CHEMICAL ENGINEERING THERMODYNAMICS-II

Course Code: 15CH1110

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Course Outcomes:

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

CO 1 Evaluate the heat effects that accompany physical and chemical operations.

CO 2 Apply Raoult's law and the cubic equations of state to perform vapor liquid equilibrium calculations.

CO 3 Develop the theoretical formulations for application of thermodynamics to gas mixtures and liquid solutions and formulate activity – coefficient correlations to predict vapor liquid equilibrium data.

CO 4 Identify phase equilibria in chemical engineering operations.

CO 5 Evaluate the extent of reaction, effect of temperature on equilibrium constant and equilibrium conversion for single reaction and multiple reactions.

UNIT-I (10 Lectures)

Heat effects: Sensible heat effects, Evaluation of sensible heat integral, Latent heats of pure substances, standard heat of reaction, standard heat of formation, standard heat of combustion, temperature dependence of heat of reaction, Heat effects of Industrial Reactions.

UNIT-II (10 Lectures)

VLE at low to moderate pressure, the nature of equilibrium, the phase rule, VLE qualitative behaviour, Dew point and Bubble point calculations using Raoult's law and Modified Raoult's law.

VLE from K-value correlation, flash calculations, Dew point & bubble point calculations and Flash calculations for non-ideal solutions (Algorithms and flow charts only)

Thermodynamic properties and VLE from equations of state: properties of fluids from the virial equations of state, VLE from Van der Waals equations of state.

UNIT-III (10 Lectures)

SOLUTION THERMODYNAMICS: THEORY

Fundamental property relation, chemical potential as a criterion for phase equilibrium, partial molar properties, ideal gas mixtures, fugacity and fugacity coefficient for pure species, fugacity and fugacity coefficient for species in solutions, generalized correlations for Fugacity coefficient, ideal solutions, excess properties.

SOLUTION THERMODYNAMICS: APPLICATIONS

Models for the excess Gibbs energy (Margules, Van Laar and Wilson models), calculating the two constants for Margules, Van Laar and Wilson models from experimental data. VLE estimations using Margules, Van Laar and Wilson equations.

Basics of UNIFAC model, NRTL model, UNIQUAC model (Qualitative treatment only).

UNIT-IV (10 Lectures)

Topics in phase Equilibria: Equilibrium and stability, liquid-liquid equilibrium (LLE), vapor- liquid–liquid equilibrium (VLLE), solid-liquid equilibrium (SLE), solid vapor equilibrium (SVE), equilibrium absorption of gases on solids (Qualitative treatment only)

UNIT-V (10 Lectures)

Chemical - Reaction Equilibria: The reaction coordinate, application of equilibrium criterion to chemical reactions, the standard Gibb's energy change and the equilibrium constant, effect of temperature on equilibrium constant, relation of equilibrium constant to composition, equilibrium conversion for single reaction, and multiple reactions, Phase rule for reacting systems.

TEXT BOOK:

1. Smith J.M. and Van Ness H.C, *"Introduction to Chemical Engineering Thermodynamics"*, 7th Edition, Tata McGraw Hill, 2009.

REFERENCES:

1. Rao Y.V. C., *"Chemical Engineering Thermodynamics"*, University Press Ltd., 2001.
2. Narayanan K. V., "Chemical Engineering Thermodynamics", PHI, 2000.
3. Kyle B.G., *"Chemical and Process Thermodynamics"*, 3rd Edition, Pearson, Prentice Hall, 1999.
4. Abbott M.M. and Van Ness H.C. *"Thermodynamics with chemical applications"*, 2nd Edition, Tata McGraw-Hill Publishing company Limited, 2005.