ADVANCED CHEMICAL ENGINEERING THERMODYNAMICS

Course Code: 15CH2102

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Prerequisites: The student should have a basic knowledge of phase and solution thermodynamics.

Course outcomes: On successful completion of the course, the student should be able to

CO1: Formulate phase equilibria for single and multicomponent mixtures.

CO2: Derive the relations for thermodynamic properties to evaluate fugacity of a component in a mixture using van der Waals equation of state.

CO3: Use Virial equation of state to calculate the fugacities in gas mixtures

CO4: Discuss and apply models and theories of solutions to evaluate activity coefficients in liquid mixtures.

CO5: Discuss the effect of pressure, temperature, on gas solubility and recognize the suitable model to estimate the gas solubility.

UNIT-I (10-Lectures)

Classical Thermodynamics of Phase Equilibria:

Homogeneous Closed Systems, Homogeneous Open Systems, Equilibrium in a Heterogeneous Closed System, The Gibbs-Duhem Equation, The Phase Rule, The Chemical Potential, Fugacity and Activity, A Simple Application: Raoult’s Law

Thermodynamics Properties from Volumetric Data:

Thermodynamic Properties with Independent Variables P and T, Fugacity of a Component in a Mixture at Moderate Pressures, Fugacity of a Pure Liquid or Solid, Thermodynamic Properties with Independent

Variables V and T, Fugacity of a Component in a Mixture according to vander Waals' Equation, Phase Equilibria from Volumetric Properties, References, Problems.

UNIT-II (10-Lectures)

Fugacities in Gas Mixtures:

The Lewis Fugacity Rule, The Virial Equation of State, Extension to Mixtures, Fugacites from the Virial Equation, Calculation of Virial Coefficients from Potential Functions, virial Coefficients from Corresponding-States Correlations, The 'Chemical" Interpretation of Deviations from Gas-Phase Ideality, Strong Dimerization: Carboxylic Acids, Weak Dimerization and Second Virial Coefficients, Fugacities at High Denstites, Solubilities of Solids and Liquids in Compressed Gases.

UNIT-III (10-Lectures)

Fugacities in Liquid Mixtures: Excess Functions:

The Ideal Solution, Fundamental Relations of Excess Functions, Activity and Activity Coefficients, Normalization of Activity Coefficients, Activity Coefficients from Excess Functions in Binary Mixtures, Activity Coefficients for One Component from those of the Other components, Partial Pressures from Isothermal Total-Pressure Data, Testing Equilibrium Data for Thermodynamic Consistency, Wohl's Expansion for the Excess Gibbs Energy, Wilson, NRTL, and UNIQUAC Equations, Excess Functions and Partial Miscibility, Upper and Lower Consulate Temperatures.

UNIT-IV (10-Lectures)

Fugacities in Liquid Mixtures: Models and Theories of Solutions

The Theory of van Laar, The Scatchard-Hildebrand Theory, Excess Functions From an Equation of State, the lattice Model, Activity Coefficients from Group-Contribution Methods, Chemical Theory, Activity Coefficients in Associated Solutions, Associated Solutions With Physical Interactions, Activity coefficients in solvated solutions, Solutions Containing Two(or More) Complexes, Distribution of a Solute between Two Immiscible Solvents.

UNIT-V (10-Lectures)

Solubilities of Gases in Liquids:

The Ideal Solubility of a Gas, Henry's Law and Its Thermodynamic Significance, Effect of Pressure on Gas Solubility, Effect of Temperature on Gas Solubility, Estimation of Gas Solubility, Gas Solubility in Mixed Solvents, Chemical Effects on Gas Solubility

TEXT BOOK:

1. Prausnitz J.M, Lichtenthaler R.N, Edmundo Gomes de Azevedo *"Molecular Thermodynamics of Fluid Phase Equilibria",* 3rd Edition, Prentice Hall, New Jersey, 1998.

REFERENCE:

1. Sandler S.I, *"Chemical, Biochemical and Engineering Thermodynamics"*, 4th Edition, Wiley Student Edition, 2006.