GUJARAT TECHNOLOGICAL UNIVERSITY

Bachelor of Engineering
Subject Code: 3140507
Semester –IV
Subject Name: Chemical Engineering Thermodynamics-II

Type of course: Professional Core Course

Prerequisite: Chemical Engineering Thermodynamics-I

Rationale: This subject introduces the concepts of fugacity, activity coefficient and other important thermodynamic properties and its evolution for pure components and solutions. Starting with ideal gas mixtures and ideal solutions, the concepts of bubble and dew points are introduced to enable flash calculations and design of process components. Subsequently, various levels of non-ideality and complexity are introduced. The course also provides fundamental insight into the underlying thermodynamic principles of phase equilibria and reaction equilibria to solve complex problems.

Teaching and Examination Scheme:

Teaching Scheme			Credits	Examination Marks				Total Marks
L	T	P	C	Theory Marks		Practical Marks		
				ESE (E)	PA (M)	ESE (V)	PA (I)	
3	1	0	4	70	30	0	0	100

Content:

Sr. No.	Content	Total Hrs
1	**PHASE EQUILIBRIA:** **VAPOUR/LIQUID EQUILIBRIUM (VLE):** Introduction, The Nature of Equilibrium, The Phase Rule; Duhem's Theorem, VLE-Qualitative Behaviour, Azeotropic Mixtures, Retrograde condensation, Simple Models for Vapour/Liquid Equilibrium ,Raoult's Law, Dewpoint and Bubblepoint Calucations with Raoult's Law , Henry's law, VLE by Modified Raoult's Law, VLE from K-Value Correlations, Flash Calculations, The Gamma / Phi Formulation of VLE, An introduction to Equilibrium and stability, liquid- liquid equilibrium (LLE), solid-liquid equilibrium, Vapor-Liquid-liquid equilibrium (VLLE), Solid-Liquid equilibrium (SLE), Solid-Vapor equilibrium (SVE) etc..	15
2	**SOLUTION THERMODYNAMICS:** **THEORY** Fundamental Property Relation, The Chemical Potential as a Criterion for Phase Equilibria, Partial Properties, Equations Relating Molar and Partial Molar Properties , The Partial Molar Gibbs Energy and the Generalized Gibbs-Duhem Equation, Partial Properties in Binary Solutions, Relations among Partial Properties, The Ideal Gas Mixture model, The Partial Molar Gibbs Energy and Fugacity, Fugacity and Fugacity Coefficient: Pure Species and for Species in Solution ,The Ideal Solution Model , The Lewis/Randall	18

	Rule , Excess Properties , The Excess Gibbs energy and activity coefficient, nature of excess property **APPLICATIONS** Liquid-Phase Properties from VLE Data ,Composition Dependence of Liquid- Phase Fugacities for Species in a Binary Solution, Excess Gibbs Energy, Data Reduction, Thermodynamic Consistency by Integral or Area Test Method, Models for the Excess Gibbs Energy, Margules Equations, VanLaar Equations, Local Composition Models such as NRTL Equation, UNIQUAC Equation, UNIFAC Method	
3	**CHEMICAL REACTION EQUILIBRIA:** The reaction coordinates, Application of equilibrium criteria to chemical reactions, The standard Gibbs free energy change and the equilibrium constant, Effect temperature on equilibrium constant, Evaluation of the equilibrium constant, Relation of equilibrium constant to composition for gas phase and liquid phase reactions, calculation of equilibrium conversion for single reaction, The phase rule and Duhem's theorem for reacting systems, introduction to multi-reaction equilibria	12

Suggested Specification table with Marks (Theory):

Distribution of Theory Marks					
R Level	**U Level**	**A Level**	**N Level**	**E Level**	**C Level**
7	28	28	7	0	**0**

Legends: R: Remembrance; U: Understanding; A: Application, N: Analyze and E: Evaluate C: Create and above Levels (Revised Bloom's Taxonomy)

Reference Books:

1. Smith J.M, Van Ness H.C., Abbott M. M, "Introduction to Chemical Engineering Thermodynamics", the McGraw Hill Companies, Inc., USA, 7th Ed., 2005.
2. Elliot J. R. and Lira C.T., "Introductory Chemical Engineering Thermodynamics", Prentice Hall, 1999.
3. Hougen O.A., Watson K.M., and Ragatz R.A., "Chemical Process Principles Part,II" Thermodynamics, John Wiley 1970.
4. Perry's chemical engineers handbook, 7th edition, McGraw,Hill, USA, 2000.
5. K.V.Narayanan "A Text book of chemical Engineering thermodynamics", Prentice Hall of India
6. Stanley I. Sandler, "Chemical, Biochemical and Engineering Thermodynamics", Wiley India Pvt. Ltd., 4th ed., 2007.
7. B.G. Kyle,"Chemical Process Thermodynamics", 2nd Edn., Prentice Hall of India Pvt.Ltd., New Delhi, 2000.
8. J.M.Prausnitz, R.N. Litchtenthaler, Molecular thermodynamics of fluid phase Equilibria, 3rd Edition,Prentice Hall.
9. Stanley M. Walas, Phase-Equilibria in Chemical Engineering,Wiley India Private Limited

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Course Outcomes:

Students should be able to

Sr. No.	CO statement	Marks % weightage
CO-1	Explain fundamentals of Solution thermodynamics, phase equilibria and reaction equilibria.	10
CO-2	Apply fundamental property relations to find thermodynamic properties of solutions	15
CO-3	Calculate maximum extent of separation possible under prevailing operating conditions for various multiphase multi component systems	30
CO-4	Determine thermodynamic properties like fugacity, activity coefficients, constants of model equations etc.. for solutions	20
CO-5	Determine equilibrium conversions of reaction systems and its dependence on various operating parameters	25

List of Tutorials: Numericals/problems based on topics of each theme of content.

Major Equipment: None

List of Open Source Software/learning website:
1. Students can refer to video lectures available on the websites including NPTEL.
2. Students can refer to the CDs which are available with some reference books for the solution of problems using softwares. Students can develop their own programs for the solutions of problems.
3. XSEOS–an Open Software for Chemical Engineering Thermodynamics