moodle, normally 11:59 pm on Fridays. Late homework submissions receive 20% grade deduction and accepted until 11:59 pm on Saturday following the due date.

Homework format:
- ✓ Handwritten homework must be done on plain white paper or using digital tablet.
- ✓ Many of the problems will ask to plot the dependencies graphically. Any software can be used to electronically generate the plot. Using Wolfram Mathematica is highly recommended. The resulting plots can be copied and pasted to the homework electronic files.
- ✓ Write only on one side.
- ✓ Begin each problem on a new page, and *box all final answers*.
- ✓ All parts of each problem in a completed assignment must be easily legible.
- ✓ On the first page, write your name and surname, and the problem set number.
- ✓ Problems should be submitted in the same order they appear in the homework assignment.
- ✓ *Points may be deducted for not following these guidelines*.
- ✓ Turn in any homework by scanning/taking pictures and submitting them through Gradescope (Course ID: **789899**; Entry Code: **DK56P3**) Please ensure that the files are legible before sending them.

Homework regrades: If you believe an error was made in grading your homework, send the regrade request using Gradescope. Write a short explanation of your claim. Regrade requests may be submitted up to one week after the graded homework is returned; it will not be accepted afterwards. If you disagree with the decision on the regrade request and response provided, please email the instructor and explain the reason for your disagreement.

- **Exams:** There will be two in-term exams during the semester. Each exam will test all of the material covered up to the week before the exam. The grade of each exam will

contribute 25% of the final grade of the course. <u>Exams are closed-book and closed-note</u>. Any form of communication by or with the students, including sharing of class materials, during an exam is strictly forbidden. Failure to comply with these guidelines will result in a failing grade for the class, and will be *immediately* reported to the Office of Student Conduct.

- **Exam regrades:** If you believe an error was made in grading your exam, send the regrade request using Gradescope. Provide an explanation of your claim. Exam regrade requests must be submitted up to one week after the graded exam is returned, and will not be accepted afterwards. If you disagree with the decision on the regrade request and response provided, please email the instructor and explain the reason for your disagreement. Note that *<u>the entire exam may be regraded</u>* to ensure consistency and fairness.

- **Missed exams:** If you know you will miss an exam <u>for a legitimate reason</u>, let the instructor know at least one week in advance. Schedule conflict, i.e. taking other classes at the same time, is *not* considered a legitimate reason. If you miss an exam for a legitimate reason, you may take a comprehensive makeup exam near the end of the semester. Only one such exam will be given, you cannot take more than one makeup exam.

- **Academic integrity**: Students are required to comply with the university policy on academic integrity found in the Code of Student Conduct found at http://policies.ncsu.edu/policy/pol-11-35-01. It is the instructor's understanding and expectation that the student's signature on any test or assignment means that the student contributed to the assignment in question (if a group assignment) and that they neither gave nor received unauthorized aid. Authorized aid on an individual assignment includes discussing the interpretation of the problem statement, sharing ideas or approaches for solving the problem, and explaining concepts involved in the problem. Any other aid would be unauthorized and a violation of the academic integrity policy. Unauthorized aid additionally includes consulting or providing tests from previous years (unless explicitly sanctioned by the instructors). In addition, any computer work submitted must be completed on your own personal computer or from your own account to avoid confusion about the origin of the file, and no sharing of files in any way is allowed. Proper referencing of any source of information you use in your homework is required (e.g. Table B.1 of Felder & Rousseau, Perry's Chemical Engineers' Handbook pp. XX-YY, full URL and date accessed for any online resource, etc.). All cases of academic misconduct will be submitted to the Office of Student Conduct. Students found guilty of academic misconduct will be subject to **getting a zero for that entire course component** (e.g. a zero for the homework portion of the final grade), or a failing grade in the course, depending on the nature of the violation. In addition, if you are found guilty of academic misconduct in the course, you will be on academic integrity probation

for the remainder of your years at NCSU and may be required to report your violation on future professional school applications. It's not worth it!

Example: It is found that student A violated the course rules when doing homework set #8. Zero credit can be given to student A not only for homework set #8, but also for *all the preceding and all the following homework sets*, i.e. **the entire course component** (because the presumption of innocence no longer applies to student A.) The final decision remains at the instructor's discretion and depends on the type of violation.

- **Digital course components:** Moodle will be used to host the class website. This will be the primary means of communication (besides lectures and office hours) between the instructor, teaching assistants, students, and support staff. For in-class activities we will use Top Hat (Class code: **198870**). Homework assignments will often require using software to carry out calculations, including but not limited to numerically solving nonlinear equations and nonlinear systems of equations as well as analytical and numerical integration or differentiation. Wolfram Mathematica software will be used for class examples and homework. Turnitin will be used to check submissions for plagiarism and the use of unapproved tools such as AI chatbots.

- **Wolfram Mathematica** is a highly recommended tool for solving numerical (and even analytical) problems offered within the Course. It can be downloaded for free using the NCSU credentials. The link below provides the detailed instructions: **https://software.ncsu.edu/software/mathematica/**

- **Personally identifiable information:** Students may be required to disclose personally identifiable information to other students in the course, via digital tools, such as email or web-postings, where relevant to the course. Examples include online discussions of class topics, and posting of student coursework. All students are expected to respect the privacy of each other by not sharing or using such information outside the course.

