ECH 4123 Phase and Chemical Equilibria
Summer 2019

Instructor: Spyros A. Svoronos

Office Phone: 352-392-9101 (preferred over e-mail)
Home Phone: 352-378-1342 (only way to reach me during weekends)
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E-mails must include a call-back phone number. Without it, they may not receive a response.

Office: 264 Chemical Engineering Student Center
Office Hours: Tuesdays, 3:00 - 5:00 PM, Thursdays 1:15 - 3:15 PM
- In addition, I have an open door policy, but I am not available 45 minutes before class time or mornings

Teaching Assistant or Grader: None

Course Objectives:
- To teach the concepts of thermodynamic phase and chemical equilibria.
- To teach how to evaluate chemical potentials and fugacities in pure components and mixtures.
- To apply thermodynamic phase and chemical equilibrium theory to liquid-liquid, vapor-liquid, and solid-liquid systems.
- To effectively utilize the thermodynamic packages of software such as UniSim

Impact on Program Objectives:

This course will significantly contribute in achieving B.S. program objectives a, e, and k (see https://www.che.ufl.edu/accreditation/)

Course Topics:

1. Class introduction, notation, review of energy balances, introduction to UniSim.
2. Review of entropy balances.
3. Review of thermodynamic state variables and their differentials for closed and open systems.
4. Review of Maxwell relationships and expressions for the dependence of state variables on temperature, pressure, and volume. Departure functions
5. Review of equations of state and the principle of corresponding states
6. Criteria for equilibrium of single component systems
7. Fugacity
8. Phase transitions and the Antoine equation (and others)
9. UniSim modeling of phase transitions
10. Calculation of vapor pressure for cubic equation models and coding for it
11. Thermodynamic properties of small systems
12. Multicomponent systems and partial molar quantities
13. Experimental determination of partial molar enthalpy and volume. UniSim simulation
14. Criteria for equilibrium of multiple component systems without reactions
15. Criteria for equilibrium of multiple component systems with reactions
16. Gibbs phase rule
17. Ideal gas mixtures
18. Ideal mixtures and excess properties
19. Activity coefficients and calculations for phase equilibria
20. Activity coefficient models and creation of $T_{xy}$ and $P_{xy}$ diagrams using Excel and regression
21. Creation of $T_{xy}$ and $P_{xy}$ diagrams using UniSim
22. Chemical reaction equilibria
23. Reaction standard enthalpies and Gibbs free energies

**Required Text:**

*Chemical, Biochemical, and Engineering Thermodynamics.* By Stanley I. Sandler, edition used in ECH3101

**Recommended Additional Text:**

*Essential Thermodynamics* by Panagiotopoulos, Drios Press

**Computer:** Laptop computer running Windows and Excel is **required**

**Course Assessment:**

- Homework 10%
- Class Participation 10%
- Paper Exam 1, **Friday June 21,** 7:00-? 30%
- Software Exam, **Friday August 2,** 7:00-? 20%
- Paper Exam 2, **Friday August 9,** 7:00-? 30%

**Detailed Explanation of Grading:**

1. For each student, Overall Points are calculated as follows:

   \[
   \text{Overall Points} = 0.30 \times \text{Paper Exam 1 Grade} + 0.20 \times \text{Software Exam Grade} + 0.30 \times \text{Paper Exam 1 Grade} + 0.10 \times \text{Homework Grade} + 0.10 \times \text{Class Participation Grade}
   \]

   where
   - Exam grades are 0-100
   - HomeworkGrade = \((\text{Total homework points earned})/(\text{maximum possible points})\) *100
   - Class participation grade:
     - 88 if student never misses class (without excuse) and never speaks. This number is multiplied by my estimate of the fraction of times the student was present in class.
Then the grade is raised according to how frequently a student answers or asks questions. Corrections of my lecture errors are especially noted. However, if a student is engaged in obvious non-class activity (reading paper, having laptops on when lecture is not involving computer, etc), that student is considered absent. If you are using your laptops for taking class notes, you are encouraged to notify me of that (I may sometimes ask you to see your notes after a class).

