GUJARAT TECHNOLOGICAL UNIVERSITY

CHEMICAL (COMPUTER AIDED PROCESS DESIGN) (16)

Advance Chemical Engineering Thermodynamics

SUBJECT CODE: 3711612

SEMESTER: I

Type of course: Program Elective – 2

Prerequisite: Under graduate course in Chemical Engineering Thermodynamics

Rationale: This core course aims to connect the concepts and laws of classical thermodynamics to applications that require knowledge of thermodynamic properties at macroscopic level .The purpose is to present a broad understanding of phase equilibria and chemical reaction equilibria typically applied in the design of chemical engineering separation processes. Phase and Chemical equilibria of multi-component systems are covered. While on the other hand postulation approach of the subject is introduced and statistical thermodynamics is introduced to understand multi component interactions on a molecular level.

Teaching and Examination Scheme:

Teaching Scheme			Credits	Examination Marks				Total Marks
L	T	P	C	Theory Marks		Practical Marks		
				ESE(E)	PA (M)	PA (V)	PA (I)	
3	0	0	3	70	30	0	0	100

Content

Sl. No.	Topic	Teaching Hours	Module Weightage (%)
1	**Vapour –liquid equilibria**: Vapour –liquid equilibria of multi component , non ideal systems, evaluations of activity coefficient and fugacity coefficient, dew point and bubble point calculations, , P-T Flash calculations, Adiabatic Flash calculations, Block diagrams of these calculations.VLE from K value correlation. Data reduction. Computational methods for checking consistency of VLE data. Activity coefficient equations for multi component , non ideal systems like NRTL,UNIFAC,UNIQUAC methods and computations .	12	22
2	**Liquid-liquid equilibria :** Criteria of equilibrium, Different types of liquid-liquid solubility diagram, evaluation of LLE data. **Vapour- liquid- liquid equilibria:** Criteria of equilibrium, Pxy diagram at constant temperature. Txy diagram of VLLE at constant pressure and for several pressures, **Solid-liquid Equilibria :** Criteria of equilibrium, Txz plots	10	19
3	**Chemical Reaction equilibria:** Evaluation of equilibrium extent of reaction and equilibrium constant for exothermic, endothermic, reversible, irreversible reactions and various combinations. Thermodynamic analysis of some important industrial reactions. Liquid phase and heterogeneous reactions,	11	20

	Multi reaction equilibria, Simultaneous, consecutive reactions and various combinations, adiabatic reactions		
4	**Refrigeration:** Vapour Compression Cycle, Industrial vapor compression cycle, Vapour absorption cycles, Industrial vapour absorption cycles. Selection criteria, Calculations of net refrigeration effect, TR, COP, steam required, solvent required etc, Advances in refrigeration processes like ejector refrigeration, diffusion absorption refrigeration ,solar vapour absorption system etc.	10	19
5	**Postulational thermodynamics:** Introduction to postulational thermodynamics ,basic concepts and approach, postulates. **Quantum mechanics:** Introduction to quantum mechanics **Statistical thermodynamics:** Introduction to statistical thermodynamics, Boltzmann statistics, Fermi –Dirac statistics and Bose – Einstein statistics	11	20

Reference Books:

1. Smith J.M, Van Ness H.C., Abbott M. M, "Introduction to Chemical Engineering Thermodynamics", The McGraw Hill Companies Inc., USA, 7th Ed., 2005.
2. Don Green and Robert Perry, "Perry's Chemical Engineers Handbook", 8th edition, McGraw-Hill, USA. 2008.
3. Elliott J. R. and Lira C.T, "Introductory Chemical Engineering Thermodynamics ",2nd Edn. Prentice Hall, 2012.
4. Hougen O.A., Watson K.M., and Ragatz R.A. , "Chemical Process Principles Part-II(Thermodynamics)", 2nd Edition ,John Wiley 2004.
5. S.I.Sandler; " Chemical ,Biochemical and Engineering Thermodynamics" 5th Wiley India Edition,2016.
6. B.G.Kyle; " Chemical and Process Thermodynamics" Prentice –Hall Inc.1991.
7. Pedro Dinis Gasper and Pedro dinho da Silva; "Hand book of research on advances and applications in refrigeration systems and technologies Volume -I & II " IGI Global ,2015.
8. Y.V.C.Rao ; " Postulational and statistical Thermodynamics" Allied Publishers,1994.
9. M.W.Hanna; " Quantum mechanics in Chemistry" 2nd Edn.W.A.Benjamin Inc. 1969.
10.H.B.Callen: "Thermodynamics and Introduction to Thermo statistics" (Indian Edition)John Willy ,2005.
11.Kenneth Denbeigh ; " The Principals of Chemical Equilibrium", Cambridge University Press ,1981.

Course Outcome:

After learning the course the students should be able to:

1) Solve the phase equilibrium problems for complex systems based on classical and molecular thermodynamics.
2) Calculate thermodynamic properties from experimental data and able to reduce experimental data.
3) Know about advancement in refrigeration processes.
4) Predict the equilibrium conversion and composition of the constituents participating in multi-chemical reaction processes.

List of Open Source Software/learning website:

1. Students can refer to video lectures available on the websites including NPTEL lecture series.
2. Students can refer to the CDs available with some reference books for the solution of problems using softwares/spreadsheets. Students can develop their own programs/spreadsheets for the solution of problems.