BIRLA INSTITUTE OF TECHNOLOGY AND SCIENCE, PILANI, HYDERABAD CAMPUS
INSTRUCTION DIVISION
FIRST SEMESTER 2015-2016
Course Handout for Advanced Chemical Engineering Thermodynamics

                                                                                    Date:

Course No.   :   **CHE G622**
Course Title   :   **Advanced Chemical Engineering Thermodynamics**
Instructor-in-Charge :   I SREEDHAR

1. Course Description: Review of basic undergraduate concepts in thermodynamics including
   Legendre transformations and Maxwell's relations, Phase equilibria in multi-component and multi-
   phase systems, Chemical Equilibrium, Statistical Thermodynamics

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.

3. Text Book (TB):

   Stanley I. Sandler, "Chemical, Biochemical and Engineering Thermodynamics", Wiley, 2006, 4th
   Edition

   J. M. Smith, H. C. Van Ness and M. M. Abbott, "Introduction to Chemical Engineering
   Thermodynamics", MGHFSE, 7th Edition

4. 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

4. Course Plan:

Lecture No.	Learning Objectives	Topics to be covered	Reference
1 – 2	Introduction	Review of Basics, First Law of Thermodynamics, Second Law of Thermodynamics Entropy, Entropy balance and Reversibility, Third Law of Thermodynamics	Chap. 1,2,3,4 TB/Lecture notes / Chap 1,2, 5 T2
3	Equations of state (EOS),, Generalized Correlations for PVT behaviour	PVT behaviour, Review of Virial Equation, Cubic Equations of State, Generalized correlations for gases and liquids (Review only)	Chap. 6.6, 6.7 TB / Chap 3 T2
4 – 5	Thermodynamic Properties of Fluids	Fundamental Property relations, Equilibrium, Review of Maxwell equations	Chap. 6 T2
6 – 8	Thermodynamic Potentials	Legendre Transformations, Thermodynamic potentials, Criteria for equilbrium, Energy minimum and maximum principle	Chap. 6 RB1/ Chap 7. TB
9 – 10	Stability of Thermodynamic systems	Stability criteria, Application of equilibrium and stability criteria to equation of state	Chap. 7 TB / Chap. 10 RB1
11 – 12	Multi-component mixtures	Thermodynamic description of mixtures, review of partial molar property, Chemical potential, Generalized Gibbs-Duhem Equations	Chap. 8 TB / Chap. 9 RB1
13 – 15	Multi-component mixtures	Criteria for phase equilibrium in multi-component systems, Criteria for chemical equilibrium and combined chemical and phase equilibrium	Chap. 8 / TB
16 - 17	Gibbs energy calculations	Review of fugacity and estimation of fugacity and fugacity coefficient for pure gas, Fugacity co-efficient of species in mixture	Chap. 7/9 TB / Chap 9 RB1
18 – 19	Gibbs energy calculations for real gas mixtures	Mixing rules, Estimation of pure component fugacity for real gas mixtures	Chap. 9 TB / Chap 9 RB1
20 – 21	Gibbs energy calculations for solutions	Lewis Randall rule, Excess properties, concept of activity coefficient, Gibbs Duhem relation	Chap. 9 TB / Chap 11 RB1

22 – 24	Gibbs energy calculations for solutions	Correlative activity coefficient models	Chap. 9 TB / Chap 11 RB1
25 – 26	Vapor-Liquid Equilibrium	Fundamental VLE equation, VLE at low and moderate pressures (review only), Azeotropic system	Chap. 10 TB / Chap 12 RB1
27 – 28	Vapor-Liquid Equilibrium	Multi-component VLE, Thermodynamic consistency test of VLE data, Descriptive VLE	Chap. 10 TB / Chap 12 RB1
29 - 30	Other Fluid – Fluid equilibria	The solubility of gas in a liquid, Vapour liquid-liquid equilibrium & Liquid-Liquid equilibrium, solid liquid equilibrium	Chap. 11 TB/ Chap 14 T2
31	Chemical Reaction Equilibria (review)	Review of multi-reaction Stoichiometry, standard Gibbs free energy change and Equilibrium constant, vant' Hoff equation, Relation between equilibrium constants and species activities at equilibrium	Chap. 13 TB / Chap 14 RB1
32 – 34	Chemical Reaction Equilibria	Homogeneous gas and liquid phase reactions Equilibrium with simultaneous reactions, Heterogeneous reactions	Chap. 13 TB / Chap 14 RB1
35 – 36	Statistical Thermodynamics	Introduction, Quantum mechanical aspects, Role of statistical 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 for the same	Chap. 6 RB2 /Lecture notes
40 – 42	Statistical Thermodynamics	Thermodynamic properties in terms of partition functions, Partition functions of polyatomic molecules	Chap. 6 RB2 / Lecture notes

4. Evaluation Scheme:

Component	Duration	Weightage	Date & Time	Remarks
Test I	60 min	15%		CB
Test II	60 min	15%		OB
Seminars /Projects/Assignments		40%	To be announced	OB
Comprehensive Exam	3 hours	30 %		CB/OB

5. Chamber Consultation Hours: To be announced in the class.

6. Notice: Notices will be put on CMS

7. Make-up will be granted for genuine cases only. Prior permission of IC is compulsory.

Instructor-in-charge CHE G622