GUJARAT TECHNOLOGICAL UNIVERSITY

Program Name: Bachelor of Engineering

Level: UG

Branch: Chemical Engineering (Green Technology and Sustainability Engineering)

Subject Code: BE03044011

Subject Name: Chemical Engineering Themodynamics

w. e. f. Academic Year:	2024-25
Semester:	3
Category of the 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.

Course Outcome:

After Completion of the Course, Student will 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

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Teaching and Examination Scheme:

Teaching - Learning Scheme (in Hours per Semester)					Total Credits = TH/30	Assessment Pattern and Marks					Total Marks
						Theory		Tutorial / Practical			
L	T	P	PBL*	TH		ESE (E)	PA (M)	PA/ (I)	PBL (I)	ESE (V)	
45	15	0	60	120	04	70	30	0	30	0	130

Where L = Lecture, T= Tutorial, P= Practical, TW/SL = Term-Work / Self-Learning, TH = Total Hours, ESE = End-Semester Examination, PA = Progressive Assessment

*** Problem Based Learning (PBL) aims to accommodate learning beyond syllabus as per clause 9.4 of NBA manual.**

Course Content:

SR. NO.	CHAPTER NAME & CONTENT	TOTAL HRS.	% weightage
1	**Introduction, Laws of Thermodynamics & their applications:** 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	**Volumetric Properties of Pure Fluids:** 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 Pc, Tc, Vc. Generalized Correlations for gases and liquids.	05	**15**
3	**Second Law Of Thermodynamics:** Statements of second law of thermodynamics, Heat engines, Thermodynamic Temperature Scales, Concept of entropy, Entropy changes of an Ideal Gas, Third law of thermodynamics. **Refrigeration and Liquefaction** Carnot refrigerator, Vapour compression cycle, Absorption refrigeration, Choice of refrigerant, Heat pump, Liquefaction processes	05	**15**
4	**Thermodynamics Properties of Fluids:** The fundamental property relations for homogeneous phases, Maxwell's equations, Residual properties, Mathematical relations among thermodynamic properties, Two phase systems, Thermodynamic diagrams.	04	**07**

5	**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, 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	**13**
6	**Solution Thermodynamics** THEORY: 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 APPLICATIONS: 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	**20**
7	**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	08	**20**

Suggested Specification table wit 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.

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
10. "Chemical and Process Thermodynamics"; B.G. Kyle, Prentice-Hall Inc. 5. "Introduction to Thermodynamics"; Y.V.C. Rao, 2nd Edition, Wiley Eastern Limited

List of Open Source Software/learning website:

- Students can refer to video lectures available on the websites including NPTEL.
- 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.
- XSEOS–an Open Software for Chemical Engineering Thermodynamics

- **List of suggested activities for Problem Based Learning:**

Sl. No.	Name of the activity	No. of hours	Evaluation Criteria
1.	Industry/Research laboratory visit	Visit = 5h, Report preparation = 5h Total = 10h	Based on report submitted. Report should contain observations and calculations based on industry/ lab data.
2.	Technical Video based learning related to the subject	Duration of video = 5h Report preparation = 5h Total = 10h	Report /presentation based on the video learning outcomes.
3.	Assignment writing. Numerical based assignment is preferable.	5 assignments of 2h each. Total = 10h	Based on the assignment submitted.
4.	Self learning on-line course	Minimum duration of the course should be 10h.	Examination based assessment at the end of course. Based on the certificate produced.
5.	Complex problem solving	Maximum 2 problem. Study of the problem and solution finding, Total = 10h	Based on the depth of the solution submitted.
6.	Videos on Industrial safety aspects based on subject	Duration of video = 5h Report preparation = 5h Total = 10h	Based on quiz/report submitted
7.	Poster/chart/power point preparation on technical topics	Duration = 6 h	Based on poster/chart preparation and presentation skills
8.	Industrial exposure for 2-3 days to observe and provide tentative solutions on society/environment/health/any other issue	Duration = 15 h for industrial exposure Problem identification and tentative solution = 10 h Total = 20 h	Based on evaluation of critical problems and solutions
9.	Group Discussion on emerging/trending technical topics based on subject	Duration = 1 h each	Based on performance in group discussion, technical depth, knowledge etc.

Note:

- All the suggested activity should be related to the subject.

- The number of hours is suggestive. Faculty can sub-divide the number of hours based on the activity. However, total number of hours is fixed.
- Rubrics for the evaluation can be prepared by the faculty.
- All records pertaining to the evaluation and assessment of self-learning activities must be properly maintained and preserved at the institute level. These records should be made available to the university upon request. •
- Institutes are encouraged to utilize digital platforms, such as Microsoft Teams, for effective recordkeeping and to ensure transparency in the evaluation and assessment of self-learning activities.

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