CBE 501
Chemical Engineering Thermodynamics
Fall 2011

COURSE OUTLINE

Engr. B2
Dr. David (Qiang) WANG
Office: 108 Glover

TEXTBOOK: Tester & Modell, *Thermodynamics and its Applications*.

REFERENCE BOOKS: Callen, *Thermodynamics and an Introduction to Thermostatistics;*
Prausnitz et al., *Molecular Thermodynamics of Fluid-Phase Equilibria;*
McQuarrie, *Statistical Mechanics;*
Allen & Tildesley, *Computer Simulation of Liquids.*

ORGANIZATION: The course consists of 2 lecture periods per week, T&R 3:30-4:45pm.

HOMEWORK: There will be 6~8 homework assignments. Students are encouraged to work in groups, but copying is not allowed. Assignments are due at the beginning of class. Each assignment must be submitted on the indicated due date and will be graded. Late homework may (and should!) be turned in, but 20% will be deducted for each day that it is late. Students who are unable to attend class may submit assignments early by placing them in my mailbox in Glover 100. ***Homework done using homework solutions from any source will receive 0 credit.*** **Homework results represent 40% of the grade for the course**.

PROJECT: There will be one project on “Special Topics in Thermodynamics”. Each student will be required to give a mini-lecture on a selected topic and to answer any questions from the audience (including rest of the class and instructor). The project will be graded by the audience. **The project results represent 10% of the grade for the course**.

EXAMINATIONS: There will be one quiz, one mid-term and one final exam for this course, all of which are closed book, but 1-page (letter-size) notes and a calculator can be used. There will be no makeup exam and students will receive 0 credit for any exam they fail to take unless the absence is excused. Requests for an excused absence from an examination must be submitted in writing to the instructor prior to the next scheduled lecture following the exam. All exams will be comprehensive. **Results of the mid-term and final exams will each represent 20% of the grade for this course, and those of the quiz will represent 10%**.

OFFICE HOURS: T&R, 4:45-5:30pm. Office: 108 Glover. To meet with me outside regular office hours call 491-2763, or better yet, e-mail me at q.wang@colostate.edu.

COMMENTS: The primary objective of this course is to develop additional depth in understanding the fundamentals of chemical engineering thermodynamics. This will be accomplished largely through solution of realistic engineering problems more complicated than those attempted in an introductory undergraduate course. In addition, introductory materials on statistical thermodynamics will be taught to provide molecular-level understanding of classical thermodynamics. **Thermodynamics and Calculus at the undergraduate level are needed for taking this course.**

Additional Information

Academic Integrity Policy

A statement of the university's academic integrity policy can be found in the General Catalog at http://www.catalog.colostate.edu/FrontPDF/1.6POLICIES1112f.pdf (See "Students' Responsibilities" on pages 7-11). The policy is zero tolerance. The ***minimum*** action taken for academic dishonesty will be a failing grade for the course. In particular:

- Students may not copy any part of a homework assignment or an exam from other students, ***including those in previous years***. The student who knowingly provides his/her assignment or exam to be copied is also in violation of the CSU policy. Students, however, are allowed and encouraged to work in groups on homework assignments.
- Students are forbidden to use solution manuals from any source. The resources that the students are allowed to use for homework and exams are limited to textbook, reference or similar books, lecture notes and handouts, and data handbooks. For the project, other resources may be used.
- Discussing the content of an exam with someone who has not taken the exam is not allowed.

Mini-Lecture on "Special Topics in Thermodynamics"

Examples of the topic are: "*History of Thermodynamics*", "*What Is Entropy?*", "*Thermodynamic Analysis of … Process*", "*Clean the Mess of Mixtures*", "*Computation of Multi-Component Phase Equilibrium*", "*Applications of Molecular Dynamics (or Monte Carlo Simulations) in …*", etc. Each student should discuss with the instructor about his/her selected topic and scope. The lecture should be well organized (no longer than 20 minutes). Blackboard and computer projector are available for the presentation. All mini-lectures will be given in the last week of classes, and will be graded by the audience on a scale of 1~10 (1 for the worst and 10 for the best lecture you've ever had).

Learning objectives (can also be used as your study guide for exams)

The student successfully completing this course will be able to:

1. Apply the mass, energy and entropy balance to open systems;
2. Derive the relations among various thermodynamic quantities (transform derivatives);
3. Apply the criteria of thermodynamic equilibrium and stability for pure materials and binary mixtures;
4. Given an equation of states, calculate property changes of pure materials;
5. For mixtures, explain the concepts of partial property, mixing function, departure function, excess function, and their combinations (e.g., partial molar excess mixing Gibbs free energy);
6. Calculate fugacity coefficient given an equation of state, and activity coefficient given an excess Gibbs free energy (or Gibbs free energy of mixing) model;
7. Select appropriate thermodynamic models and solve phase equilibrium problems for both pure materials and mixtures;
8. Explain the concepts of statistical ensembles and partition functions, and their connections to classical thermodynamics;
9. Explain why and how molecular dynamics and Monte Carlo simulations work;
10. Derive the acceptance criteria for Monte Carlo trial moves in various ensembles;
11. Derive the lattice theories for binary liquid mixtures (including polymers) using statistical-mechanical approach.

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Preliminary Class Schedule (8-16-11)

Week	**Day**	**Topic**	**Textbook**
1	Aug. 23 Aug. 25	Introduction and Basic Concepts The First Law	Chap. 1&2 Chap. 3
2	Aug. 30 Sep. 1	 ***No Class – ACS Meeting***	
3	Sep. 6 Sep. 8	The Second Law	Chap. 4
4	Sep. 13 Sep. 15		
5	Sep. 20 Sep. 21 Sep. 22	Calculus and Mathematical Transforms ***Quiz*** (7~8pm in classroom) Equilibrium and Stability Criteria	Chap. 5 Chap. 6&7
6	Sep. 27 Sep. 29	 Pure Materials	 Chap. 8
7	Oct. 4 Oct. 6	 Mixtures	 Chap. 9
8	Oct. 11 Oct. 13		
9	Oct. 18 Oct. 20	***No Class – AIChE Meeting*** Phase Equilibrium and Stability	 Chap. 15
10	Oct. 25 Oct. 26 Oct. 27	 ***Mid-term Exam*** (6~9pm in classroom) Statistical Mechanics and Molecular Dynamics	 Chap. 10
11	Nov. 1 Nov. 3	Statistical Ensembles	
12	Nov. 8 Nov. 10		
13	Nov. 15 Nov. 17	Ideal Gas & Maxwell Distribution of Velocity Monte Carlo Simulations	
14	Nov. 22 Nov. 24	***No Class This Week – Fall Recess***	
15	Nov. 29 Dec. 1	 Lattice Theory	 Chap. 11
16	Dec. 6 Dec. 8	***Mini-Lectures***	
	Dec. 14	***Final Exam*** (11:50am~1:50pm in classroom)	

Note: this schedule may be changed as the course progresses.