FIRST SEMESTER 2015-2016
Course Handout for Advanced Chemical Engineering Thermodynamics

Date: 03.08.2015

Course No.	**:**	**CHE G622**
Course Title	**:**	**Advanced Chemical Engineering Thermodynamics**
Instructor-in-Charge	**:**	**Arvind Kumar Sharma**

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. [*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)**

Sandler, Stanley I., *Chemical, Biochemical and Engineering Thermodynamics*, 4th Edition, Wiley (India Pvt. Ltd. : Wiley Student Edition), 2006 (Reprint 2013!).

4. **Reference Books (RB)**

RB1: Rao, Y V C, *Chemical Engineering Thermodynamics*, Universities Press, 1997.
RB2: Smith, J M, H C Van Ness and M M Abbott (Adapted by B I Bhatt), *Introduction to Chemical Engineering Thermodynamics (in SI Units)*, 7th Edition, Tata McGraw Hill Education Pvt. Ltd., 2005 (Special Indian Edition 2010, Latest Reprint!).
RB3: Rastogi, R P and R R Mishra, *An Introduction to Chemical Thermodynamics*, 6th Revised Edition, Vikas Publishing House Pvt. Ltd., 1995.
RB4: Prausnitz, John M, Rüdiger N. Lichtenthaler, Edmundo Gomes de Azevedo, *Molecular Thermodynamics of Fluid Phase Equilibria*, 3rd Edition, Prentice Hall, 1998!.
RB5: Rajaram J and J C Kuriacose, *Chemical Thermodynamics - Classical, Statistical and Irreversible*, Pearson, 2013 (Chap. 7 on Statistical Thermodynamics).
RB6: Atkins P and Julio De Paula, *(Atkins') Physical Chemistry*, 9th Edition, Oxford University Press, 2010 (1st Indian Ed. 2011) [2 chapters on Statistical Thermodynamics].
RB7: McQuarrie D A and John D Simon, *Molecular Thermodynamics*, Viva Books (by arrangement with University Science Books), 1st Indian Edition 2004 (reprinted 2014).
RB8: McQuarrie D A, Statistical Mechanics, Viva Books (by arrangement with University Science Books), 1st Indian Edition 2003 (reprinted 2013).
RB9: Cengel, Y A and M A Boles, *Thermodynamics : An Engineering Approach (SI Units)*, 7th Edition, Tata McGraw Hill Education (India) Pvt. Ltd., (Special Indian Edition, 2011: Sixth Reprint, 2013!)

5. 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 RB2
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 RB2
4 – 5	Thermodynamic Properties of Fluids	Fundamental Property relations, Equilibrium, Review of Maxwell equations	Chap. 6 RB2
6 – 8	Thermodynamic Potentials	Legendre Transformations, Thermodynamic potentials, Criteria for equilibrium, 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 RB2
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 RB3 / Lecture notes
37 – 38	Statistical Thermodynamics	Molecular basis of residual entropy, Boltzmann's Distribution Law, Partition function and expressions for the same	Chap. 6 RB3 / Lecture notes
39 – 40	Statistical Thermodynamics	Thermodynamic properties in terms of partition functions, Partition functions of polyatomic molecules	Chap. 6 RB3 / Lecture notes

6. Evaluation Scheme*

EC No.		Evaluation Component	Duration	Weightage (%)	Date, Time	Remarks**
A	1.	Midsem. Test	90 min	25	8/10 10:00 - 11:30 AM	CB + OB
B	2.	Project (s)	-	40 (exact split-up will be shared in classes)	-	-
	3.	Assignment (s) of varied natures / Surprise Test (s) … etc	-		-	-
	4.	Constructive (Class) Participation	-		-	-
C	5.	Comprehensive Exam.	3 hrs	35	8/12 AN	CB + OB

***If any change in this / rest of the handout : it will be communicated in Classes – pls follow them.**

** **CB** = Close Book **OB** = Open Book

- **Chamber consultation hour** will be announced in the class.
- The **notices,** if any**,** concerning the course, will be displayed on the notice board of the Department of Chemical Engineering **only**.
- **Make-up** will be granted for **genuine cases only**. Certificate from authenticated doctor, say from the Medical Center, must accompany make-up application (*only prescription or vouchers for medicines will not be sufficient*). Prior permission of IC is compulsory.

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