# CHEMICAL ENGINEERING THERMODYNAMICS

Course Outcomes: At the end of the course the student shall be able to CO1: Apply laws of thermodynamics to closed and open systems (L2)

CO2: Discuss the importance of various equations of state (L2)

CO3: Evaluate thermodynamic property relations to solutions (L5)

CO4: Discuss the nature of VLE and LLE (L2)

CO5: Evaluate the heat effects in single and multiple reactions (L5)

## **UNIT-I**

### 10 Lectures

**Laws of thermodynamics**: Basics of thermodynamics, first law of thermodynamics for closed and open systems, two phase systems (for pure component), Clausius-Clapeyron equation, second law of thermodynamics and entropy, third law of thermodynamics, applications to process equipment like turbines, compressors, pumps, nozzles, boilers and valves.

# **Learning outcomes:**

- Define laws of thermodynamics (L1)
- Apply law of thermodynamics to various process equipment (L3)
- Describe the importance of entropy (L2)
- Calculate the amounts of vapour and liquid in a two-phase system (L3)

### **UNIT-II**

#### 10 Lectures

**Volumetric equations of state**: Various equations of state (van der Waals, Pitzer and virial equations of state), fundamental property relations for homogeneous fluids of constant composition, discussion of Maxwell equations and their importance, Gibbs free energy as the generating function and residual properties.

# **Learning outcomes:**

- Apply various equations of state (L3)
- Discuss Maxwell's equations (L2)
- Calculate residual properties (L3)
- Describe the importance of Gibbs free energy as the generating function (L2)

## UNIT-III

## 10 Lectures

**Solution thermodynamics:** Fundamental property relations, Chemical potential and phase equilibria, Partial molar properties, The Gibbs-Duhem equation, Fugacity of pure component, Ideal gas mixture, Fugacity of a species in solution, Ideal solution, Lewis Randall rule, Excess properties, Activity coefficient using One parameter and two parameter Margules equations and van Laar equations.

## **Learning Outcomes:**

- Define the partial properties (L1)
- Explain the concept of chemical potential and fugacity (L2)
- Calculate excess properties (L3)
- Calculate the activity coefficient using the given models (L3)

# UNIT- IV 10 Lectures

**Vapor-liquid equilibrium:** Qualitative behaviour of VLE, P-x-y and T-x-y diagrams, Models for VLE, Raoult's law for VLE, VLE by modified Raoult's law, Henry's law, Bubble and dew point calculations, azeotropic systems, Vapor-liquid phases coexistence line.

Liquid –Liquid equilibrium: Criterion of equilibrium and stability Learning outcomes:

- Show P-x-y and T-x-y diagrams (L3)
- Calculate bubble point and dew points of a binary system (L3)
- Describe the importance of entropy (L2)
- Define the limits of stability for LLE (L1)

UNIT-V 10 Lectures

**Chemical Reaction Equilibria:** Temperature dependence of the heat of reaction, Theoretical flame temperature, Reaction coordinate, Equilibrium criteria for chemical reaction equilibrium, Equilibrium constant, vant Hoff equation, Equilibrium conversion for single and multiple reactions for the ideal gas and ideal solution, Phase rule for reacting systems.

### **Learning outcomes:**

- Discuss the effect of T on heat of reaction (L2)
- Describe the mole fractions in terms of reaction coordinate (L2)
- Discuss the effect of T and P on equilibrium constant (L2)
- Calculate the equilibrium conversion for single and multiple reactions (L3)

#### **Text Book:**

Smith J.M., Van Ness H.C., Abbott M.M., Swihart M.T., Introduction to Chemical Engineering Thermodynamics, 8th Edition, Tata McGraw Hill, 2018.

#### **References:**

- 1. Koretsky M.D.Engineering and Chemical Thermodynamics, 2nd Edition, John Wiley & Sons, Inc., 2013.
- 2. Narayanan K. V., Chemical Engineering Thermodynamics, PHI, 2000.
- 3. Rao Y.V. C., Chemical Engineering Thermodynamics, University Press Ltd., 2001
- 4. Kyle B.G., Chemical and Process Thermodynamics, 3rd Edition, Pearson, Prentice Hall, 1999.