Chemical Engineering Thermodynamics

ENCH 610

Mondays & Wednesdays, 4:00-5:15 pm
CHE 2136
Fall 2010

Instructor: Prof. Jeffery B. Klauda
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Office hours: Monday, 11-noon or Thursday, 10-noon

Course Description

This course will focus on the theory and application of classical thermodynamics and give an introduction to statistical thermodynamics. Traditional topics covered in an undergraduate chemical engineering thermodynamics course will be reviewed, e.g., the first and second laws of thermodynamics, thermodynamic properties, phase equilibrium, and equations of state. Methods used to describe and predict phase equilibrium involving all three states of matter will be covered (liquid activity coefficient models, solid-liquid models, partition coefficients, etc.). Thermodynamic concepts will be applied to chemical reaction equilibria and various applications in biology (solubility, protein folding, membrane potentials, etc.). Statistical thermodynamics will be introduced with a focus on the concepts of ensembles, applications to the ideal and imperfect gas phase, and relations to classical thermodynamics. Class time will be devoted to a variety of activities, including lecture, individual or small group problem solving, and quizzes.

Course Objectives for Students

- Understand and apply the three laws of thermodynamics.
- Determine appropriate methods for predicting phase equilibrium of various mixtures in all three states of matter.
- Apply thermodynamic concepts to research in many areas of chemical engineering.
- Understand how to relate properties at the atomic or molecular level to macroscopic properties via statistical thermodynamics.
- Improve communication skills by classroom discussion, problem solving, and written assignments.

Required Course Readings

Textbooks

- S.I. Sandler. (2006). *Chemical, Biochemical, and Engineering Thermodynamics.* (4th Ed.). USA: Wiley. ISBN: 978-0-471-66174-0
- T.L. Hill. (1986). *An Introduction to Statistical Thermodynamics.* USA: Dover Publication, Inc. ISBN: 0-486-65242-4

Useful Websites

- webbook.nist.gov/chemistry/
- www.wiley.com/college/sandler

Computer Software

Some homework problems may require the use of software, such as Excel, Matlab, or MATHCAD. The resource CD for Prof. Sandler's book contains a 120 day free trial of MATHCAD. Other programs are available at many campus computing centers (www.oit.umd.edu/projects/wheretogo/).

Lecture

The lecture time will consist of an overview of the topics given in the course calendar for that day. Students are expected to read the material to be covered that day before class. The lectures serve as an overview and *details are left for the student to understand outside of class*. Many lecture periods will also consist of in-class problem solving in groups based on the lecture material. Therefore, **always bring your textbook and a calculator to class**.

Class Participation

Students will be expected to participate in class and during group problem solving activities. Solutions to these problems will be discussed and presented by students. Everyone is expected throughout the semester to contribute to these discussions. Dr. Klauda will determine the grade for class participation based on the student's involvement.

Quizzes

Short quizzes, one or two problems, will be given throughout the semester. These will NOT be announced ahead of time and are open book/notes/calculator (another reason to bring a textbook/calculator to class). The grades will be scored on a 3 pt scale. The lowest grade on a quiz will not be counted in the final grade.

Homework

Homework problems will be assigned regularly and will be graded. These will consist of problems that only require pencil and paper to those that require software. You are allowed to help each other on the homework problems but **each person must turn in their own work**. Homework that is copied from another student is in violation the university's Code of Academic Integrity. Similarly, you are not allowed to use the publisher's solution manual or those from previous students.

Exams

There will be two midterm exams (**October 4 and November 3)** and a final exam (**December 18**). The midterm exams will only cover the material listed on the course calendar. The final is comprehensive but about half of the exam will be on problems related to the final third of the course. All exams are open book, open notes, and a calculator is allowed.

Term Project

The details of the term project will be given during the semester.

Grading Summary

Homework	30%
Exam 1	15%
Exam 2	15%
Final Exam	20%
Class participation	5%
Quizzes	5%
Term Project	10%

Class Policies

Absences from class: If you must miss class for any reason, I strongly recommend that you ask a classmate for any notes, handouts, or announcements you may have missed. In addition, please notify me as far in advance as possible if you know that you are going to miss class for a university-approved reason, so that we can discuss any necessary arrangements. Please see the Undergraduate Catalog's description of university-approved reasons for absence (http://www.umd.edu/catalog).

Academic integrity: The University of Maryland, College Park has a nationally recognized Code of Academic Integrity, administered by the Student Honor Council. This code sets standards for academic integrity at Maryland for all undergraduate and graduate students. As a student you are responsible for upholding these standards for this course. It is very important for you to be aware of the definitions and consequences of cheating, fabrication, facilitation, and plagiarism. For more information on the Code of Academic Integrity or the Student Honor Council, please visit http://www.shc.umd.edu. Violations of the code will not be tolerated in this class.

Accommodations for students with disabilities: In order to receive accommodations, students with learning disabilities must provide a written request and documents from the University of Maryland Disability Support Services (http://counseling.umd.edu/DSS). Please submit any requests by **September 8**.

Cell phones: Please keep cell phones and other communicative devices silent and out of sight during class. Text messaging is not allowed during class and will be reflected in the class participation grade.

