

ACADEMIC-GRADUATE STUDIES AND RESEARCH DIVISION

FIRST SEMESTER 2023-2024

Course Handout for Advanced Chemical Engineering Thermodynamics

Date:
12/08/2023

Course No. : CHE G622
Course Title : Advanced Chemical Engineering Thermodynamics
Instructor-in-Charge : Prof. D. Purnima
Instructor : Prof. Vikramth Kumar Surasani
Lab Instructor : Ms. D.Vidya, Prof. D.Purnima, Prof. Vikranth Kumar Surasani

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.

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 – 6	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
7-9	Equations of state (EOS), Generalized Correlations for PVT behavior	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
10-13	Thermodynamic Properties of Fluids	Fundamental Property relations, Equilibrium, Review of Maxwell equations	Chap. 6 TB2
14-16	Thermodynamic Potentials	Thermodynamic potentials, Criteria for equilibrium, Energy minimum and maximum principle	Chap. 6 RB1/ Chap 6 TB2
17 – 18	Stability of Thermodynamic systems	Stability criteria, Application of equilibrium and stability criteria to equation of state	Chap. 7 TB2 /Chap. 10 RB1
19-21	Multi-component mixtures	Thermodynamic description of mixtures, review of partial molar property, Chemical potential, Generalized Gibbs-Duhem Equations	Chap. 11TB2 /Chap. 9 RB1
22-24	Multi-component mixtures	Criteria for phase equilibrium in multi-component systems, Criteria for chemical equilibrium and combined chemical and phase equilibrium	Chap.11 / TB2
24 – 25	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
26 – 27	Gibbs energy calculations for real gas mixtures	Mixing rules, Estimation of pure component fugacity for real gas mixtures	Chap. 11 TB2 / Chap 9 RB1
28-30	Gibbs energy calculations for solutions	Lewis Randall rule, Excess properties, concept of activity coefficient, Gibbs Duhem relation	Chap. 12 TB2 / Chap 11 RB1
31	Gibbs energy calculations for solutions	Correlative activity coefficient models	Chap. 12 TB2 / Chap 11 RB1
32-33	Vapor-Liquid Equilibrium	Fundamental VLE equation, VLE at low and moderate pressures (review only), Azeotropic system	Chap. 10 TB 2/ Chap 12 RB1
34-35	Vapor-Liquid Equilibrium	Multi-component VLE, Thermodynamic consistency test of VLE data, Descriptive VLE	Chap. 10 TB2 / Chap 12 RB1
36-37	Other Fluid – Fluid equilibria	The solubility of gas in a liquid, Vapour liquid-liquid equilibrium & Liquid-Liquid equilibrium, solid liquid Equilibrium	Chap. 10 TB2/
38	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	Chap. 13 TB2 / Chap 14 RB1

		species activities at equilibrium	
37-39	Chemical Reaction Equilibria	Homogeneous gas and liquid phase reactions Equilibrium with simultaneous reactions, Heterogeneous reactions	Chap. 13 TB2 / Chap 14 RB1
40	Statistical Thermodynamics	Introduction, Quantum mechanical aspects, Role of statistical mechanics, Thermodynamic probability, Probability and entropy. Molecular basis of residual entropy, Boltzmann's Distribution Law, Partition function and expressions for the same. Thermodynamic properties in terms of partition functions, Partition functions of polyatomic molecules	Chap. 6 RB2

5. Plan for Lab experiments

Practical. No	Topic	Experiment Name
1	Introduction to ASPEN Plus: Getting Started	Introduction to Aspen Plus property
2	Physical Properties	Introduction to data models
3	Pure Component Properties	Flash Calculation in Aspen Plus
4	Vapor Pressure	Heat of vaporization using Aspen plus
5-6	Thermodynamic Data	Steam engine simulation with Aspen Plus
	Flash Model & Heat of Evaporation	Maximum Fill up in Propane Tanks with Aspen Plus – Using calculator block
7	Stream Engine and Refrigeration	Usage ASPEN calculator block to perform custom calculations
8	Txy Diagram –VLLE	Txy examples with Aspen Plus
9	Ternary Maps LLE	Txy in VLLE system
10	Residue Curve Maps	PT envelope in Aspen Plus
11-12	Material and Energy Balances	Retrograde Behavior Illustrated with Aspen Plus
13	Simulation of distillation and reactor models and Networks (Note: Students need to perform individual projects during these practical Hrs.)	Thermodynamic Equilibrium with Sensitivity

6. Evaluation Scheme:

Component	Duration	Weightage	Date & Time	Remarks
Mid sem tests	90 min	20%	09/10 - 4.00 - 5.30PM	OB
Lab	120mins	15%		OB
Project /Seminar(Assignments)	TBA	20%		OB
Quiz	20mins	10%		OB
Comprehensive Exam	3 hours	35 %	07/12 AN	OB

- 7. Chamber Consultation Hours:** To be announced in the class.
- 8. Notice:** Notices will be put on CMS
- 9. Make-up will be granted for genuine cases only. Prior permission of IC is compulsory.**
- 10. 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