2. The students are sorted in the order of decreasing overall points. Grades are then decided as follows:

Division between A and A- : Largest gap between two students with $90 \geq$ overall points $> 85$
Division between A- and B+ : Largest gap between two students with $85 \geq$ overall points $> 80$
Division between B+ and B : Largest gap between two students with $80 \geq$ overall points $> 75$
Division between B and B- : Largest gap between two students with $70 \geq$ overall points $> 65$
Division between B- and C+ : Largest gap between two students with $65 \geq$ overall points $> 60$
Division between C+ and C : Largest gap between two students with $60 \geq$ overall points $> 55$
Division between C and C- : overall points $\geq 50$ (no gap here, 50 is C, 49.9 C-)
Division between C- and D+ : Largest gap between two students with $40 \geq$ overall points $> 35$
Division between D+ and D : Largest gap between two students with $30 \geq$ overall points $> 25$
Division between D and D- : Largest gap between two students with $5 \geq$ overall points $> 0$

E: Given to students for honesty violations

The class participation grade is designed so that a student who attends class regularly will not have an A grade lowered even if s/he never speaks. It helps attending students with lower overall points.

Other:

Do not hesitate to ask questions both in class and outside class.
ADDITIONAL INFORMATION

Students Requiring Accommodations

Students with disabilities requesting accommodations should first register with the Disability Resource Center (352-392-8565, https://www.dso.ufl.edu/drc) by providing appropriate documentation. Once registered, students will receive an accommodation letter which must be presented to the instructor when requesting accommodation. Students with disabilities should follow this procedure as early as possible in the semester.

Course Evaluation

Students are expected to provide feedback on the quality of instruction in this course by completing online evaluations at https://evaluations.ufl.edu/evals. Evaluations are typically open during the last two or three weeks of the semester, but students will be given specific times when they are open. Summary results of these assessments are available to students at https://evaluations.ufl.edu/results/.

University Honesty Policy

UF students are bound by The Honor Pledge which states, “We, the members of the University of Florida community, pledge to hold ourselves and our peers to the highest standards of honor and integrity by abiding by the Honor Code. On all work submitted for credit by students at the University of Florida, the following pledge is either required or implied: “On my honor, I have neither given nor received unauthorized aid in doing this assignment.” The Honor Code (https://www.dso.ufl.edu/sscr/process/student-conduct-honor-code/) specifies a number of behaviors that are in violation of this code and the possible sanctions. Furthermore, you are obligated to report any condition that facilitates academic misconduct to appropriate personnel. If you have any questions or concerns, please consult with the instructor or TAs in this class.
**Campus Resources:**

**Health and Wellness**

**U Matter, We Care:**
If you or a friend is in distress, please contact umatter@ufl.edu or 352 392-1575 so that a team member can reach out to the student.

**Counseling and Wellness Center:** [http://www.counseling.ufl.edu/cwc](http://www.counseling.ufl.edu/cwc), and 392-1575; and the University Police Department: 392-1111 or 9-1-1 for emergencies.

**Sexual Assault Recovery Services (SARS)**
Student Health Care Center, 392-1161.

**University Police Department** at 392-1111 (or 9-1-1 for emergencies), or [http://www.police.ufl.edu/](http://www.police.ufl.edu/).

**Academic Resources**

**E-learning technical support**, 352-392-4357 (select option 2) or e-mail to Learning-support@ufl.edu. [https://lss.at.ufl.edu/help.shtml](https://lss.at.ufl.edu/help.shtml).

**Career Resource Center**, Reitz Union, 392-1601. Career assistance and counseling. [https://www.crc.ufl.edu/](https://www.crc.ufl.edu/).

**Library Support**, [http://cms.uflib.ufl.edu/ask](http://cms.uflib.ufl.edu/ask). Various ways to receive assistance with respect to using the libraries or finding resources.

**Teaching Center**, Broward Hall, 392-2010 or 392-6420. General study skills and tutoring. [https://teachingcenter.ufl.edu/](https://teachingcenter.ufl.edu/).

**Writing Studio, 302 Tigert Hall**, 846-1138. Help brainstorming, formatting, and writing papers. [https://writing.ufl.edu/writing-studio/](https://writing.ufl.edu/writing-studio/).

**Student Complaints Campus:**