GUJARAT TECHNOLOGICAL UNIVERSITY

CHEMICAL ENGINEERING (05)
CHEMICAL ENGINEERING THERMODYNAMICS – II
SUBJECT CODE: 2150503
B.E. 5th SEMESTER

Type of course: Chemical Engineering

Prerequisite: Chemical Engineering Thermodynamics- I

Rationale: This course introduces the basic thermodynamics concepts of multiphase equilibrium in pure and multi-component systems. 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: 1) activity coefficient models for non-ideal liquid mixtures, 2) fugacity calculations of gas and liquid phases from equations-of-state, 3) systems with chemical reactions. The course provides fundamental insight into the underlying thermodynamic principles, as well as practice with advanced computational techniques to solve complex problems.

Teaching and Examination Scheme:

Teaching Scheme			Credits	Examination Marks						Total Marks
				Theory Marks			Practical Marks			
L	T	P	C	ESE (E)	PA (M)		ESE (V)		PA (I)	
					PA	ALA	ESE	OEP		
3	2	0	5	70	20	10	30	0	20	150

Content:

Sr. No.	Content	Total Hrs	% Weightage
1	Vapour/Liquid Equilibrium (VLE): Introduction The Nature of Equilibrium, the Phase Rule, Duhem's Theorem, VLE-Qualitative Behaviour, Azeotropic Mixtures, Maximum Boiling Azeotrope, Minimum Boiling Azeotrope, Simple Models for Vapour/Liquid Equilibrium ,Raoult's Law, Dewpoint and Bubblepoint Calucations with Raoult's Law ,VLE by Modified Raoult's Law,VLE from K,Value Correlations, Flash Calculations	12	22
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 , The Partial Molar Gibbs Energy and Fugacity, Fugacity and Fugacity Coefficient: Pure Species, Fugacity and Fugacity Coefficient: Species in Solution ,The Ideal Solution Model , The Lewis/Randall Rule , Excess Properties , The Excess Gibbs Energy and the Activity Coefficient, Nature of Excess Property	12	22
3	Solution Thermodynamics: Applications Liquid-Phase Properties from VLE Data ,Composition Dependence of Liquid- Phase Fugacities for Species in a Binary Solution, Excess Gibbs	12	22

	Energy, Data Reduction, Thermodynamic Consistency, Integral or Area Test Method , Models for the Excess Gibbs Energy, Margules Equations, VanLaar Equations, Calculations with Margules and VanLaar Equations, Local Composition Models, NRTL Equation, UNIQUAC Equation, UNIFAC Method, Enthalpy/ Concentration Diagrams		
4	Chemical Reaction Equilibria: The reaction coordinates, Application of the criteria for equilibrium 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, calculation of equilibrium conversion for single reaction, The phase rule and Duhem's theorem for reacting systems, multireaction Equilibria	12	22
5	Phase Equilibria: The Gamma / Phi Formulation of VLE, Equilibrium and stability, liquid-liquid equilibrium, solid- liquid equilibrium, osmotic equilibrium and osmotic pressure	6	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**	**21**	**7**	**7**	**-**

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

Note: This specification table shall be treated as a general guideline for students and teachers. The actual distribution of marks in the question paper may vary slightly from above table.

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

Course Outcome:

After learning the course the students should be able to:

1. Solution thermodynamics fundamentals. Application of Raoult's law and its variation to obtain VLE for binary systems.
2. Understand partial molar properties of components in a particular phase, and apply to calculations of heat of mixing, volume, and entropy changes on processing of ideal and real mixtures.
3. Azeotrope and its importance.
4. Estimating thermodynamic properties like fugacity, activity from the network of equations.
5. Solution Thermodynamics calculating the thermodynamic properties from experimental data. Different Activity coefficient models.
6. Data reduction to get constants of different activity coefficient models.
7. Predict the equilibrium products and their concentration in equilibrium when dealing with systems involving chemical reactions. The topic will include Homogeneous and Heterogeneous reaction. You will also get an introductory knowledge of multi reaction equilibrium.

List of Open Source Software/learning 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/spreadsheets. Students can develop their own programs/spreadsheets for the solution of problems.

ACTIVE LEARNING ASSIGNMENTS: Preparation of power-point slides, which include videos, animations, pictures, graphics for better understanding theory and practical work – The faculty will allocate chapters/ parts of chapters to groups of students so that the entire syllabus to be covered. The power-point slides should be put up on the web-site of the College/ Institute, along with the names of the students of the group, the name of the faculty, Department and College on the first slide. The best three works should submit to GTU.