Chemical Engineering Thermodynamics - Course Outline and suggested reading for 6th edition of Smith, Van Ness and Abbott

I. Introduction to Course

II. Properties of Pure Substances and Constant Composition Fluids

A. PVT Properties of Pure Substances (3.1 - 3.6)

1. Review of Phase Diagram
2. Representation by Equations of State
   a. Ideal Gas Law
   b. Virial Equation
   c. Cubic Equations (e.g. van der Waals)
   d. Other Equations of State
   e. Principle of Corresponding States

B. Other Thermodynamic Properties (6.1)

1. Development of Equations for Changes in H, U and S
   a. The Fundamental Property Relation
   b. Definitions of Convenience Functions
   c. Property Relations, Total Differentials, and Maxwell Relations
   d. Definition of the Heat Capacities
   e. Final *General* Equations for dS, dH and dU
2. Changes in H, U and S for *Ideal* Gases (6.1)
3. Changes in H, U and S for *Nonideal* Gases (6.2, 6.3)
   a. Definition of Residual Properties
   b. Evaluation of Residual Properties Using an Equation of State
   c. Evaluation of Residual Properties Using Corresponding States

C. Phase Equilibria of a Pure Substance (6.4)

1. Criteria of Equilibrium
2. Practical Aspects
   a. Clapeyron Equation
   b. Clausius-Clapeyron Equation
   c. Vapor Pressure Equations

D. Fugacity of a Pure Substance (11.5, 11.7)

1. Definition and Motivation for its Use
2. Fugacity as a Criterion of Phase Equilibrium
3. Evaluation of Fugacity
   a. From an Equation of State
   b. Using Corresponding States
   c. Approximations for Compressed Liquids
4. Use of Fugacity to Calculate Saturation Properties of a Pure Substance (14.2 - pure species only)

III. Thermodynamics of Solutions

A. Partial Molar Properties (11.3)

1. Definition
2. Physical Importance

B. Property Relations for Mixtures - Part I

1. Fundamental Property Relation for Open Systems (11.1)
   a. Definition of Chemical Potential
   b. Relation between $_i$ and Partial Molar G
   c. Temperature and Pressure Dependence of $_i$
2. Fugacity of a Component in a Mixture (11.6)
3. Criteria of Phase Equilibrium for Mixtures (11.2)

C. Ideal Solutions (11.8)

1. The Ideal (Lewis-Randall) Solution
   a. Definition
   b. Consequences
2. Vapor-Liquid Equilibria (VLE) for Ideal Solns (Class Notes, 10.4)
   a. Low Pressure
   b. Moderate to High Pressure
   c. Typical Calculations
   d. Phase Diagrams for Ideal Systems

D. Property Relations for Mixtures - Part II

1. Component Fugacities from an Equation of State (11.6)
2. Equations of State for Mixtures (11.4, 11.7, 14.2)
   a. Ideal Gas
   b. Virial Equation
   c. Cubic Equations
3. Component Fugacities from Excess Functions (11.9)
   a. Definition of the Activity Coefficient
   b. Definition of Excess Properties
   c. Relation between Activity Coefficient and Excess Gibbs Free Energy
   d. Temperature, Pressure and Mole Dependence of the Excess Gibbs Free Energy
4. Two Methods for Performing VLE Calculations
   a. The Equation of State Approach
   b. The Gamma-Phi Approach

E. Vapor-Liquid Equilibrium by the Gamma-Phi Method (12.1, 12.2, 10.5, 14.1)

1. Review of Various Approximations in Gamma-Phi Method
2. Obtaining Activity Coeficients from Experimental Data
3. Correlation of Activity Coefficients - Binary Systems
   a. Method
   b. Composition Dependence
      i. Boundary Conditions
      ii. Historical Models
      iii. Local Composition Models
   c. Activity Coefficients from Infinite Dilution Data
4. Phase Diagrams for Nonideal Mixtures - Azeotropy
5. Activity Coefficients for Multicomponent Systems
6. Thermodynamic Consistency and the Gibbs-Duhem Equation
   a. The Area Test for Isothermal VLE Data

F. Vapor-Liquid Equilibrium by the Equation of State Approach

1. Qualitative Aspects of VLE at Elevated Pressure (10.3)
2. Analysis of Equations and Unknowns (14.2)

G. Flash Calculations (10.6)

1. Mass Balances and Phase Equilibria Relationships
2. Evaluation of the K-Factors

H. Property Changes on Mixing (12.3, 12.4)

1. Definition of Property Change on Mixing
2. Heat Effects

I. Chemical Reaction Equilibria (13.1-13.9,15.9,4.3,4.4,4.6)

1. Criteria of Equilibrium and Reaction Stoichiometry
2. Definition of the Equilibrium Constant
   a. Typical Standard States
3. Solving for Equilibrium Compositions of Single Reactions in One Phase
4. Temperature Dependence of the Equilibrium Constant
5. Heterogeneous Reactions
   a. Each Reactant or Product in a Single Phase
   b. Each Reactant or Product in Every Phase
6. Multiple Chemical Reactions
   a. Theory
   b. Choosing a Set of Independent Reactions
   c. Solution Strategies