GUJARAT TECHNOLOGICAL UNIVERSITY

Bachelor of Engineering
Subject Code: 3163612

Semester – VI
Subject Name: Fundamentals of Reaction Engineering

Type of course: Professional Core Course

Prerequisite: Reactor design uses information, knowledge and experience of areas like fluid mechanics, heat transfer and mass transfer & mathematics.

Rationale: The Fundamentals of Reaction Engineering principles learned in these subjects can also be applied in area such as waste water treatment and living systems in addition to the more traditional area of the manufacture of chemicals and pharmaceuticals. Reaction engineering is that engineering activity concerned with the exploitation of chemical reaction on commercial scale.

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)	
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, variables affecting reaction rate, concentration dependent term of rate equation for single, multiple, elementary and non-elementary reactions. Molecularity and order of reaction. Kinetic models for non-elementary reactions. Temperature dependant term of rate equations from Arrhenius theory and comparison with collision and transition state theory. Activation Energy and Temperature Dependency. Temperature dependency from thermodynamics, comparison of theories. Prediction of reaction rate by theories. Searching for the mechanism.	**7**
2	**Conversion and reactor sizing** Batch reactor design equations, Design equation of flow reactors: CSTR, PFR and PBR. 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. Introduction to semi batch reactor.	**10**
3	**Collection and Analysis of Rate Data** Constant volume batch reactor, Differential method of analysis, Integral Method, Method of Half-lives, Method of initial rates.	**10**
4	**Multiple Reactions** Types of reaction, series – parallel reactions, concept of instantaneous and overall yield, Reactor/reactors selection based on yield of the desired product.	**8**
5	**Temperature and pressure effects** Single Reactions Calculations of heats of reactions and equilibrium constants from thermodynamics, equilibrium conversion, General graphical design procedure.	**7**

	Adiabatic and non-adiabatic operations, strategies for heat transfer for reactors for exothermic reactions.	
6	**Introduction to Heterogeneous catalysis** Catalyst, Promoter, Inhibitor, Catalyst properties, classification of catalyst, Steps in a catalytic reaction. Synthesizing rate law, Mechanism and rate limiting step, Deactivation of catalyst.	**9**

Suggested Specification table with Marks (Theory): (For BE only)

Distribution of Theory Marks					
R Level	U Level	A Level	N Level	E Level	C Level
20	**15**	**15**	**10**	**5**	**5**

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

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. L. D. Schmidt, "The Engineering of Chemical Reactions", Oxford Press.
4. J.M. Smith, "Chemical Engineering Kinetics", 2nd, McGraw-Hill.
5. J. J. Carberry, "Chemical and Catalytic Reaction Engineering", McGraw Hill, New York, 1976.

Course Outcomes:

Sr. No.	**CO statement**	**Marks % weightage**
CO-1	Build basic knowledge of classification of reactions, kinetics of competing reactions and their influence on product yield and selectivity.	15%
CO-2	Describe the batch, CSTR, and PFR and Derive performance equations from general material balances.	20%
CO-3	Apply the fundamentals of kinetics including definitions of rate and forms of rate expressions	20%
CO-4	Develop the skills to choose the right reactor among single, multiple, recycle reactors etc.	15%
CO-5	Explain the concepts of heat capacity, latent heat, heat of reaction, heat of combustion, and heat of formation.	15%
CO-6	Classify catalysts and predict physical properties of catalyst, surface area, void volume and Understand the nature and mechanism of catalytic reactions.	15%

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List of Experiments:

1. Integral Method of analysis
2. Differential method of analysis
3. Kinetics by Half Lives Method
4. Activation Energy & Frequency factor calculation
5. Isothermal CSTR
6. Plug Flow reactor
7. Adiabatic Batch reactor
8. Study experiment on preparation techniques for catalyst
9. Study experiment on characterization techniques for catalyst

Major Equipment:

Batch Reactor, Isothermal CSTR, PFR, Cascade CSTR, Combined Flow Reactors.

List of Open Source Software/learning website:

- Literature available on internet
- Research articles
- NPTEL Lectures