**BIRLA INSTITUTE OF TECHNOLOGY AND SCIENCE, PILANI,HYDERABAD CAMPUS**

**FIRST SEMESTER 2019-2020**

**Handout II**

|  |  |  |
| --- | --- | --- |
|  |  | **Date: 17/8/2022** |
| **Course No.** | **:** | **CHE G622** |
| **Course Title** | **:** | **Advanced Chemical Engineering Thermodynamics** |
| **Instructor-in-Charge** | **:** | Prof. Vikranth Kumar Surasani |
| **Instructor** |  | Mr. DasikaPrabhatSourya |

1. **Course Description**: Review of fundamental principles; statistical foundations; thermodynamic properties of pure substances and mixtures, their estimation and correlation; stability and equilibrium criteria for homogeneous and heterogeneous systems; thermodynamics of irreversible processes.
2. **Scope & Objective**:

The objective of this course is to learn how to apply thermodynamics to phenomena and processes of interest to chemical engineers. The content is advanced and based on prior knowledge of courses taken at the undergraduate level. This course aims to provide further depth with major focus on phase equilibrium thermodynamics. Solving phase equilibria problems involves general computational techniques that have widespread application in other areas of engineering. Another objective of this course is to provide experience in fitting mathematical models to experimental data, using phase equilibria calculations. A small part of the course is devoted to statistical mechanics and its relation to thermodynamics.

Learning objective :

At the end of the course student will be able to

* Apply the principles of thermodynamics for the energy requirements , feasibility of the processes and predict reaction equilibria
* Predict the phase behavior and properties of multicomponent system.
* Use tools such as ASPEN for solving calculations useful in thermodynamics.

1. **Text Book (TB):**

J. M. Smith, H. C. Van Ness and M. M. Abbott, “Introduction to Chemical EngineeringThermodynamics”, MGHFSE, 7th Edition

**Reference Books: (RB)**

**RB1:** Y. V. C. Rao, “Chemical Engineering Thermodynamics”,Universities Press, 1997

**RB2:** R. P. Rastogi& R. R. Mishra, “An Introduction to Chemical Thermodynamics”, Vikas

Publishing House Pvt. Ltd., 6th Revised Edition (1995)

**RB2:** John M.Prausnitz; Rüdiger N. Lichtenthaler; Edmundo Gomes de Azevedo,

“Molecular Thermodynamics of Fluid Phase Equilibria”, Prentice Hall, 3rd Edition

1. **Course Plan**:

