Advanced Chemical Engineering Thermodynamics
Chemical Engineering 808, Spring 2000

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Class hours: T R 10:30-11:48
Location: 330 Koffolt Labs
Textbook: *Molecular Thermodynamics of Fluid-Phase Equilibria*
Prausnitz, Lictenthaler, Azevedo, 3rd Edition (1999)
Prerequisites: Chem Eng 509 or equivalent

Course Description and Objectives

Graduate students in this course learn how to apply thermodynamics to phenomena and processes of interest to chemical engineers. The content is advanced, building upon prior courses in thermodynamics taken at the undergraduate level. The goal of this course is to provide further depth in the area of process thermodynamics (energy, entropy, heat, work), with special emphasis given to phase equilibrium thermodynamics. A small part of the course is devoted to statistical mechanics and its relation to thermodynamics.
Solving phase equilibria problems involves general computational techniques that have widespread application in other areas of engineering. For example, we often need to determine whether a particular activity coefficient model accurately describes a given set of experimental data and, if so, to calculate values of the model parameters that result in the best fit. Thus, another objective of this course is to provide students experience in fitting mathematical models to experimental data, using phase equilibria calculations as an example of one type of problem for which this excercise is important.

By the end of the quarter, you should:

- be able to apply the first and second laws in the analysis of chemical processes;
- know how to qualitatively and quantitatively describe the effect of intermolecular interactions on the thermodynamic properties of real gases, liquids, and mixtures;
- be able to solve phase equilibria problems; this includes the ability to determine which of a variety of models best describes a given set of data, and to calculate the model parameters.

Course Policies

Homework will be assigned approximately once per week and, unless instructed otherwise, must be submitted no later than noon on the due date. The solution to each assignment will be posted

at this time, so no credit will be given for late homework. Late homework must still be completed and submitted within one week of the due date to receive a score of zero. A score of -10 will be given for each assignment not submitted before the one week deadline.
You may discuss homework assignments with classmates, but each student must do his/her own work. You may **not** copy solutions from a classmate or from solution sets from previous years to which you might have access. Presenting someone else's work as your own is plagiarism. Your are expected to be familiar with the university's policies regarding academic misconduct. I am obligated to initiate proceedings in all cases where I suspect any impropriety.
Exams are open-book and open-notes. You should **not** assume this means you do not have to study as long or prepare as thoroughly as you would for a closed book test. Numerous past students have convincingly proven this theory to be wrong!

Excused Absences

Situations may arise when, due to sickness or emergency, you miss an exam or do not submit a homework assignment on time. It is your responsibility to contact me as early as possible and explain why you were absent. If you do so to my satisfaction, you will not be penalized and I will make arrangements for you to do make-up work. If you are too sick to attend class, you should seek professional medical attention and ask the doctor for a written acknowledgement that you did so. Professors are generally understanding and lenient when students keep them informed in a timely manner in these situations.

Computers

You should already be familiar with the computer labs in KL 132, 134, and 135. Be sure to check the course homepage and your email on a regular basis, as we will make full use of these resources for distributing information about the course. If you use the networked printers in the computer labs, please be aware that you have a quota of 300 pages per quarter - it is your responsibilty to manage your quota and insure that you don't run out before the end of the quarter.

Regrades

If you believe a mistake was made and that you deserve more points on a homework or exam, you must write a short note of explanation and resubmit your work directly to Dr. Rathman. You must do this within one week after the assignment in question is returned. Assignments resubmitted after one week will not be considered for correction. ***Do not complain about a grade to the T.A. or expect her to change your score.***

Format for Homework and Exams

- Assignments must be worked on engineering paper. Write only on one side of each sheet of paper and start each problem on a new page.

- At the top of the first page, write your full name, student ID number, date, and your personal mailbox number. Each subsequent page must be numbered and have your name written at the top.
- At the start of each problem, briefly describe the problem and for what you are expected to solve. When appropriate, draw and label a flowchart for the process described in the problem statement.
- When necessary, graphs should be prepared either on graph paper or (preferably) using a computer graphing program. Spreadsheet programs such as Microsoft Excel or Lotus 1-2-3 or Quatro Pro are adequate for preparing graphs. Do not use engineering paper - the grid used on engineering paper is too course for preparation of accurate graphs. Graphs should include a descriptive title and each axis should be properly labeled.
- Clearly define any algebraic variables used in your solution - be consistent with those used in the text and during lecture. State all assumptions you make and cite sources of data used in your calculations.
- All steps of a solution should be shown and easy to follow and your final results must be clearly indicated (boxed or underlined) - don't make us hunt for your answers!
- Numerical answers must have correct units - a number without proper units is as meaningless as units without a number. Correct use of significant figures is also important.
- Your assignment must be stapled together when submitted- we are not responsible for lost pages if you do not staple your work.

After solving a problem, always take a second look at your answer and ask yourself whether or not it seems reasonable. If not, don't attempt to "fudge" your calculation, but write a brief comment indicating that you suspect your answer is incorrect. For example, if you end up with a negative absolute pressure, we will be more lenient grading your work if you tell us you know this is an impossible result. We will not be lenient if you report the negative value with no comment, or if you simply change the negative sign to a positive and try to fool us.

Evaluation

Final grades will be based on the components listed in the table below. All scores will be used - none of the scores will be dropped. To insure confidentiality, I will never post grades or scores - instead, you will receive email from me on a regular basis throughout the quarter listing the scores I have recorded for you and your current standing in the class. This will make sure we catch any mistakes early, and will help you know how you're doing as the quarter progresses. Please contact me with any questions - there should never be any mysteries or surprises when you receive your final grade at the end of the quarter.

Components Used to Determine Final Grade

	# Points	% of Total
Homework	100 pts	31.25
Midterm Exams	140 = 2 x 70 pts/ea	43.75
Final Exam	80	25.00

Total	**320**	**100**

Schedule of Exams and Reading Assignments

Dates	Textbook	Topics to be covered
Mar 28, 30	1, 2 Appendix A	review of undergraduate thermodynamics: energy and entropy balances, equilibrium criteria, chemical potential, fugacity, activity, Raoult's Law
Apr 4, 6	3	thermodynamic properties from volumetric and thermal data; equations of state; fugacity of components in a mixture; phase equilibria from an equation of state
Apr 11, 13	4.1 - 4.6	intermolecular forces and potential functions: ion-ion, dipole, induction, and dispersion forces
Apr 18, 20	4.7 - 4.12	repulsion, specific chemical forces; hydrophobic interaction and entropy effects; theory of corresponding states
Apr 25, 27	4.12 - 4.14 Appendix B	theory of corresponding states (cont.); introduction to statistical mechanics
May 3	**1 - 4 Appendix B**	**Exam #1 (Time to be announced.)**
May 2, 4	5.1 - 5.7	fugacities in gas mixtures: virial equations of state
May 9, 11	6 Appendix D	fugacities in liquid mixtures: ideal solutions; excess functions; Gibbs-Duhem equation
May 16, 18	6 Appendix E	Wilson, NRTL, and UNIQUAC equations; partial miscibility (liquid-liquid equilibrium); multicomponent mixtures
May 24	**1 - 6 Appendices**	**Exam #2 (Time to be announced.)**
May 23, 25	7.1 - 7.4	fugacities in liquid mixtures: van Laar theory, Scatchard-Hildebrand theory, equations of state, lattice model
May 30 Jun 1	7.7 - 7.10	two-liquid model; chemical theory; associated solutions
Jun 6	**1 - 7**	**Final Exam (9:30 am - 11:18 am)**