GUJARAT TECHNOLOGICAL UNIVERSITY

ENVIRONMENTAL SCIENCE AND TECHNOLOGY (35)
BASICS OF THERMODYNAMICS & KINETICS
SUBJECT CODE: 2163508
B.E. 6th SEMESTER

Type of course: Environmental Science & Technology

Prerequisite: A good fundamental backup of basics properties of fluids, law of conservation of energy, Mathematics and Chemical engineering principles

Rationale: The main objective of this subject is to make students aware about the basics of thermodynamics & kinetics and the fundamentals of chemical engineering principles which are very useful in developing a proper understanding of the basic principles of chemical engineering thermodynamics and its calculations.

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.	Content	Total Hrs.	% Weightage
1	**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 properties of single phase and two phase systems, 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.	12	25
2	**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, Qualitative treatment for phase behavior at low pressures, P-x, y, T-x, y, x-y diagrams, , V-L equilibrium of ideal and non-ideal solutions, Henry's Law, Raoult's Law, modified Raoult's law, Constructions of various diagram from data, Evaluation of K and construction of K-charts, Non ideal system, Dew point and bubble point calculations, BUBLP, DEWP, BUBLT and DEWT calculations, P-T Flash calculations.	8	25
3	**Chemical Reaction Equilibria:** Criteria of chemical reaction equilibrium, Equilibrium extent of reaction, Equilibrium constant, Effect of temperature	10	

	and pressure on K, Evaluation of K by various methods, Evaluation of equilibrium extent of single reactions for exothermic, endothermic, reversible, irreversible reactions and various combinations. Thermodynamic analysis of some important industrial reactions		20
4	**Introduction to chemical reaction kinetics:** Classification of reactions, reaction rate, elementary and non-elementary reactions, molecularity and order of reaction, rate constant k, Arrhenius law, collision theory, transition state theory, integral and differential method of analysis for irreversible reactions Introduction to heterogeneous catalysis Catalyst, catalyst properties, steps in catalytic reaction, basics of catalyst deactivation and its types	12	30

Suggested Specification table with Marks (Theory):

Distribution of Theory Marks					
R Level	U Level	A Level	N Level	E Level	C Level
24	**29**	**22**	**14**	**11**	**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",
3. Rao Y.V.C., "Introduction to Chemical Engineering Thermodynamics", Wiley Eastern. 1994
4. H. Scott Fogler, "Elements of Chemical Reaction Engineering", Eastern Economy Edition.
5. Octave Levenspiel, "Chemical Reaction Engineering", Wiley student Edition

Course Outcome:

After learning this course the students would have:

1) Understanding about the important application of thermodynamics laws in chemical engineering and processes used in industry.
2) Information about the calculation of BUBL P, BUBL T, DEW P, DEW T and flash calculation
3) Hands on knowledge for thermodynamic analysis of chemical reactions.
4) Practical knowledge of basic chemical reaction kinetics

List of Experiments:

1. Determination of BUBL P value theoretically and using simulation
2. Determination of BUBL T value theoretically and using simulation
3. Determination of DEW P value theoretically and using simulation

4. Determination of DEW T value theoretically and using simulation
5. Determination of order of reaction and rate constant. (Integral and differential method).
6. Determination of activation energy.
7. Kinetic study of half life method.

Design based Problems (DP)/Open Ended Problem:

Students are free to select any area of science and technology based on chemical engineering 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
4) Reaction mechanism
5) Deactivation of catalyst

Major Equipment:

Computer, reactor

List of Open Source Software/learning website:

1. Literature available under R&D of thermodynamics
2. Literature available on internet
3. Journals / e-journals
4. Software available like Thermo-Calc/Open cal phad/Thermo solver

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.