GUJARAT TECHNOLOGICAL UNIVERSITY

CHEMICAL ENGINEERING - 30

Advanced Chemical Engineering Thermodynamics (Elective – II)

SUBJECT CODE: 3713019

M.E. Semester: I

Type of course: Program specific Elective-II

Prerequisite: Introductory Chemical Engineering Thermodynamics (CET-I and CET-II)

Rationale:

Efficient separation operations and many other chemical processes depend on a thorough understanding of the properties of gaseous and liquid mixtures. This course is advanced, building upon prior courses in thermodynamics covered at graduate level. The goal of this course is to interpret, correlate, and predict thermodynamic properties used in mixture related phase-equilibrium and reaction equilibrium calculations. Solving phase equilibria problems involves general computational techniques that have widespread applications in chemical engineering.

Teaching and Examination Scheme:

Teaching Scheme			Credits	Examination Marks				Total Marks
				Theory Marks		Practical Marks		
Th	Tut	Lab	C	ESE(E)	PA (M)	ESE (V)	PA(I)	
3	0	2	4	70	30	30	20	150

Content:

Sr. No.	Content	Total Hrs	%Weightage
1	**Review of Chemical Engineering Thermodynamics** Introduction to Molecular Thermodynamics of Fluid Phase Equilibria, Basic Differences among Classical, Statistical and Molecular Thermodynamics, Fundamental Concepts of Statistical Thermodynamics, Classical Thermodynamics of Phase Equilibrium, Gibbs-Duhem Equation, Chemical Potential, Fugacity and Activity, Estimation of Physical Properties, Estimation Methods for Vapour-Liquid Critical Properties Tc, Pc and Vc	6	11
2	**Thermodynamics Properties from Volumetric Data** Fugacity of a Component in a Mixture at Moderate Pressures, Fugacity of a Pure Liquid or Solid, Thermodynamics Properties With Independent Variables V and T, Fugacity of a Component in a Mixture According to Van der Waals' Equation	6	11
3	**Fugacities in Gas Mixtures** The Virial Equation of State, Extension to Mixtures, Fugacities from the Virial Equation, Calculation of Second and Third Virial Coefficients	6	11
4	**Fugacities in Liquid Mixtures: Excess Functions** The Ideal Solution, Fundamental Relations of Excess Functions, Temperature and Pressure dependency of Activity Coefficients, Activity Coefficients from Excess Functions in Binary Mixtures, Testing Equilibrium Data for the Thermodynamic Consistency, Wohl's Expansion for the Gibbs Energy, Wilson NRTL and UNIQUAC Equations, Excess Functions and Partial Miscibility, Upper and Lower Consolute	21	39

	Temperatures, Excess Functions for Multicomponent Mixtures, Wilson, NRTL, and UNIQUAC Equations for Multicomponent Mixtures		
5	**Chemical reaction Equilibria** Review of Reaction Equilibrium Principle, Equilibrium Conversion, Calculation and Construction of Equilibrium Conversion Charts, Algorithmic Calculation of Equilibrium Conversion, Homogeneous and Heterogeneous reaction Systems, Phase Rule for Reacting Systems, Chemical Reaction Equilibria for Complex and Multiple Reactions, Lagrange's Undetermined Multiplier's Methods, Various Methods Computation of Equilibrium Composition of Complex Multiphase Systems	**15**	**28**

Reference Books:

1. J. M. Prausnitz, R. N. Litchtenthaler, E. G. de Azevedo, Molecular Thermodynamics of Fluid Phase Equilibria, 3rd Edition, Prentice Hall.
2. S. M. Walas, Phase Equilibria in Chemical Engineering, Butterworth .
3. J. M. Smith, H. C. VanNess, M. M. Abbott, Introduction to Chemical Engineering Thermodynamics, 7th Edition, McGraw-Hill.
4. Bruce E. Poling, John M. Prausnitz, John P. O'Connell, The Properties of Gases and Liquids, 5th Edition, McGraw-Hill.

Course Outcome:

After learning the course the students should be able to:

- Apply chemical engineering thermodynamics to a variety of systems and problems, including phase and reaction equilibrium.
- Use theoretical concepts to describe and interpret solution properties.
- Know how to qualitatively calculate the equilibrium properties of real liquid mixtures.
- Solve phase equilibria problems; this includes the ability to determine which of a variety of models best describes a given set of data, and to calculate the model parameters.

List of Open Source Software/learning website:

- Students can refer to video lectures available on the websites including NPTEL lecture series.
- Students can refer to the CDs available with some reference books for the solution of problems using softwares/spreadsheets. Students can develop their own programs/spreadsheets for the solution of problems.