Gyanmanjari Innovative University

Course Syllabus
Gyanmanjari Institute of Technology
Semester-1 (M.Tech)

Subject: Advanced Chemical Engineering Thermodynamics-METCH11501

Type of course: Major (Core)

Prerequisite: Basics of Chemical Engineering Thermodynamics

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.

Teaching and Examination Scheme:

Teaching Scheme			Credits	Examination Marks					Total Marks
				Theory Marks		Practical Marks		CA	
CI	T	P	C	ESE	MSE	V	P	ALA	150
4	0	2	5	60	30	10	20	30	

Legends: CI-Classroom Instructions; T – Tutorial; P - Practical; C – Credit; ESE – End Semester Examination; MSE- Mid Semester Examination; CA - Continuous Assessment; ALA-Active Learning Activities.

Course Content:

Sr. No	Course content	Hrs	% 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.	12	20
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. **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.	12	20
3	**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.	12	20

4	**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.	12	20
5	**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.	12	20

Continuous Assessment:

Sr. No	Active Learning Activities	Marks
1	**Preparation of Multimedia Presentations on Thermodynamic Concepts:** Students will prepare PowerPoint presentations that include videos, animations, pictures, and graphics for better understanding of advanced thermodynamic principles such as phase equilibrium, fugacity, and reaction equilibrium. Each group will be assigned a topic or chapter by the faculty to ensure full syllabus coverage. The presentation file will be submitted on the GMIU Web Portal.	10
2	**Case Study on Phase and Reaction Equilibria:** Students will conduct a case study involving the analysis of phase equilibrium or chemical reaction equilibrium in an industrial process. They will identify relevant thermodynamic models, evaluate equilibrium constants, and present their findings in a report or poster format on the GMIU Web Portal.	10
3	**Virtual Lab Experiments and Simulation Study:** Students will perform or simulate thermodynamic experiments such as Binary Vapour-Liquid Equilibrium, Adsorption Isotherm, and Phase Change using virtual labs or spreadsheet simulations. A detailed experiment report with results and analysis will be prepared and uploaded on the GMIU Web Portal	10
Total		30

Suggested Specification table with Marks (Theory): 60

Distribution of Theory Marks (Revised Bloom's Taxonomy)						
Level	Remembrance (R)	Understanding (U)	Application (A)	Analyze (N)	Evaluate (E)	Create (C)
Weightage	10%	40%	40%	05%	05%	00%

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 Outcome:

After learning the course, the students should be able to:	
CO1	Apply chemical engineering thermodynamics to a variety of systems and problems, including phase and reaction equilibrium.
CO2	Use theoretical concepts to describe and interpret solution properties.
CO3	Know how to qualitatively calculate the equilibrium properties of real liquid mixtures.
CO4	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.

List of Suggested Practical

Sr. No	Suggested Practical
1	Binary Vapour Liquid Equilibrium
2	Ebulliometric Determination of Vapour Pressure
3	Adsorption Isotherm

4	Vib-rotational Spectroscopy of Carbon dioxide
5	Simultaneous estimation method for multicomponent samples: Principle of additivity of absorbance
6	Study of Phase Change
7	Sample Preparation for TEM analysis (Bulk metal, Powder sample, Brittle material)

Instructional Method:

The course delivery method will depend upon the requirement of content and the needs of students. The teacher, in addition to conventional teaching methods by black board, may also use any tools such as demonstration, role play, Quiz, brainstorming, MOOCs etc.

From the content 10% topics are suggested for flipped mode instruction. Students will use supplementary resources such as online videos, NPTEL/SWAYAM videos, e-courses. The internal evaluation will be done on the basis of Active Learning Assignment.

Practical/Viva examination will be conducted at the end of semester for evaluation of performance of students in the laboratory.

Reference Books:

[1]. J. M. Prausnitz, R. N. Litchtenthaler, E. G. de Azevedo, "Molecular Thermodynamics of Fluid Phase Equilibria" 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