- **Students with disabilities:** Reasonable accommodations will be made for students with verifiable disabilities. In order to take advantage of available accommodations, students must register with the Disability Resource Office at Holmes Hall, Suite 304, Campus Box 7509, 919-515-7653. For more information on NC State's policy on working with students with disabilities, please see the **Academic Accommodations for Students with Disabilities Regulation (REG02.20.01) (http://policies.ncsu.edu/regulation/reg-02-20-01)**

- **Equal Opportunity:** NC State University provides equality of opportunity in education and employment for all students and employees. Accordingly, NC State affirms its commitment to maintain a work environment for all employees and an

academic environment for all students that is free from all forms of discrimination. Discrimination based on race, color, religion, creed, sex, national origin, age, disability, veteran status, or sexual orientation is a violation of state and federal law and/or NC State University policy and will not be tolerated. Harassment of any person (either in the form of quid pro quo or creation of a hostile environment) based on race, color, religion, creed, sex, national origin, age, disability, veteran status, or sexual orientation also is a violation of state and federal law and/or NC State University policy and will not be tolerated. Retaliation against any person who complains about discrimination is also prohibited. NC State's policies and regulations covering discrimination, harassment, and retaliation may be found at **http://policies.ncsu.edu/policy/pol-04-25-05** or **http://www.ncsu.edu/equal_op** Any person who feels that he or she has been the subject of prohibited discrimination, harassment, or retaliation should contact the Office for Equal Opportunity (OEO) at 919-515-3148.

- **NC State Policies, Regulations, and Rules (PRR):** Students are responsible for reviewing the NC State University PRR's located at **http://oucc.ncsu.edu/course-rights-and-responsibilities**, which pertains to their course rights and responsibilities.

- **Policy on incomplete grades:** If an extended deadline is not authorized by the instructor or department, an unfinished incomplete grade will automatically change to an F after either (a) the end of the next regular semester in which the student is enrolled (not including summer sessions), or (b) the end of 12 months if the student is not enrolled, whichever is shorter. Incompletes that change to F will count as an attempted course on transcripts. The burden of fulfilling an incomplete grade is the responsibility of the student. The university policy on incomplete grades is located at **http://policies.ncsu.edu/regulation/reg-02-50-03**.

- **Classroom Capture:** Please be advised this course will be recorded for current and potential future educational purposes. By your continued participation in this recorded course, you are providing your permission to be recorded.

- **Supporting Fellow Students in Distress:** As members of the NC State Wolfpack community, we each share a personal responsibility to express concern for one another and to ensure that this classroom and the campus as a whole remains a safe environment for learning. Occasionally, you may come across a fellow classmate whose personal behavior concerns or worries you. When this is the case, you are encouraged to report this behavior to the Division of Academic Affairs: **https://prevention.dasa.ncsu.edu/nc-state-cares/referring-a-student/.**
Although you can report anonymously, it is preferred that you share your contact information so they can follow-up with you personally.

- **Religious/Cultural Observance:** Persons who have religious or cultural observances that coincide with this class should let the instructor know in writing (by e-mail for example) by the end of the second week of class. I strongly encourage you to honor your cultural and religious holidays. However, if I do not hear from you by the end of the second week of class, I will assume that you do not have any attendance conflicts of this sort.

- **Title IX Statement:** Title IX makes it clear that violence and harassment based on sex or gender is a Civil Rights offense, subject to the same kinds of accountability and the same kinds of support applied to offenses against other protected categories such as race or national origin. If you or someone you know has been harassed or assaulted, you can find the appropriate resources at **https://diversity.ncsu.edu/title-ix/**

- **Inclusion Statement:** At NCSU, administrators, faculty, and staff are committed to the creation and maintenance of "inclusive learning" spaces, where you shall be treated with respect and dignity and where all individuals are provided equitable opportunity to participate, contribute, and succeed. In this course, all students are welcome regardless of race/ethnicity, gender identities, gender expressions, sexual orientation, socio-economic status, age, disabilities, religion, regional background, Veteran status, citizenship status, nationality and other diverse identities that we each bring to class. The success of an inclusive classroom relies on the participation, support, and understanding of you and your peers. We encourage you to speak up and share your views, but also understand that you are doing so in a learning environment in which we all are expected to engage respectfully and with regard to the dignity of all others.

- **Reporting Form:** A new departmental Anonymous Reporting Form is now online for use by students, staff, and faculty at **https://ncsu.qualtrics.com/jfe/form/SV_cAY9R8mKN4nFRe6?jfefe=new** Using it, you can communicate incidents and suggestions related to unprofessional behavior and departmental climate, including but not limited to cheating, bullying, and harassment.

- **Pronoun Use:** I will gladly honor your request to address you by your chosen name or gender pronoun. Please advise me of this at any point in the semester so that I may make appropriate changes to my records.

- **ClassEval:** Course and instructor evaluations: Online class evaluations will be available for students to complete during the last two weeks of class. Students will receive an email message directing them to a website where they can login using their Unity ID and complete evaluations. All evaluations are confidential; instructors

will never know how any one student responded to any question, and students will never know the ratings for any particular instructors:

- ✓ ClassEval website: **https://isa.ncsu.edu/for-the-pack/classeval/**
- ✓ Student help desk: **classeval@ncsu.edu**
- ✓ Schedule: Online class evaluations will be available for students to complete during the last 2 weeks of class and become unavailable before finals begin. A reminder will be posted on the class website.
- ✓ ClassEval Survey Link: **https://classeval.ncsu.edu/secure/prod/cesurvey**