GUJARAT TECHNOLOGICAL UNIVERSITY

Program Name: M.E. in Chemical Engineering
Level: Post Graduate Degree
Branch: Chemical Engineering
Course / Subject Code: ME01030021
Course / Subject Name: Advanced Chemical Engineering Thermodynamics

w.e.f. Academic Year:	A.Y. 2024-25
Semester:	1st Semester
Category of the Course:	PCC

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.

Course Outcome:

After Completion of the Course, Student will be able to:

No	Course Outcomes
01	Apply chemical engineering thermodynamics to a variety of systems and problems, including phase and reaction equilibrium.
02	Use theoretical concepts to describe and interpret solution properties.
03	Know how to qualitatively calculate the equilibrium properties of real liquid mixtures.
04	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.

Teaching and Examination Scheme:

Teaching Scheme (in Hours)			Total Credits L+T+(PR/2)	Assessment Pattern and Marks				Total Marks
				Theory		Tutorial/ Practical		
L	T	PR	C	ESE (E)	PA/ CA (M)	PA/CA(I)	ESE (V)	
3	0	2	4	70	30	20	30	150

Course Content:

Unit No.	Content	No. of Hours	%of 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, **Fundamental of Statistical thermodynamics** Combinatorial Analysis of statistical thermodynamics, Distinguishable and indistinguishable particles, ensemble method, microstates and macrostates, most probable macrostate, Postulates of statistical thermodynamics, Maxwell-Boltzmann Statistics, Bose-Einstein statistics, Fermi Dirac statistics, Most probable particle distribution.	**9**	**19**
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, Recent advancements in the above topic.	**5**	**10**
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, Recent advancements in the above topic.	**5**	**10**
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 Temperatures, Excess Functions for Multicomponent Mixtures, Wilson, NRTL, and UNIQUAC Equations for Multicomponent Mixtures, Recent advancements in the above topic.	**11**	**25**
5.	**Solubility of Gases in liquids** The ideal solubility of gas, Henry's Law and its significance, Effect of Pressure and Temperature on gas solubility, Gas solubility in mixed solvents, Chemical effects on Gas solubility, Recent advancements in the above topic.	**5**	**10**

6.	**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 for Computation of Equilibrium Composition of Complex Multiphase Systems, Recent advancements in the above topic.	**10**	**25**
	Total	**45**	**100**

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

Where R:Remember; U:Understanding; A:Application, N:Analyze and E:Evaluate C:Create(as per Revised Bloom's Taxonomy)

References/Suggested Learning Resources:

(a) Books:

1. J. M. Prausnitz, R. N. Litchtenthaler, E. G. de Azevedo, "Molecular Thermodynamics of Fluid PhaseEquilibria" 3rd Edition, Prentice Hall.
2. S. M. Walas, "Phase Equilibria in Chemical Engineering", Butterworth-Heinemann .
3. J. M. Smith, H. C. Van Ness, M. M. Abbott, "Introduction to Chemical Engineering Thermodynamics", 7th Edition, McGraw-Hill Education.
4. Poling, Bruce E., John M. Prausnitz, and John P. O'Connell. 2001. "Properties of Gases and Liquids". 5th Edition, New York: McGraw-Hill Education.
5. Laurendeau, N. M. (2005). Statistical Thermodynamics: Fundamentals and Applications. United Kingdom: Cambridge University Press.

(b) Open source software and website:

1. Students can refer to video lectures available on the websites including NPTEL lecture series.
2. Students can refer to the CDs available with some reference books for the solution of problems

using software's /spreadsheets. Students can develop their own programs/spreadsheets for the solution of problems.

Suggested Course Practical List: List of Virtual lab experiments:

- Binary Vapour Liquid Equilibrium
- Ebulliometric Determination of Vapour Pressure
- Adsorption Isotherm
- Vib-rotational Spectroscopy of Carbon dioxide
- Simultaneous estimation method for multicomponent samples: Principle of additivity of absorbance
- Study of Phase Change
- Sample Preparation for TEM analysis (Bulk metal, Powder sample, Brittle material)

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