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Lec. No.** | **Learning Objectives** | | **Topics to be covered** | **Reference** | |
| **1 – 2** | Introduction | | Review of Basics, First Law of Thermodynamics,Second Law of Thermodynamics Entropy, Entropybalance and Reversibility, Third Law ofThermodynamics | Chap. 1,2,3,4  TB/Lecture  notes / Chap  1,2, 5 T2 | |
| **3** | Equations of state(EOS),, GeneralizedCorrelations forPVT behaviour | | PVT behaviour, Review of Virial Equation, CubicEquations of State, Generalized correlations forgases and liquids (Review only) | Chap. 6.6, 6.7  TB / Chap 3  T2 | |
| **4 – 5** | ThermodynamicProperties of Fluids | | Fundamental Property relations, Equilibrium, Review ofMaxwell equations | Chap. 6 T2 | |
| **6 – 8** | ThermodynamicPotentials | | Legendre Transformations, Thermodynamic potentials,Criteria for equilbrium, Energy minimum and maximumprinciple | Chap. 6 RB1/  Chap 7. TB | |
| **9 – 10** | Stability ofThermodynamicsystems | | Stability criteria, Application of equilibrium andstability criteria to equation of state | Chap. 7 TB /  Chap. 10 RB1 | |
| **11 – 12** | Multi-componentmixtures | | Thermodynamic description of mixtures, review ofpartial molar property, Chemical potential, GeneralizedGibbs-Duhem Equations | Chap. 8 TB /  Chap. 9 RB1 | |
| **13 – 15** | Multi-componentmixtures | | Criteria for phase equilibrium in multi-componentsystems, Criteria for chemical equilibrium and combinedchemical and phase equilibrium | Chap. 8 / TB | |
| **16 - 17** | Gibbs energycalculations | | Review of fugacity and estimation of fugacity andfugacity coefficient for pure gas, Fugacity co-efficient ofspecies in mixture | Chap. 7/9 TB /  Chap 9 RB1 | |
| **18 – 19** | Gibbs energycalculations for realgas mixtures | | Mixing rules, Estimation of pure component fugacity forreal gas mixtures | Chap. 9 TB /  Chap 9 RB1 | |
| **20 – 21** | Gibbs energycalculations forsolutions | | Lewis Randall rule, Excess properties, concept ofactivity coefficient, Gibbs Duhem relation | Chap. 9 TB /  Chap 11 RB1 | |
| **22 – 24** | Gibbs energycalculations forsolutions | | Correlative activity coefficient models | Chap. 9 TB /  Chap 11 RB1 | |
| **25 – 26** | Vapor-LiquidEquilibrium | | Fundamental VLE equation, VLE at low and moderatepressures (review only), Azeotropic system | Chap. 10 TB /  Chap 12 RB1 | |
| **27 – 28** | Vapor-LiquidEquilibrium | | Multi-component VLE, Thermodynamic consistencytest of VLE data, Descriptive VLE | Chap. 10 TB /  Chap 12 RB1 | |
| **29 - 30** | Other Fluid – Fluidequilibria | | The solubility of gas in a liquid, Vapour liquid-liquidequilibrium & Liquid-Liquid equilibrium, solid liquidequilibrium | Chap. 11 TB/  Chap 14 T2 | |
| **31** | Chemical ReactionEquilibria (review) | | Review of multi-reaction Stoichiometry, standard Gibbsfree energy change and Equilibrium constant, vant’ Hoffequation, Relation between equilibrium constants andspecies activities at equilibrium | Chap. 13 TB /  Chap 14 RB1 | |
| **32 – 34** | Chemical ReactionEquilibria | | Homogeneous gas and liquid phase reactionsEquilibrium with simultaneous reactions, Heterogeneousreactions | Chap. 13 TB /  Chap 14 RB1 | |
| **35 – 36** | StatisticalThermodynamics | | Introduction, Quantum mechanical aspects, Role ofstatistical mechanics, Thermodynamic probability,Probability and entropy | Chap. 6 RB2 /  Lecture notes | |
| **37-39** | Statistical Thermodynamics | | Molecular basis of residual entropy, Boltzmann’s Distribution Law, Partition function and expressions forthe same | Chap. 6 RB2 /Lecture notes | |
| **40 – 42** | Statistical Thermodynamics | | Thermodynamic properties in terms of partitionfunctions, Partition functions of polyatomic molecules | Chap. 6 RB2 / Lecture notes | |
| **Practical. No** | | **Topic** | | |
| **1** | | Introduction to ASPEN Plus: Getting Started | | |
| **2** | | Physical Properties | | |
|  | | 1. Pure Component Properties | | |
| 1. Vapor Pressure | | |
| **3-6** | | Thermodynamic Data | | |
|  | | 1. Flash Model & Heat of Evaporation | | |
| 1. Stream Engine and Refrigeration | | |
| 1. Txy Diagram –VLLE | | |
| 1. Ternary Maps LLE | | |
| 1. Residue Curve Maps | | |
| **7-8** | | Material and Energy Balances | | |
| **9-13** | | Simulation ofdistillationand reactor models and Networks  (Note: Students need to perform individual projects during these practical Hrs.) | | |

1. **Evaluation Scheme:**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Component** | **Duration** | **Weightage** | **Data&Time** | **Remark** |
| Mid Term | 90 minutes | **20** | 05/11 11.00 -12.30PM | CB |
| Comprehensive | **180 minutes** | **40** | **29/12 FN** | **OB** |
| **Class Tests (min 3)** | **20 minutes** | **15** |  | **CB** |
| **Project + Practical** | **-** | **25** |  | **OB** |

1. **Chamber Consultation Hours:** To be announced in the class.
2. **Notice:** Notices will be put on CMS
3. Make-**up** will be granted for genuine cases only. Prior permission of IC is compulsory.
4. **Academic Honesty and Integrity Policy**: Academic honesty and integrity are to be maintained by all the students throughout the semester and no type of academic dishonesty is acceptable.

**Instructor-in-chargeCHE G622**