



# GUJARAT TECHNOLOGICAL UNIVERSITY

Bachelor of Chemical Engineering

Subject : Chemical Engineering Thermodynamics

Subject Code : 3134401

Semester: III

**Type of Course:** Professional Core

**Prerequisite:** None

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

SR. NO.	CHAPTER NAME & CONTENT	TOTAL HRS.	% weightage
1	<b>Introduction, Laws of Thermodynamics &amp; their applications:</b> The scope of thermodynamics, Force, temperature, pressure, work, energy, heat, etc. Internal Energy, Enthalpy, The first law of thermodynamics, Energy balance for closed systems, Equilibrium, The reversible process, Heat capacity, Application of first law of thermodynamics to steady state flow process.	05	10
2	<b>Volumetric Properties of Pure Fluids:</b> PVT behavior of pure substances, Ideal and non-ideal gases, Equation of states, Virial, Cubic, Vanderwaals EOS, Redlich/Kwong (RK) EOS etc., Calculation of constants in terms of $P_c$ , $T_c$ , $V_c$ . Generalized Correlations for gases and liquids.	05	15
3	<b>Second Law Of Thermodynamics:</b> Statements of second law of thermodynamics, Heat engines, Thermodynamic Temperature Scales, Concept of entropy, Entropy changes of an Ideal Gas, Third law of thermodynamics. <b>Refrigeration and Liquefaction</b> Carnot refrigerator, Vapour compression cycle, Absorption refrigeration, Choice of refrigerant, Heat pump, Liquefaction processes	05	15
4	<b>Thermodynamics Properties of Fluids:</b> The fundamental property relations for homogeneous phases, Maxwell's equations, Residual properties, Mathematical relations among thermodynamic properties, Two phase systems, Thermodynamic diagrams.	04	07



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<b>5</b>	<b>Phase Equilibria: Vapour/Liquid Equilibrium (VLE):</b> 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, Dew point and Bubble point Calculations 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	08	<b>13</b>
<b>6</b>	<b>Solution Thermodynamics</b> <b>THEORY:</b> The Chemical Potential as a Criterion for Phase Equilibria, Equations Relating Molar and Partial Molar Properties, Partial Properties in Binary Solutions, 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, Rule , Excess Properties , The Excess Gibbs energy and activity coefficient <b>APPLICATIONS:</b> 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	10	<b>20</b>
<b>7</b>	<b>Chemical Reaction Equilibria</b> 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	08	<b>20</b>

**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.



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7. B.G. Kyle, "Chemical Process Thermodynamics", 2nd Edn., Prentice Hall of India Pvt.Ltd., New Delhi, 2000.
8. J.M.Prausnitz, R.N. Litchenthaler, Molecular thermodynamics of fluid phase Equilibria, 3<sup>rd</sup> Edition, Prentice Hall.
9. Stanley M. Walas, Phase-Equilibria in Chemical Engineering, Wiley India Private Limited
10. "Chemical and Process Thermodynamics"; B.G. Kyle, Prentice-Hall Inc. 5. "Introduction to Thermodynamics"; Y.V.C. Rao, 2nd Edition, Wiley Eastern Limited

**Suggested Specification table with Marks (Theory):**

Distribution of Theory Marks					
R Level	U Level	A Level	N Level	E Level	C Level
15	24	23	8	0	0

**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.

**Course Outcomes:**

**Students should be able to**

Sr. No.	CO Statement	Marks % Weightage
CO-1	Develop fundamental understanding of the basic principles of thermodynamics, related calculations and its uses and applications.	10
CO-2	Evaluate changes in different thermodynamic properties for pure fluids using equations of state (EOS).	15
CO-3	Apply thermodynamic principles to the analysis of chemical processes and equipment such as turbines, compressors, heat pumps etc	15
CO-4	Explain fundamentals of Solution thermodynamics, phase equilibria and reaction equilibria and its application to find thermodynamic properties of solutions	20
CO-5	Determine thermodynamic properties like activity coefficients, constants of model equations for solutions to calculate maximum extent of separation possible for various multiphase multi component systems	20
CO-6	Determine equilibrium conversions of reaction systems and its dependence on various operating parameters	20

**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