Inclement weather: In the event of inclement weather, I will comply with the University's decision regarding whether classes are going to be held or not. Any assignments due on the day of a cancellation will be due instead at the next class meeting.

Late Homework: These items are due at the designated time stated on each assignment. Email submissions will not be accepted, unless approved by myself. The penalty for lateness without a university-approved reason for absence on the due date is half credit up to 24 hours late and no credit after 24 hours.

Make-ups: Exams and quizzes may only be made up if you are absent for a documented, university-approved reason. If you miss class without a university-approved reason on a day that an exam or quiz takes place, you will not be able to make it up.

Religious observation: If you will miss class on the day of an exam or on the date that an assignment is due because of a religious observation that is not officially recognized by the university, you must contact me **at least 2 weeks before your anticipated absence** in order to discuss alternative dates for the exam or assignment.

Blackboard (www.elms.umd.edu): On Blackboard, I will post this syllabus, assignments, and any major changes to the course calendar. In addition, I may sometimes post handouts utilized in class and links to useful web sites. You will also be able to access your grades via Blackboard.

CourseEvalUM (www.courseevalum.umd.edu)**:** Your participation in the evaluation of courses through CourseEvalUM is a responsibility you hold as a student member of our academic community. Your feedback is confidential and important to the improvement of teaching and learning at the University as well as to the tenure and promotion process. CourseEvalUM will be open for you to complete your evaluations for fall semester courses between Tuesday, November 30 and Sunday, December 12. Please go directly to the website to complete your evaluations starting November 20. By completing all of your evaluations each semester, you will have the privilege of accessing online, at Testudo, the evaluation reports for the thousands of courses for which 70% or more students submitted their evaluations.

Course Calendar

Note: Students should read the chapter associated with the lecture PRIOR to class. Homework (HW) assignment dates are tentatively listed; due dates will be listed on the assignment.

Day	Date	Topic	Chapter/Section	HW
Mon	Aug 30	Introduction and nomenclature Conservation of mass	Ch. 1 & 2	
Wed	Sep 1	Conservation of energy Energy balances	Ch. 3	
Mon	Sep 6	Holiday		
Wed	Sep 8	Applications of energy balances	Ch. 3	#1
Mon	Sep 13	Entropy balance Reversibility	Ch. 4	
Wed	Sep 15	Applications of entropy balances	Ch. 4	#2
Mon	Sep 20	Mechanical explosions Thermodynamic partial derivatives	Ch. 5.3 Ch. 6	
Wed	Sep 22	Ideal gas Equations of state (EOS)	Ch. 6	#3
Mon	Sep 27	Criteria for equilibrium EOS and phase equilibrium Free Energy/Fugacity	Ch. 7.1-7.2 Ch. 7.3 Ch. 7.4	
Wed	Sep 29	Phase transitions and the Gibbs phase rule	Ch. 7.5-7.8	#4
Mon	Oct 4	**EXAM 1**	Covered Material in Chapters 1-6	
Wed	Oct 6	Thermo of Mixtures: partial molar quantities Reactions	Ch. 8.1-8.6	#5
Mon	Oct 11	Phase & Chemical Equilibrium Ideal Gas Mixtures	Ch. 8.7-8.9 Ch. 9.1-9.3	
Wed	Oct 13	Fugacity of mixtures Activity coefficient models	Ch. 9.4 Ch. 9.5-9.6	#6
Mon	Oct 18	Combined EOS/G^{ex} models Electrolyte Solutions	Ch. 9.7-9.9 Ch. 9.10 & App. 9.3	
Wed	Oct 20	Vapor-liquid Equilibrium (VLE)	Ch. 10	#7
Mon	Oct 25	VLE/Gas solubility	Ch. 10 & Ch. 11.1	
Wed	Oct 27	LLE/VLLE Partitioning between liquid phases	Ch. 11.2-11.3 Ch. 11.4	#8
Mon	Nov 1	Solid Equilibrium	Ch. 12	
Wed	Nov 3	**EXAM 2**	Covered Material in Chapters 7-10	
Mon	Nov 8	Chemical Equilibrium	Ch. 13.1-13.2	
Wed	Nov 10	Chemical Equilibrium	Ch. 13.3-13.4	#9
Mon	Nov 15	Biochemical applications	Ch. 15.1-15.2	
Wed	Nov 17	Solubilities & pH, ligand binding, and biochemical reactions and protein folding	Ch. 15.3-15.5	#10
Mon	Nov 22	**PROJECT (may move)**		
Wed	Nov 24	**PROJECT (may move)**		
Mon	Nov 29	Stat Mechanics: Introduction & Ensembles	Hill: Ch. 1-3	
Wed	Dec 1	Ideal Monotonic Gases	Hill: Ch. 4	#11
Mon	Dec 6	Ideal Diatomic & Polyatomic Gases	Hill: Ch. 8-9	
Wed	Dec 8	Imperfect Gases & Applications	Hill: Ch. 15	#12
Sat	Dec 18	**FINAL EXAM, 1:30-3:30pm (tentative)**	All course material	