Birla Institute of Technology & Science, Pilani
Hyderabad Campus

FIRST SEMESTER 2019-2020

Course Handout Part II

01-08-2019

In addition to part-I (General Handout for all courses appended to the time table) this portion gives further specific details regarding the course.

Course No. : *CHE F213*
Course Title : Chemical Engineering Thermodynamics
Instructor-in-Charge : Dr. Angan Sengupta

Scope and Objective of the Course: The purpose of this course is to provide a comprehensive treatment of essential chemical-industry oriented problems using the versatile thermodynamics approach (maintaining the standard of rigor demanded by sound thermodynamic analysis). The most important aspects a chemical engineer must be able to cope up with will be emphasized, viz. mass and energy balances for reacting as well as for non-reacting physical and chemical process. The course will deal with the determination of equilibrium constants for chemical reactions and for the transfer of chemical species between phases and also the fundamental understanding of the need for thermodynamics in performing the process design of various extensively used equipment (e.g. distillation column and flash drum) in the chemical industries.

Learning objectives:

- The student will be able to estimate the mass and energy requirements for various processes taking place in chemical engineering and also able to evaluate the feasibility of a process.
- Able to predict the PVT behavior for various substances which deviate from ideal behavior
- Able to predict the phase behavior of ideal and non-ideal systems
- Able to study the reaction equilibrium

Textbooks:

1. J. M. Smith, and H.C. Van Ness, "Introduction to Chemical Engineering Thermodynamics", TMH, 7th ed.,2005.
2. YVC Rao, "Chemical Engineering Thermodynamics", Universities Press, 1997.

Reference books

1. KV Narayanan, "A Textbook of Chemical Engineering Thermodynamics". Prentice Hall of India, 2001.

Course Plan:

Lecture No.	Learning objectives	Topics to be covered	Chapter in the Text Book
1-2	Introduction	Course content and evaluation scheme. Motivation on the need & the scope of thermodynamics in chemical	TB: 1& 2

		engineering. Basic Concepts on types of systems, surroundings, equilibrium and steady state systems, irreversible and reversible processes and types of characteristic variables. Mixing rule. Understanding of control mass and control volume.	
3-4	Conservation of extensive Property (Mass)	Mass conservation of non-reacting and reacting systems.	TB: 1 & 2
5-6	Conservation of extensive Property (Energy)	Development of energy balance equation, obtaining 1st Law of Thermodynamics from the energy balance equation. Application of 1st Law of Thermodynamics to a constant temperature, constant pressure, constant volume and adiabatic systems.	TB: 1 & 2
7-9	Conservation of Energy	Applications of 1st Law to a few industrial systems. Cubic EoS (van der Waals, RK, SRK, PR) and understanding the concept of phases and degree of freedom (Gibb's Phase Rule). Principle of Corresponding States.	TB: 1 & 2
10	Heat effects	Understanding the heat effects (sensible heat, latent heat, the heat of reaction, heat of formation, specific heats; e.g. c_p and c_v). Hess's Law.	TB: 1 & 2
11-12	Conservation of extensive Property (Entropy)	Understanding what Entropy is. Clausius Inequality and the development of the entropy balance equation. Understanding the connection between 2nd Law of thermodynamics and entropy, Clausius statement and Kelvin statement of 2nd Law of thermodynamics. Entropy balance for cyclic and reversible processes.	TB: 1 & 2
13-15	Conservation of Entropy	Irreversibility, Free energies	TB: 1 & 2

		(Helmholtz, Gibb's). Entropy change calculation for Ideal gas mixing (identical and non-identical), Entropy change of non-ideal gas during phase change, determining the feasibility of a process.	
16-17	Application of 1st and 2nd Law	Nozzles, diffusers, Turbine, Compressor, Throttle valve (Joule Thomson coefficient, inversion curve). Carnot cycle, Heat engines, Heat Pump and Refrigeration unit.	TB: 1
18-19	System Integration	Rankine heat generation cycle, Vapour compression cycle. Practical problems	TB: 1
20-22	Thermodynamic properties	Partial thermodynamic properties of fluids, Maxwell's relations. Generalized properties of ideal and non-ideal gases, residual properties. Zeroth & 3rd Law of thermodynamics.	TB: 1 & 2
23-26	Vapour Liquid Phase Equi--libria (VLE)	Physical understanding of phase equilibria. Phase equilibria in terms of free energies (1st order transition). Stability analysis. EoS revisited for understanding phase equilibria. Simple models to predict phase equilibria (Raoult's Law, Henry's Law, Modified Raoult's Law). Clapeyron equation, Clausius-Clapeyron equation and Antoine equation.	TB: 1 & 2
27-29	Phase equilibria in non-ideal gas	Concept of fugacity for deviation from an ideal gas, fugacity coefficient, relationship with residual properties and also with compressibility factor. Poynting expression. Industry oriented problems.	TB: 1
30-33	Phase behavior of multi-component system	An analogy with pure component VLE, azeotropes,	TB: 1 & 2

		Dew point and Bubble point, partial molar properties, excess properties, plotting P-xy and T-xy data. Gibb's – Duhem equation, Gibb's theorem, Lewis – Randall rule.	
34-36	Application of multi-component VLE data	Thermodynamic consistency, Heat effect on mixing, K – value correlation, thermodynamic design calculation of flash drum. Interpreting VLE data for distillation column design.	TB: 1 & 2
37-38	VLE models for multi-Component system	Margules equation, Redlich-Kister equation, Wohl's equation, van-Laar equation, NRTL equation.	TB: 2
39-42	Chemical Reaction Equilibria	Reaction coordinate, Equilibrium criteria for chemical reactions, Equilibrium constants and their variation with temperature, Evaluation of Equilibrium constants, Relation of Equilibrium Constants with Compositions, Equilibrium conversions for Single Reactions, Phase Rule and Duhem's theorem for Reacting Systems and Multi-reaction Equilibria.	TB: 2

Note: Topics that are highlighted are to be self-studied.

Evaluation Scheme:

Component	Duration	Weightage (%)	Date & Time	Nature of Component
Mid-semester exam	90 min.	30	1/10 (9:00 am to 10:30 am)	CB
Comprehensive exam	180 min.	40	6/12 (9:00 am to 12:00 noon)	CB
Surprise Quizzes	To be decided	10	Surprise Component	CB
Class/ Take-home Assignments	Continuous Evaluation	20	Continuous Evaluation	OB

Closed Book Test: No reference materials (**except thermodynamic tables**) of any kind will be permitted inside the exam hall.

Open Book Exam: Use of any text/ reference books are permitted. Loose sheets will not be permitted. Computers/mobile of any kind will not be allowed inside the exam hall. No exchange of any material will be allowed.

Chamber Consultation Hour: Thursday 5:00 pm to 6:00 pm in D-216.

Notices: All notices concerning this course will be displayed in Chem. Engg. Notice Board or CMS.

Make-up Policy: Make-up for the test may be granted with prior permission from Instructor-in-charge only for candidates having minimum 80% attendance or for any genuine case (certificate from an authenticated doctor from the Medical Center must accompany the make-up application. Only prescription or vouchers for medicines will not be sufficient).

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.

Dr. Angan Sengupta
INSTRUCTOR-IN-CHARGE