

ChBE 3130 Chemical Engineering Thermodynamics II (required course)

Note: This course was previously numbered 3110

Credit: 3-0-3

Instructor: Carson Meredith

Textbook: *Introduction to Chemical Engineering Thermodynamics*, Seventh Ed., by Smith, Van Ness, and Abbott, McGraw Hill, ISBN: 0-07-310445-0.

Catalog Description: Phase and chemical reaction equilibria. Vapor-liquid, liquid-liquid, and solid-vapor phase equilibrium. Fugacity and activity coefficients. Multi-reaction equilibrium.

Prerequisites: Chemical Process Principles (ChBE 2100), Numerical Methods (ChBE 2120), and Chemical Engineering Thermodynamics I (ChBE 2130), minimum grade of "C" in each course.

Learning Outcomes: By the end of this course, a student should be able to:

1. Understand the origin of chemical potential and fugacity (Student outcomes a, e)
2. Understand the molecular basis for ideal mixtures and calculate equilibrium phase compositions by relating chemical potential of fugacity to composition. Also apply in calculating boiling point elevation, osmotic pressure and other colligative properties. (Student outcomes a, b, e, k)
3. Determine the fugacity of a pure component non-ideal gas and of pure liquids and solids under high pressure. (Student outcomes a, e)
4. Understand partial molar properties of components in a particular phase and apply to calculations of the heat of mixing, volume, and entropy changes on processing of ideal and real mixtures. (Student outcomes a, e)
5. Calculate phase compositions for real mixtures at equilibrium based on EOS for gas phases, and activity coefficient models for non-ideal liquid or solid behavior. Understand the molecular interaction theory behind common models. (Student outcomes a, b, e, k)
6. Apply the above tools to equilibrium separations including flash distillation and batch distillation. (Student outcomes a, c, k)
7. Understand when phase equilibrium calculations require use of an EOS applicable to all phases, and perform such calculations using computer software. (Student outcomes a, b, c, e, k)
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. (Student outcomes a, c, e)
9. Determine the effects on reaction equilibrium composition of temperature, pressure, diluents, mole ratios of reactants, and other variables, and determine the heat requirements to reach equilibrium. (Student outcomes a, b, c, e, k)

10. Calculate the activity of electrolytes in solution. Apply Debye-Huckel theory to calculate mean ionic activity coefficients. (Student outcomes a, e)
11. Understand the effect of surface energy on vapor-liquid equilibrium. (Student outcomes a, e)

Topical Outline

1. Pure-component multi-phase systems
 - a. VLE and saturation pressure
 - b. chemical potential, fugacity and fugacity coefficient
2. Ideal multi-component systems
 - a. chemical potential, fugacity and fugacity coefficient
 - b. Ideal solutions and gas mixtures, VLE
 - c. Raoult's law, phase-diagrams
 - d. Flash drum calculations
3. Non-ideal multi-component systems
 - a. EOS calculations of fugacity and chemical potential
 - b. VLE calculations from EOS
 - c. Activity models for non-ideal liquid mixtures, modified Raoult's law
 - d. Excess Gibbs free energy: relating models to experimental data
 - e. LLE, SLE, and VLLE calculations
4. Molecular thermodynamics
 - a. Association and solvation
 - b. Equilibrium criteria on molecular level
 - c. Ideal chemical theory
5. Reacting systems
 - a. Reaction coordinates and equilibrium for ideal solutions
 - b. Pressure and temperature effects
 - c. Electrolyte thermodynamics
6. Special topics
 - a. Electrochemistry
 - b. Thermodynamics of biomacromolecules or polymers
 - c. Surface thermodynamics

Prepared by: Carson Meredith

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