



GUJARAT TECHNOLOGICAL UNIVERSITY

Program Name: Master of Engineering

Level: PG

Branch: Computer Aided Process Design

Subject Code: ME02072111

Subject Name: Thermodynamics for Phase and Chemical Reaction Equilibria

w.e.f. Academic Year:	2024-25
Semester:	2
Category of the Course:	Professional Elective Course

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.

Course Out comes:

After Completion of the Course, Student will able to:

No	Course Outcomes	
01	Solve the phase equilibrium problems for complex systems	A,N,E,C
02	Calculate thermodynamic properties from experimental data and able to reduce experimental data.	A,N,E
03	Solve problems related to refrigeration and know about advancement in refrigeration processes	A,N,E
04	Predict the equilibrium conversion and composition of the constituents participating in multi- chemical reaction processes	A,N,E

Teaching and Examination Scheme:

			Total Credits L+T+(PR/2)	Assessment Pattern and Marks				Total Marks
L	T	PR	C	Theory		Tutorial/Practical		
				ESE (E)	PA/CA (M)	ESE(V)	PA/CA(I)	
3	1	0	4	70	30	0	20	120



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Course Content:

Unit No.	Content	No.of Hours	%of 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 to solve the problems using Excel and Aspen plus	10	10
2.	Liquid-liquid equilibria : Criteria of Liquid –liquid equilibrium, Different types of liquid-liquid solubility diagram, evaluation of LLE data. Vapour- liquid- liquid equilibria, Pxy diagram at constant temperature. Txy diagram at constant pressure and for several pressures, Solid- liquid Equilibria : Txz plots.	8	14
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 Multi reaction equilibria, Simultaneous, consecutive reactions and various combinations, adiabatic reactions	10	22
4.	Refrigeration: Carnot refrigerator, Vapour Compression Cycle, 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.	8	19
5	Thermodynamic properties and VLE from equation of state: Properties of fluids from virial equation of state, Properties of fluids from cubic equation of state, Properties of fluids from	9	19



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correlations of the Pitzer type, VLE from cubic equation of state, vapor pressure for a pure species, VLE from cubic equations of state, VLE from K-value correlations		
Total	45	100

Suggested Specification Table with Marks (Theory):

Distribution of Theory Marks					
R Level	U Level	A Level	N Level	E Level	C Level
-	-	20	35	35	10

Where R:Remember; U:Understanding; A:Application, N:Analyze and E:Evaluate C:Create (as per Revised Bloom's Taxonomy)

References/ Suggested Learning Resources:

(a) 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. H.B.Callen: "Thermodynamics and Introduction to Thermo statistics" (Indian Edition)John Willy ,2005.
9. Kenneth Denbeigh ; " The Principals of Chemical Equilibrium", Cambridge University Press ,1981.

(b) Open-source software and website:

1. NPTEL lecture series.
2. DWSIM

Suggested Course Practical List: If any

List of Tutorials: -



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Tutorials/Presentation/Practical based on above topics.

1. Solve Problems related to phase equilibrium
2. Solve Problems related to experimental data reduction
3. Solve Problems related to refrigeration
4. Solve Problems related to equilibrium conversion
5. Prepare presentation related to advances in refrigeration processes