**Chemical Engineering Thermodynamics**

1.1 Course Number: CH262

1.2 Contact Hours: 3-1-0 Credits: 11

1.3 Semester -Offered: 2nd Year-odd

1.4 Prerequisite: Engineering Thermodynamics

1.5 Course Committee Members: Dr Amit Ranjan, Dr V S Sistla

2. **Objective**

To covers the key features of chemical engineering thermodynamics for prediction of thermodynamic properties for real gas, liquid and solid mixtures at equilibrium.

3. **Course Content:**

Unit wise distribution of content and number of lectures

| Unit # | Topics | Sub-topics | Lectures |
|---|---|---|---|
| 1 | Combining 1st and 2nd laws | Accounting energy and entropy in flow systems after combining 1st and 2nd laws. Thermodynamic potentials. | 2 |
| 2 | Review of Mathematical preliminaries | Review of calculus of multiple variables and applying them to thermodynamic variables. Maxwell's relations. | 2 |
| 3 | Thermodynamic relationships | Response functions in single phase systems. Thermodynamic relationships in one component single phase closed systems. | 2 |
| 4 | Real systems | Real systems vs ideal systems. Various equations of state in real systems and their use in thermodynamic property calculation. Departure functions from EoS. | 2 |
| 5 | Phase equilibrium in unary systems | Equilibrium of single component multiple phases systems. Phase transitions. Clausius equation, Clausius Clapeyron Equation. Fugacity. | 3 |
| 6 | Mixtures | Thermodynamic Properties of mixtures. Partial molar properties. Partial molar Gibbs energy and generalized Gibbs Duhem Equation. | 3 |
| 7 | Multicomponent phase equilibrium | Phase equilibrium in multicomponent mixtures. Gibbs phase rule. Ideal gas mixtures. Partial molar G and fugacity. Ideal mixture and excess properties. | 3 |

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|---|---|---|---|
| 8 | Fugacity calculation for predicting phase equilibrium | Fugacity calculation in gaseous, liquid, and solid mixtures. Mixture activity coefficient models. Non-simple mixtures. Combined EoS and excess G models. Reference states. | 4 |
| 9 | Vapor liquid equilibrium in simple mixtures | Vapor liquid equilibrium in ideal mixtures. Raoult's law and Henry's law. Low pressure non-ideal mixtures. high pressure VLE using EoS (phi-phi method). | 4 |
| 10 | Equilibrium in non-simple mixtures | Non-simple mixtures. Solubility of gases in liquids. Liquid liquid equilibrium. Solid liquid equilibrium. | 5 |
| 11 | Applications | Applications to phase equilibrium based separation processes. | 2 |
| 12 | Chemical reaction thermodynamics | Combined chemical and phase equilibria. Balance equations in reacting single phase mixtures. Multiphase reacting mixtures. Heterogeneous chemical reactions. | 5 |
| 13 | Statistical thermodynamics | Statistical thermodynamics: Relating microscopics to Macroscopics. Energy states. Partition functions. Statistical mechanical principles. Connecting with classical thermodynamics | 3 |
| | | **Total** | **40** |

4. **Readings**

4.1 Text Books:

1. Chemical, Biochemical, and Engineering Thermodynamics, by Stanley Sandler.

4.2 Reference Books:

1. Introduction to Chemical Engineering Thermodynamics, by Van Ness, Smith, and Abbott.
2. Chemical Engineering Thermodynamics, by Y. V. C. Rao.

5. **Outcome of the Course:**

Thermodynamics is the heart of all macroscale engineering. The subject itself has evolved by engineering practices and developed by engineers. It is indispensable for chemical engineers. This course will help students understand e.g. how to evaluate and design a chemical process having optimum efficiency, or how to understand multiphase equilibria in multicomponent mixtures, and apply phase equilibrium concepts to processes such as distillation, extraction, and absorption etc. This course also introduces the idea of statistical thermodynamics as a bridging link between the molecular behavior and the bulk thermodynamic behavior of fluids.