GUJARAT TECHNOLOGICAL UNIVERSITY

CHEMICAL TECHNOLOGY (36)
CHEMICAL ENGINEERING THERMODYNAMICS & KINETICS
SUBJECT CODE: 2163611
B.E. 6th SEMESTER

Type of course: Chemical Technology

Prerequisite: studied previous semesters' subjects and should have knowledge of basic properties and law of conservation of energy

Rationale: The main objective of this subject is to understand the laws of thermodynamics and its application in different domain of chemical technology.

Teaching and Examination Scheme:

Teaching Scheme			Credits	Examination Marks						Total Marks
L	T	P	C	Theory Marks			Practical Marks			
				ESE (E)	PA (M)		ESE (V)		PA (I)	
					PA	ALA	ESE	OEP		
3	1	2	6	70	20	10	20	10	20	150

Content:

Sr. No.	Topic	Teaching Hours	Module Weightage (%)
01	**Introduction:** Conservation of energy and first law of thermodynamics, application to steady state flow process; enthalpy, internal energy, equilibrium state, phase rule, irreversible vs. reversible process, heat capacity and specific heat.	4	10
02	**Properties of pure substances:** PVT behavior of pure substances, ideal and non-ideal gases, equation of states, Virial, Van der Waals, Redlich kwong equation , RKS equation, PR equation, Berthelot equation etc., Calculation of constants in terms of Pc, Tc, Vc, condition to be satisfied by any equation of state, reduced forms of equations of state, principles of corresponding states.	6	14
03	**Second Law of thermodynamics:** Second law of thermodynamics, Thermodynamic temperature scale, Ideal gas temperature scale, Concept of entropy, entropy change and irreversibility, Introduction to third law of thermodynamics.	6	14
04	**Thermodynamic properties of fluids**: Network of thermodynamic equations, mathematical relations among thermodynamic functions, Maxwell relations, Interrelations between H, S, G, E, Cp, Cv, etc. in terms of PVT relations (exhaustive treatment), Thermodynamic	8	20

	properties of single phase and two phase systems, Effect of temperature and pressure, on various properties and their evaluations, Types of thermodynamic diagrams, generalized correlations of thermodynamics properties of ideal gas mixtures. Residual properties, Partial Molar properties, Mathematical model for the chemical potential, Ideal and non-ideal solutions, Fugacity, Pure component fugacity, Fugacity coefficient and its evaluation, Effect of Pressure and Temperature on Fugacity, Fugacity of mixtures, Gibb's Duhemn Theorem, Composition in phase equilibrium, Excess properties of mixtures.		
05	**Phase Equilibrium:** Criteria of Phase equilibrium, Duhemn theorem, VL Equilibrium idealization, Phase diagram for miscible systems, Immiscible systems, Partial miscible systems, Testing of VLE data, Gibbs Duhemn Equation, Van Laar equation, Margules equation, Evaluation of various constants, Excess properties of mixtures, Qualitative treatment for phase behavior at low pressures, P-x, y, T-x, y, x-y diagrams, Qualitative treatment for phase behavior at high pressures, V-L equilibrium of ideal and non-ideal solutions, Henry's Law, Raoult's Law, Positive and negative deviations, Constructions of various diagram from data, Quantitative treatment for phase behavior at high pressures, Evaluation of K and construction of K-charts, Non ideal system, Evaluations of activity coefficient and fugacity coefficient, Dew point and bubble point calculations, BUBLP, DEWP, BUBLT and DEWT calculations, P-T Flash calculations, Adiabatic Flash calculations, Block diagrams of these calculations.	9	21
06	**Chemical Reaction Equilibria:** Criteria of chemical reaction equilibrium, Equilibrium extent of reaction, Equilibrium constant, Effect of temperature and pressure on K, Evaluation of K by various methods, Evaluation of equilibrium extent of reaction for exothermic, endothermic, reversible, irreversible reactions and various combinations. Thermodynamic analysis of some important industrial reactions, Liquid phase and heterogeneous reactions, Adiabatic reactions	9	21

Suggested Specification table with Marks (Theory):

Distribution of Theory Marks					
R Level	U Level	A Level	N Level	E Level	C Level
60	**11**	**9**	**11**	**9**	**00**

Legends: R: Remembrance; U: Understanding; A: Application, N: Analyze and E: Evaluate C: Create and above Levels (Revised Bloom's Taxonomy)

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. Narayanan K.V., "Chemical Engineering Thermodynamics", Prentice Hall, 1999.
3. Rao Y.V.C., "Introduction to Chemical Engineering Thermodynamics", Wiley Eastern. 1994 Karapetyants M. Kh., "Chemical Thermodynamics" Mir Publishers. 5 Elliot J. R. and Lira C.T, "Introductory Chemical Engineering Thermodynamics ",
4. Kyle B.G., "Chemical and Process Thermodynamics"3rd Ed., Prentice Hall, 1999
5. Sandler S.I, "Chemical Engineering Thermodynamics", John Wiley and Sons, Inc., New York, 3rd Ed., 1999
6. Dodge B.F., `Chemical Engineering Thermodynamics', McGraw Hill.1960
7. Weber H.C. and Meissner J.P., "Thermodynamics for Chemical Engineers", Wiley Eastern

Course Outcome:

1. Understanding of three laws of thermodynamics and the thermodynamic properties
2. Can explain the behaviour of real gas on the basis of different equation of state
3. Concept of entropy
4. Can explain thermodynamic property relation of fluids, Maxwell equation and its importance
5. Can describe partial molar properties and excess properties of mixture.
6. Concept of fugacity and fugacity coefficient
7. Vapour liquid equilibrium and qualitative behaviour of that
8. Calculation of BUBL P, BUBL T, DEW P, DEW T and flash calculation
9. Thermodynamic analysis of chemical reactions

List of Experiments:

1. Joule experiment
2. Calculation of degree of freedom from phase rule
3. Determination of BUBL P value theoretically and using simulation
4. Determination of BUBL T value theoretically and using simulation
5. Determination of DEW P value theoretically and using simulation
6. Determination of DEW T value theoretically and using simulation

Design based Problems (DP)/Open Ended Problem:

Students are free to select any area of science and technology based on chemical technology applications to define Projects.

Some suggested projects are listed below:

1. Literature survey on any VLE system
2. Phase rule for reacting systems by taking relevant reaction
3. Study of PVT behaviour of any pure component

List of Open Source Software/learning website:

1. Literature available under R&D of thermodynamics
2. Literature available on internet
3. Journals / e-journals

ACTIVE LEARNING ASSIGNMENTS: Preparation of power-point slides, which include videos, animations, pictures, graphics for better understanding theory and practical work – The faculty will allocate chapters/ parts of chapters to groups of students so that the entire syllabus to be covered. The power-point slides should be put up on the web-site of the College/ Institute, along with the names of the students of the group, the name of the faculty, Department and College on the first slide. The best three works should submit to GTU.