CHEE 311 Thermodynamics II
Fluid Phase & Reaction Equilibria
FALL 2010

Website: http://chemeng.queensu.ca/courses/CHEE311/

Instructor: Dr. Aris Docoslis
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Teaching Assistants:

Teaching Assistant	E-mail	Location	Office Hours
Nakkiran Arulmozhi	Nakkiran.arulmozhi@chee.queensu.ca	Computer Cluster	TBA
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Textbook (required): Introduction to Chemical Engineering Thermodynamics 7th edition, Smith, Van Ness, and Abbott.

Course Description: The course is concerned with thermodynamic theory and applications to problems in phase and chemical reaction equilibria. Emphasis is placed on the study of non-ideal solutions and reaction equilibria that relate to separations and reaction engineering. The material builds on concepts introduced in CHEE 244, CHEE 221 and CHEE 222.

Timetable

Lectures: Kingston Hall 201	Monday	10:30 - 11:20
	Wednesday	13:30 - 14:20
	Friday	12:30 - 13:20
Tutorials:		
Group **B**: Dupuis Hall 217	Tuesday	16:30pm - 17:20pm
Group **A**: Dupuis Hall 215	Friday	10:30am - 11:20am

Evaluation:

Assignments	20%	Two assignments (students will work in groups of 3)
Mid term test	30%	Thursday, October 21st, 17:30 to 19:30 (tentative)
Final exam	50%	TBA

- Calculators, lecture notes and the course textbook are allowed in examination sessions. Problems and answers other than those presented in lectures are not allowed
- In accordance with the Departmental Policies governing Undergraduate Courses:
  - You must pass (>50%) all individual examination components (midterm, final) to pass the course

- No make-up midterms will be provided. Only students who miss the midterm exam due to a very important reason (e.g., course conflicts, serious illness, varsity games) can request that the weight of the midterm be transferred to the final exam. In those cases, an official note by a course instructor (doctor, or trainer, respectively) must accompany the request
- The complete set of policies can be found on our department's web site: http://chemeng.queensu.ca/PDF/DepartmentalUndergradProgramPolicies.pdf

Problem Sets, Tutorials and the Role of Teaching Assistants:

- Students will be assigned tutorial problems on a weekly basis and practice problems biweekly. The solutions to the practice problems will be posted two weeks later. A total of two marked homework assignments will be distributed at regular intervals.
- New practice problem sets, solutions to the old ones, and past tutorial problems will be posted on the web site every Friday evening. Only abbreviated versions of the solutions to the tutorial problems will be posted. You are strongly encouraged to attend the tutorial classes.
- The course instructor and TAs can provide individual assistance during scheduled office hours (or by appointment)

Communication:

Announcements will be posted on the CHEE 311 website, so please check the page frequently for information such as assigned problems, examination dates, schedule changes and special tutorials. Important announcements will also be made in class.

Learning Objectives:

At the end of the course, you will be able to:

- Explain the following abstract concepts: Entropy, Enthalpy, Chemical Potential, Fugacity, Activity Coefficients, Ideal Solution, Ideal Gas, Partial Molar Properties, Infinite Dilution, Residual Properties, Excess Properties, Equations of State, Extent of Reaction and stoichiometric number, and describe how they are used.
- Perform iterative bubble point, dew point and flash calculations for both ideal and non-ideal vapour-liquid systems at equilibrium.
- Judge when it is reasonable to make ideal gas and ideal solution assumptions in order to simplify vapour-liquid equilibrium calculations.
- Apply Gibb's Phase Rule to analyze degrees of freedom in multi-component, multi-phase systems.
- Construct P-x-y and T-x-y phase diagrams using activity coefficient correlations, and perform vapour-liquid equilibrium calculations using phase diagrams.
- Determine Margules and Van Laar parameters from experimental data, and calculate activity coefficients using Margules, Van Laar and Wilson methods.
- Use Henry's Law to perform vapour-liquid equilibrium calculations for dilute systems.
- Use equations of state for vapour-liquid equilibrium calculations.
- Calculate equilibrium constants for chemical reactions.
- Derive and solve reaction equilibrium expressions for liquid-phase, gas-phase and multi-phase reactions to determine how far a chemical reaction will proceed before equilibrium is reached.
- Determine the equilibrium point for systems involving multiple reactions.
- Apply Gibb's Phase Rule for degrees of freedom analysis when chemical reactions are involved.

Course Outline:

1. Phase Behaviour
- Phase Diagrams for Single and Multi-Component Systems
- Dew/Bubble Point Calculations - Graphical and Raoult's Law
- P,T-flash calculations

2. The Fundamental Equation for Closed Systems
- $dU = dq + dw = TdS - PdV$
- Auxiliary equations in terms of H, A,G

3. Chemical Potential and Equilibrium Criteria
- Equilibrium in terms of Gibbs energy
- Definition of Chemical Potential, μ_i
- Chemical Potential and Equilibrium

4. Development of μ_i for Ideal Systems
- Ideal Gas Mixtures
- Ideal Solutions
- Origin of Raoult's Law and the Phase Rule

5. Non-ideality in 1-component Systems
- Equations of State
- Fugacity of pure gases and liquids
- Residual properties

6. Non-ideality in Mixtures (of non-ideal components)
- Fugacity of components in mixtures
- Lewis-Randall rule
- Activity coefficients
- Excess properties

7. Thermodynamic Data for Non-Ideal Systems
- Using experimental VLE data for f_i, γ_i
- Activity coefficient models
- Property changes of mixing

8. Non-Ideal VLE at Low Pressures
- f_i, γ_i formulation of VLE problems
- Dew point, Bubble point calculations for non-ideal systems
- P,T-flash calculations
- Azeotropes
- Dilute Solution Approximations
- Solute/Solvent Systems

9. Phase Stability and Other Equilibria
- Stability Criteria for a Phase
- LLE, VLLE, SLE

10. Chemical Reaction Equilibria
- Reaction coordinate
- Equilibrium constant
- Single and multi-reaction equilibria