BIRLA INSTITUTE OF TECHNOLOGY AND SCIENCE, PILANI, HYDERABAD CAMPUS
FIRST SEMESTER 2021-2022
Course Handout for Advanced Chemical Engineering Thermodynamics

Date: 2/8/18

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

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.
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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

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, TB1/Lecture notes / Chap 1,2, 5 TB2
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 TB1 / Chap 3 TB2
4 – 5	Thermodynamic Properties of Fluids	Fundamental Property relations, Equilibrium, Review of Maxwell equations	Chap. 6 TB2
6 – 8	Thermodynamic Potentials	Thermodynamic potentials, Criteria for equilbrium, Energy minimum and maximum principle	Chap. 6 RB1/ Chap 6 TB2
9 – 10	Stability of Thermodynamic systems	Stability criteria, Application of equilibrium and stability criteria to equation of state	Chap. 7 TB2 / Chap. 10 RB1
11 – 12	Multi-component mixtures	Thermodynamic description of mixtures, review of partial molar property, Chemical potential, Generalized Gibbs-Duhem Equations	Chap. 11TB2 / 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.11 / TB2

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. 11 TB 2/ Chap 9 RB1
18 – 19	Gibbs energy calculations for real gas mixtures	Mixing rules, Estimation of pure component fugacity for real gas mixtures	Chap. 11 TB2 / Chap 9 RB1
20 – 21	Gibbs energy calculations for solutions	Lewis Randall rule, Excess properties, concept of activity coefficient, Gibbs Duhem relation	Chap. 12 TB2 / Chap 11 RB1
22 – 24	Gibbs energy calculations for solutions	Correlative activity coefficient models	Chap. 12 TB2 / Chap 11 RB1
25 – 26	Vapor-Liquid Equilibrium	Fundamental VLE equation, VLE at low and moderate pressures (review only), Azeotropic system	Chap. 10 TB 2/ Chap 12 RB1
27 – 28	Vapor-Liquid Equilibrium	Multi-component VLE, Thermodynamic consistency test of VLE data, Descriptive VLE	Chap. 10 TB2 / 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. 10 TB2/
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 TB2 / Chap 14 RB1
	Chemical Reaction	Homogeneous gas and liquid phase reactions	Chap. 13 TB2

32 – 34	Equilibria	Equilibrium with simultaneous reactions, Heterogeneous reactions	/ 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

Plan for Lab experiments

Experiment No	Lab name	Experiment Name
Expt-1	CAD LAB	Introduction to Aspen Plus property
Expt 2	CAD LAB	Introduction to data models
Expt-3	CAD LAB	Flash Calculation in Aspen Plus
Expt-4	CAD LAB	Heat of vaporization using Aspen plus
Expt-5	CAD LAB	Steam engine simulation with Aspen Plus
Expt-6	CAD LAB	Maximum Fill up in Propane Tanks with Aspen Plus – Using calculator block
Expt-7	CAD LAB	Usage ASPEN calculator block to perfom custom calculations
Expt-8	CAD LAB	Txy examples with Aspen Plus
Expt-9	CAD LAB	Txy in VLLE system
Expt-10	CAD LAB	PT envelope in Aspen Plus
Expt-11	CAD LAB	Retrograde Behavior Illustrated with Aspen Plus

Expt 12	CAD LAB	Thermodynamic Equilibrium with Sensitivity

4. Evaluation Scheme:

Component	Duration	Weightage	Date & Time	Remarks
Mid sem tests	90 min	25%		CB/OB
Lab	120mins	20%		OB
Project (2)	TBA	10%		OB
Seminar(2)	TBA	10%		OB
Comprehensive Exam	2 hours	35 %		CB/OB

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

6. Notice: Notices will be put on CMS /Chemical Engg Dept notice board

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

8. 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-charge CHE G622