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.
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3. 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

4. **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	Chap. 1,2,3,4 TB/Lecture

		Reversibility, Third Law ofThermodynamics	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
	i) Pure Component Properties
	ii) Vapor Pressure
3-6	Thermodynamic Data
	i) Flash Model & Heat of Evaporation
	ii) Stream Engine and Refrigeration
	iii) Txy Diagram –VLLE
	iv) Ternary Maps LLE
	v) 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.)

5. 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**

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

7. Notice: Notices will be put on CMS

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

9. 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