ChBE 6100
Advanced Chemical Engineering Thermodynamics

Credit: 3

Suggested Prerequisites:

- Chemical Engineering Thermodynamics I and II
- ordinary differential equations
- undergraduate organic and physical chemistry.

Recommended Textbooks:

- "Molecular Thermodynamics of Fluid-Phase Equilibria" (3rd Edition) John M. Prausnitz, Rudiger N. Lichtenthaler, Edmundo Gomes de Azevedo, Prentice-Hall (1999)

- "An Introduction to Applied Statistical Thermodynamics" Stanley I. Sandler, Wiley (2011)

Course Objectives:

Efficient separation operations and many other chemical processes depend on a thorough understanding of the properties of gaseous and liquid mixtures. This course will interpret, correlate, and predict thermodynamic properties used in mixture-related phase-equilibrium calculations. Basic statistical mechanical principles and intermolecular forces will be discussed, and applied to the correlation and prediction of thermodynamic properties and phase equilibria. Statistical thermodynamics will be shown to work with classical thermodynamics, molecular physics, and physical chemistry to solve real-world problems.

Learning Outcomes:

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

1. Apply chemical engineering thermodynamics to a variety of systems and problems, including phase and reaction equilibrium.
2. Use theoretical concepts to describe and interpret solution properties.

3. Understand the lattice-fluid and statistical associated-fluid theories, and apply these theories to polymers.
4. Apply statistical thermodynamics and molecular simulation to chemical engineering reaction systems.

Representative Topics

1. Review of undergraduate Thermodynamics: Property relationships, phase equilibria, intermolecular forces, corresponding states theory
2. Statistical thermodynamics and the partition function
    a. The partition function for ideal gases
    b. Statistical thermodynamics of mixtures
    c. Chemical equilibrium via the partition function
3. Molecular thermodynamics of real fluids
    a. Departure functions
    b. Gas phase fugacities
    c. Liquid phase fugacities
4. Theories of Solution
    a. Lattice Theory
    b. Cell Models
    c. van der Waals type models
    d. Radial Distribution Function
5. Applications
    a. Vapor-liquid equilibria
    b. Gas solubility and environmental applications
    c. Liquid-liquid and Solid-liquid equilibria
    d. Equilibria involving polymer solutions and biological molecules
    e. High pressure equilibria, supercritical fluids
6. Separation Processes
    a. Distillation
    b. Extraction
    c. Absorption
    d. Adsorption
    e. Crystallization
7. Reaction Processes
    a. Equilibria
    b. Transition State Theory