



GUJARAT TECHNOLOGICAL UNIVERSITY

Bachelor of Engineering

Subject Code: 3173518

Semester – VII

Subject Name: Basics of Reaction Engineering & Thermodynamics

Type of course: Professional Elective course

Prerequisite: The subject of reactor design uses information regarding the physical properties of reactants in different phases for conversion of raw materials into products. Prior knowledge regarding fluid flow, heat transfer, mass transfer and mathematics are essential in this regard.

Rationale: This subject Reaction Engineering and thermodynamics encompasses a process in terms of feasibility and speed at which any process will occur. At an industrial scale, the activity concerned with reactor design complying with nature's three laws of Thermodynamics.

Teaching and Examination Scheme:

Teaching Scheme			Credits C	Examination Marks				Total Marks
L	T	P		Theory Marks		Practical Marks		
				ESE (E)	PA (M)	ESE (V)	PA (I)	
3	0	2	4	70	30	30	20	150

Content:

Sr. No.	Content	Total Hrs
1	Kinetics of homogenous reactions Classification of reactions, Definitions of reactions rate, Temperature dependent term of rate equations from Arrhenius theory and comparison with collision and transition state theory.. Temperature dependency from thermodynamics, comparison of theories.	08
2	Collection and Analysis of Rate Data: Constant volume batch reactor, Differential method of analysis, Integral Method, Method of Half-lives, Method of initial rates. Variable volume batch reactor, Semi batch reactor, Batch reactor design equations, Design equation of flow reactors: CSTR, PFR. Application of design equations for continuous flow reactors, Reactors in series, combination of CSTRs and PFRs in series, Comparing the CSTR and PFR reactor volumes and reactor sequencing, space-time and space velocity, Reactor Scale up.	12
3	Multiple Reactions: Types of reaction, series – parallel reactions, Concept of instantaneous and overall yield, Reactor/reactors selection based on yield of the desired product. Maximizing the desired product in series reactions.	04
4	Introduction to Thermodynamics: Conservation of energy, Zeroth and first law of thermodynamics, application to steady state flow process, irreversible vs. reversible process, heat capacity and specific heat. Second law of thermodynamics, Temperature scale, Concept of entropy, Entropy change and irreversibility, Introduction to third law of thermodynamics.	06



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5	Thermodynamic properties of fluids: Network of thermodynamic equations, mathematical relations among thermodynamic functions, Maxwell relations, Clayperon & Clausius Clayperon equations, Types of thermodynamic diagrams, Partial Molar properties, Chemical potential, Ideal and non-ideal solutions, Fugacity, Fugacity coefficient and its evaluation, Effect of Pressure and Temperature on Fugacity	06
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Suggested Specification table with Marks (Theory):

Distribution of Theory Marks					
R Level	U Level	A Level	N Level	E Level	C Level
15	15	15	10	10	5

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

Note: This specification table shall be treated as a general guideline for students and teachers. The actual distribution of marks in the question paper may vary slightly from above table.

Reference Books:

1. Octave Levenspiel, "Chemical Reaction Engineering", 3rd Edition, John Wiley & Sons (Asia) Pvt Ltd.
2. H. Scott Fogler, "Elements of Chemical Reaction Engineering" 3rd Edition November, Prentice Hall of India Pvt Ltd.
3. Narayanan K.V., "Chemical Engineering Thermodynamics", Prentice Hall, 1999.
4. Rao Y.V.C., "Introduction to Chemical Engineering Thermodynamics", Wiley Eastern. 1994
5. Smith J.M, Van Ness H.C., Abbott M. M, "Introduction to Chemical Engineering Thermodynamics", The McGraw Hill Companies, Inc., USA, 7th Ed., 2005.
6. Kyle B.G., "Chemical and Process Thermodynamics" 3rd Ed., Prentice Hall, 1999

Course Outcomes: After learning this course, students will be able to:

Sr. No.	CO statement	Weightage
CO-1	Define the kinetics and rate law for homogeneous reactions, temperature dependency and prediction of mechanism.	15
CO-2	Illustrate various methods available for collection and analysis of rate data with continuous reactor design equations for performance of reactors and reactor sequences.	20
CO-3	Identify various steps involved in multiple reactions for reactor design based on yield of desired product.	15
CO-4	Describe various laws of thermodynamics and its relevant Environmental application.	20



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CO-5	Describe thermodynamic property relation of fluids, Maxwell equation and partial molar properties signifying their importance.	15
CO-6	Differentiate ideal and non-ideal solutions on basis of thermodynamic properties.	15

List of Experiments:

1. Activation Energy & Frequency factor calculation
2. Integral Method of analysis
3. Differential method of analysis
4. Kinetics by Half Lives Method
5. Non – linear regression simulation to obtain Antonie’s constants for single component system
6. Estimation of bubble point temperature and pressure of a multicomponent system

List of Open Source Software/learning website:

- Reference to NPTEL lectures can be made for a better understanding regarding various Reaction Engineering and concepts relating to thermodynamics.