CHEMICAL ENGINEERING THERMODYNAMICS

ENCH 254

Lecture : 3 **Year : II**
Tutorial : 1 **Part : II**
Practical : 0

Course Objectives:
The objective of this course is to provide a comprehensive understanding of the volumetric and thermodynamic properties of fluids, thermodynamics of solutions, vapor-liquid equilibrium, and chemical reactions. It aims to equip students with the theoretical knowledge and practical skills necessary to analyze, interpret and apply in chemical and process engineering.

1 Volumetric Properties of Pure Fluids (8 hours)

- 1.1 Phase rule
- 1.2 Virial equation of state, its application
- 1.3 Cubic equation of state (EOS)
  - 1.3.1 Van der Waals, Generic cubic EOS, EOS parameters, Roots of generic cubic EOS
  - 1.3.2 Redlich-Kwong (RK) EOS, Soave-Redlich-Kwong (SRK) EOS, Peng-Robinson (PR) EOS
- 1.4 Generalized correlations for gases
  - 1.4.1 Pitzer correlations for the compressibility factor
  - 1.4.2 Pitzer correlations for the second and third virial coefficient

2 Thermodynamic Properties of Fluids (7 hours)

- 2.1 Fundamental property relations, Maxwell equation
  - 2.1.1 Enthalpy and entropy as functions of T and P
  - 2.1.2 Internal energy as a function of P
  - 2.1.3 Internal energy and entropy as functions of T and V
  - 2.1.4 The Gibbs energy as a generating function
- 2.2 Residual properties: Enthalpy and entropy from residual properties

3 Solutions Thermodynamics (14 hours)

- 3.1 Fundamental property relation
- 3.2 Chemical potential and equilibrium
- 3.3 Partial Properties in binary solutions
- 3.4 Ideal-gas state mixture model

3.5 Fugacity and fugacity coefficient: Pure species
  3.5.1 Vapor-liquid equilibrium for pure species
  3.5.2 Fugacity of a pure liquid
3.6 Fugacity and fugacity coefficient: Species in solution
  3.6.1 The fundamental residual-property relation
  3.6.2 Fugacity coefficients from the virial equation of state
3.7 Generalized correlations for the fugacity coefficient
  3.7.1 Fugacity coefficients for pure species
  3.7.2 Extension to mixtures
3.8 Liquid-phase properties from VLE data: Fugacity, activity coefficient, and excess Gibbs energy for solutions

4 Thermodynamics Formulations for Vapor-Liquid Equilibrium (10 hours)

4.1 Phase rule: Duhem's theorem
4.2 Equilibrium and phase stability
4.3 Gamma-Phi formulation of VLE
4.4 Dewpoint and bubble point: Raoult's law and modified Raoult's law
4.5 Flash point
4.6 K-value correlations

5 Chemical Reaction Equilibria (6 hours)

5.1 Reaction coordinate
5.2 Standard Gibbs energy change and the equilibrium constant
5.3 Effect of temperature on the equilibrium constant
5.4 Evaluation of equilibrium constant

Tutorial (15 hours)

1. Solution of problems related to virial EOS, RK, SRK, PR EOS, and Pitzer correlation
2. Solution of problems related to enthalpy and entropy calculation from compressibility factor data
3. Solution of problems related to partial properties of binary solutions, fugacity and fugacity coefficient for pure species and mixtures
4. Solution of problems related to Fugacity, activity coefficient, and excess Gibbs energy for solutions
5. Solution of problems related to dewpoint and bubble point calculations with Raoult's law and modified Raoult's law, Flash calculations, VLE from K-value correlations
6. Solution of problems related to reaction coordinate and equilibrium constant

Final Exam

The questions will cover all the chapters in the syllabus. The evaluation scheme will be as indicated in the table below:

Chapter	Hours	Marks Distribution
1	8	10
2	7	10
3	14	19
4	10	13
5	6	8
Total	**45**	**60**

* There may be minor deviation in marks distribution.

References

1. Smith, J. M., Van Ness, H. C., Abbott, M. M. (2019). Chemical Engineering Thermodynamics. McGraw Hill Education (India) Private Limited.
2. Cengel, Y. A., Boles, M. A., Kanoğlu M. (2019). Thermodynamics: An Engineering Approach. McGraw-Hill.
3. Elliot, J., Lira C. (2012). Introductory Chemical Engineering Thermodynamics. Prentice-Hall Inc.
4. Sandler, S. I. (1998). Chemical and Engineering Thermodynamics. John Wiley and Sons, Inc.
5. Koretsky, M. D. (2012). Engineering and Chemical Thermodynamics. John Wiley and Sons Inc.