Chemical and Biomolecular Engineering Thermodynamics II
CHBE 302

Lecture: Tuesday & Thursday, 9:30-10:45 am (EGR 1202)
Recitation Section: Friday, 10:00-10:50 pm (EGR 1202)
Spring 2018

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Course Description

This course will focus on the theory and application of phase and chemical reaction equilibrium thermodynamics and give an introduction to molecular thermodynamics. Vapor/liquid equilibrium of ideal mixtures will be reviewed to form the foundation of real solution thermodynamics. Methods used to describe and predict phase equilibrium involving all three states of matter will be covered (liquid activity coefficient, solid-liquid models, equation of state, etc.). Thermodynamic concepts will be applied to chemical reaction equilibria. Specific applications of environmental concern (partitioning of chemicals), surface effects, and various applications in biology (solubility, protein folding, membrane potentials, etc.) will be included. The semester will conclude with a brief introduction to the use of molecular simulations to describe thermodynamic properties. 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 the theory behind phase equilibria between two or more phases.
- Understand the weakness and strengths of various models for predicting phase equilibria in all three states of matter.
- Apply thermodynamic concepts to areas of environmental concern and biology.
- Improve communication skills by classroom discussion, problem solving, and written assignments.

Required Course Readings

Textbook

- Stanley I. Sandler. (2017). *Chemical, Biochemical, and Engineering Thermodynamics.* (5th Ed.). USA: John Wiley & Sons, Inc. ISBN: 978-0-470-50479-6

Useful Websites

- webbook.nist.gov/chemistry/
- http://bcs.wiley.com/he-bcs/Books?action=index&itemId=0471661740&bcsId=2932

Computer Software

Some homework problems may require the use of software, such as Excel, Matlab, Mathcad or ASPEN.

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. 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**.

Recitation Section

A quiz of select problems will be posted on ELMS and graded the day before recitation. The actual recitation section will be used to go over assigned problems which the students had the most difficulty. Interactively as groups students will go through additional problems to supplement the regular lecture and/or a studio format for homework due the following week. Solutions will not be posted on ELMS and students are expected to attend.

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.

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. These will be done in groups of two students. You are allowed to help each other on the homework problems but **each group must turn in their own work**. Homework that is copied from another student/group is in violation the university's Code of Academic Integrity. Similarly, you are not allowed to use solutions from previous students.

Exams

There will be two midterm exams (**March 6 and April 12)** and a final exam (**May 14**) and are considered *Major Grading Events*. 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 *CLOSED* book, but "cheat-sheet" (front/back) and calculator are allowed.

Term Project 

The details of the term project will be given during the semester and is considered a *Major Grading Event*.

Grading Summary

Homework	10%
Exam 1	20%
Exam 2	20%
Final Exam	25%
Recitation Quiz	10%
Term Project	15%

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) and our Department's policy http://www.chbe.umd.edu/policies/index.html.

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 and our Department's policy http://www.chbe.umd.edu/policies/index.html. 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 **February 6**.

Cell phones: Please keep cell phones and other communicative devices silent and out of sight during class. Text messaging is not allowed during class.

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 Assignments (all assignments): 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 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 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.

ELMS/CANVAS (www.elms.umd.edu): On ELMS, 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. Lecture notes will be posted in the Pages section. You will also be able to access your grades via ELMS.

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. 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
Thurs	Jan 25	Introduction Review Energy & Entropy Balances	Ch. 3 & 4	#1
Tues	Jan 30	Equilibrium Criteria, Gibbs Phase Rule and Introduction to Fugacity	Ch. 7.1-7.4 and 7.6	
Thurs	Feb 1	Fugacity (Phases and with EOS) and Phase Transitions	Ch. 7.4-7.5 and 7.7	#2
Tues	Feb 6	Thermodynamics of Mixtures	Ch. 8.1-8.4	
Thurs	Feb 8	Heats of Reaction and Partial Molar Properties	Ch. 8.5-8.6	#3
Tues	Feb 13	Thermo with EOS, Ideal Gas Mixture & Fugacity of a Mixture	Ch. Notes & 9.1-9.2	
Thurs	Feb 15	Ideal Mixture and Excess Properties	Ch. 9.3	#4
Tues	Feb 20	No Class (*Biophysical Society Meeting*)		
Thurs	Feb 22	Introduction to VLE (Ideal Mixtures)	Ch. 10.1	#5
Tues	Feb 27	Non-ideal VLE and Activity Coefficient Models	Ch. 10.2 and 9.5	
Thurs	Mar 1	Predictive Act. Coef. Models and VLE	Ch. 9.6 and 10.2	#6
Tues	Mar 6	**EXAM 1**	Covered Material in Chs. 3-4 & 7-10.1	
Thurs	Mar 8	VLE at High Pressure	Ch. 10.3 and 9.4	
Tues	Mar 13	Modern VLE modeling with EoS Gas Solubility	Ch. 10.3, 9.7 & 11.1	
Thurs	Mar 15	LLE/VLLE	Ch. 11.2	#7
Tues	Mar 20	*Spring Break*		
Thurs	Mar 23	*Spring Break*		
Tues	Mar 27	VLLE/Partitioning in Environment	Ch. 11.3, 11.4 & 12.5	
Thurs	Mar 29	Adsorption, Osmotic Equilibrium & electrolytes solutions	Ch. 9.10, 11.5 & Notes	
Tues	Apr 3	Solubility of Solids and freezing point depression	12.1 & 12.3	#8
Thurs	Apr 5	Gas Hydrate Equilibrium and Equilibrium when surface forces are Important	Notes	
Tues	Apr 10	Introduction to Chemical Equilibrium	Ch. 13.1	
Thurs	Apr 12	**EXAM 2**	Covered Material in Chs. 10, 11 & 12	
Tues	Apr 17	Equilibrium Constants	Ch. 13.1	#9
Thurs	Apr 19	Heterogeneous Chemical Reactions	Ch. 13.2	
Tues	Apr 24	Multiple Reactions	Ch. 13.3	
Thurs	Apr 26	Reactions with Phase Equilibria	Ch. 13.4	#10
Tues	May 1	Ionization of Biochemicals & Ligand Binding	Ch. 15.1-15.4	
Thurs	May 3	Biochemical Reactions & Biological Osmotic Equilibrium	Ch. 15.5 &15.6	#11
Tues	May 8	No Class (*Travel to U. Illinois-UC*)		
Thurs	May 10	Introduction to Molecular Thermodynamics	Notes	
Mon	May 14	**FINAL EXAM, 8:00-10:00am (tentative)**	All course material	