CHE 3110B

**CHEMICAL ENGINEERING THERMODYNAMICS II**

**Fall Semester 2012**

**Lecture:** 11:05-11:55 MWF, Room L1205 ES&T Building

**Text:** Introduction to Chemical Engineering Thermodynamics

Seventh Edition,

by J. M Smith, H. C. Van Ness and M. M. Abbott

McGraw Hill Company

**Instructor:** Dr. S. A. Bidstrup Allen

Room 1370, ES&T Building (inside ChBE Main Office)

x4-2872

Room 308, Tech Tower (inside CoE Main Office)

X5-5053

sue.allen@chbe.gatech.edu

**Office Hours:** Tuesdays 1:00-2:00

Thursdays 2:30-3:30

(or by appointment)

**Homework:** Homework will not be accepted late. All assignments are due at the beginning of the lecture period. Homework solutions will be posted on T-Square.

**Exams:** There will be three in-class exams and a final exam. The exams will be open textbook, but closed note. The final exam is scheduled for Monday, December 12 from 8:00-10:50 AM.

**Course Grade:** Homework/Pop Quizzes 10%

First Hour Exam 20%

Second Hour Exam 20%

Third Hour Exam 20%

Final Exam 30%

**Teaching Assistants:** John Copeland:

Office: IPST 425c

Office Phone: 404-894-9702

Office Hours:

Email: [jcopeland8@gatech.edu](mailto:jcopeland8@gatech.edu)

**Course Objectives:**

This course introduces the basic thermodynamic concepts of multiphase equilibrium inpure and multi-component systems. Starting with ideal gas mixtures and ideal solutions,the concepts of bubble and dew points are introduced to enable flash calculations and design of process components. Subsequently, various levels of non-ideality and complexity are introduced: 1) activity coefficient models for non-ideal liquid mixtures, 2) fugacity calculations of gas and liquid phases from equations-of-state, 3) systems with chemical reactions. The course provides fundamental insight into the underlying thermodynamic principles, as well as practice with advanced computational techniques to solve complex problems.

**Learning Outcomes:**

By the end of this course, a student will be able to:

1. Understand the origin of chemical potential and its analog, fugacity
2. Understand the molecular basis for ideal mixtures and calculate phase compositions at equilibrium by relating chemical potential or fugacity to composition. Also apply in calculating boiling point elevation, osmotic pressure and other colligative properties.
3. Determine the fugacity of a pure component gas at non-ideal gas behavior (fugacity coefficient) and the fugacity of a pure component liquid or solid under high pressure
4. Understand partial molar properties of components in a particular phase, and apply to calculations of heat of mixing, volume, and entropy changes on processing of ideal and real mixtures.
5. Calculate phase compositions for real mixtures at equilibrium based on EOS for the gas phase, and activity coefficient models for non-ideal behavior. Understand the molecular interaction theory behind the models.
6. Apply the above tools to equilibrium separations, for example, flash distillation and batch distillation.
7. Understand when phase equilibrium calculations require use of an EOS applicable to all phases, and perform such calculations using computer software.
8. Determine the equilibrium composition of single and multi-phase reaction mixtures. Determine activity of a component in the reaction mixture and know how to determine it in solid, gas, and liquid phases.
9. Determine the effects on reaction equilibrium composition of temperature, pressure, diluents, mole ratio of reactants and other variables, and determine the heat requirements to reach equilibrium.
10. Calculate the activity of electrolytes in solutions. Apply Debye-Huckel to calculate mean ionic activity coefficients.
11. Understand the effect of surface energy on vapor-liquid equilibrium.

**ChE 3110:**

**Chemical Engineering Thermodynamics II Syllabus**

**Fall 2012**

**Textbook**

**Date Lecture Reading**

Mon. Aug. 20 Course Objectives, Summary from Thermo I Chapters 1-9

Wed. Aug. 22 Review from Thermo I Chapters 1-9

Fri. Aug. 24 Equilibrium Potential, Chemical Potential p.378-385

Mon. Aug. 27 Chemical Potential, Mixture of Ideal Gases p.391-394

Wed. Aug 29 Fugacity Concept p.394-401

Fri. Aug 31 Ideal Gas and Liquid Mixtures p. 411-413

Mon. Sept 3 Labor Day Holiday

Wed. Sept. 5\* Calculation of Fugacity from 2nd Virial Coefficient p. 401-407

Fri. Sept 7 Calculation of Fugacity from Generalized Correlations p. 407-411

Mon. Sept. 9 Simple Models for Vapor-Liquid Equilibrium p. 347-358

Wed. Sept. 12 Raoult’s and Henry’s Law p. 350-363

Fri. Sept. 14 VLE Calculations using K-Values; Flash Distillation p. 363-370

Mon. Sept. 17 Phase Rule, Qualitative VLE Behavior p. 338-347

Wed. Sept. 19 Partial Molar Properties/Gibbs-Duhem Equation p. 383-391,411-413

Fri. Sept. 21 Review for Exam 1

Mon. Sept. 24\* Exam 1

Wed. Sept. 26 Exam Review, Real Liquid Mixtures, Excess Properties p. 413-420

Fri. Sept. 28 Real Liquid Mixtures, Excess Properties p. 413-420

Mon. Oct. 1\* Activity Coefficients p. 430-435

Wed. Oct. 3\* Activity Coefficient Models p. 435-449

Fri. Oct. 5 Activity Coefficient Models, Calculation of VLE from EOS p. 556-563

Mon. Oct. 8 Calculation of VLE from Cubic Equations of State p. 556-563

Wed. Oct 10 Colligative Properties of Mixtures: Freezing Pt. Depression, Boiling notes

Elevation and Osmotic Pressure

Fri. Oct. 12 Problem Review

Mon. Oct. 15 Fall Break

Wed. Oct. 17 Liquid-Liquid Equilibrium p. 581-589

Fri. Oct. 19 Vapor Liquid Liquid Equilibrium p. 590-597

Mon. Oct. 22 Solid-Liquid Equilibiurm, Solid-Vapor Equilibrium p. 597-605

Wed. Oct. 24 Property Changes of Mixing p. 449-455

Fri. Oct. 26 Heat Effects of Mixing p. 456-469

Mon. Oct. 29\* Review

Wed. Oct. 31\* Exam II

Fri. Nov. 2\* Molecular Theory of Fluids p. 647-654

Mon. Nov. 5 Chemical Reaction Stoichiometry, Extent of Reaction p. 483-488

Wed. Nov. 7 Reaction Equilibrium Criteria, The Equilibrium Constant p. 488-498

Fri. Nov. 9 Reaction Equilibrium Criteria, The Equilibrium Constant p. 488-498

Mon. Nov. 12 Gas Phase Reactions p. 498-510

Wed. Nov. 14 Liquid Phase Reactions p. 498-510

Fri. Nov. 16 Multiphase Reaction Equilibrium p. 510-514

Mon. Nov. 19 Phase Rule, Multi-reaction Equilibria p. 514-528

Wed. Nov. 21 Multireaction Equilibria p. 518-528

Fri. Nov. 23 Thanksgiving Holiday

Mon. Nov. 26 Review p. 483-528

Wed. Nov. 27 Exam III p. 483-528

Fri. Nov. 29 Molecular Thermodynamics p. 657-673

Mon. Dec. 3 Applications TBA

Wed. Dec. 5 Applications TBA

Fri. Dec. 7 Review

Wed. Dec. 12 (8:00-10:50am) Final Exam