GUJARAT TECHNOLOGICAL UNIVERSITY

BIO-TECHNOLOGY (04)
BASICS OF REACTION ENGINEERING
SUBJECT CODE: 2150403
B.E. 5thSEMESTER

Type of course: Chemical Engineering.

Prerequisite: None.

Rationale: The objective of this course is the successful design and operation of chemical reactors. It includes study of various types of reactions and their kinetics. This course integrates knowledge from calculus, differential equations, thermodynamics, general chemistry, and material and energy balances to solve reactor design problems, To examine reaction rate data to determine rate laws, and to use them to design chemical reactors, To simulate several types of reactors in order to choose the most appropriate reactor for a given need, To design chemical reactors with associated cooling/heating equipment.

Teaching and Examination Scheme:

Teaching Scheme			Credits	Examination Marks						Total Marks
				Theory Marks			Practical Marks			
L	T	P	C	ESE (E)	PA (M)		ESE (V)		PA (I)	
					PA	ALA	ESE	OEP		
4	0	3	7	70	20	10	20	10	20	150

Content:

Sr. No.	Topic	Teaching Hours	Module Weightage (%)
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. Testing kinetic models. 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.	16	21
3.	**Interpretation of Batch Reactor data:** Constant volume batch reactor, analysis of total pressure data, Integral and differential methods of analysis of data for constant volume and variable volume cases. Temperature and Reaction rate, search for a rate equation, Kinetics of enzymes catalysis, Enzymes. Kinetics of enzymes	15	20

4.	**Introduction to Reactor Design:** Mass and energy balances around a volume element. Single ideal reactors under steady state conditions, Ideal batch reactor,ideal mixed flow & ideal plug flow reactors, space-time and space velocity. Introduction to semi batch reactor.	11	14
5.	**Design of Reactor for Single Reactions:** Ideal batch reactor, steady-state mixed flow reactor, steady-state plug-flow reactor, holding and space time for flow reactors, size comparison of single reactors- with reference to first and second order reactions for Batch reactor, mixed versus plug flow reactor, general graphical comparison. Multiple reactor system, plug flow reactors in series and parallel, equal size and different size mixed flow reactors in series, reactors of different types in series, recycles reactors and autocatalytic reactions.	10	13
6.	**Design for Parallel Reactions:** Introduction to multiple reactions, qualitative discussion about product distribution, qualitative treatment of product distribution and of reactor size, the selectivity, irreversible first order reactions in series- qualitative treatment, performance characteristics, kinetic studies, and design of plug flow and mixed flow reactor, first order followed by zero order reaction, zero order followed by first order, successive irreversible reactions of different orders, reversible reactions, irreversible series-parallel reactions-Performance characteristics, kinetic study and design for mixed and plug flow reactor,	08	15
7.	**Temperature and Pressure Effects:** (Single Reactions) Calculations of heats of reactions and equilibrium constants from thermodynamics, equilibrium conversion, General graphical design procedure. Optimum temperature progression, Exothermic reaction in mixed flow, Rules for choice of reactors and optimum operation of rectors.	07	10
8.	**Industrial Applications:** Nitration, Sulfonation & sulfation, Hydrolysis, Alkylation Esterification, Polymerization, Oxidation, Reduction, Fermentation, Chlorination, Photochlorination cracking, etc., Should be discussed with reference to types of reactors utilised in these unit process.	05	07

Suggested Specification table with Marks (Theory):

Distribution of Theory Marks					
R Level	U Level	A Level	N Level	E Level	C Level
18	19	25	8	-	-

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.

Course Outcome: After learning the course students should be able to:

1. To build basic knowledge of classification of reactions.
2. To understand kinetics of competing reactions and their influence on product yield and selectivity.
3. To understand fundamentals of kinetics including definitions of rate and forms of rate expressions and relationships between moles, concentration, extent of reaction and conversion.
4. To derive batch, CSTR, and PFR performance equations from general material balances.
5. To size and do performance calculations on single, isothermal plug-flow, CSTR, and batch reactors for a single homogeneous or heterogeneous reaction given either rate data or a rate expression.
6. Develop skills to choose the right reactor among single, multiple, recycle reactor, etc. schemes.
7. To understand and apply the concepts of heat capacity, latent heat, heat of reaction, heat of combustion, and heat of formation.

List of Experiments and Open Ended Projects:

Minimum **5** practicals to be performed and remaining time should be allotted to open-ended projects / study reports / latest outcomes in technology study **:-**

1. In the beginning of the academic term, faculties will have to allot their students at least one Open-ended Project / Study Report / Latest outcome in technology.
2. Literature survey including patents and research papers of fundamental process

- Design based small project **or**
- Study report based on latest scientific development **or**
- Technology study report/ modeling/ simulation/collection report **or**
- Computer based simulation/ web based application/ analysis presentations of basic concept field which may help them in chemical engineering.

3. These can be done in a group containing maximum **three** students in each.
4. Faculties should cultivate problem based project to enhance the basic mental and technical level of students.
5. Evaluation should be done on **approach of the student on his/her efforts** (not on completion) to study the design module of given task.
6. In the semester student should perform **minimum** 5 set of experiments and complete **one small open ended dedicated project** based on engineering applications. This project along with any performed experiment should be **EVALUATED BY EXTERNAL EXAMINER.**

PRACTICALS (ANY FIVE):

1	To determine the activation energy of the reaction between sodium thio-sulphate and HCl using Arrhenius Equation.
2	To determine order of reaction for the reaction between sodium thiosulphate and HCl
3	To measure the kinetics of a reaction between ethyl acetate and sodium hydroxide under condition of excess ethyl acetate at room temperature.
4	To determine the kinetics of the reaction between ethyl acetate and sodium hydroxide at room temperature by the integral method of analysis.
5	To determine the activation energy and frequency factor for reaction between ethyl acetate and sodium hydroxide at room temperature & at different temperature.
6	To determine the kinetics of the reaction between ethyl acetate and sodium hydroxide at room temperature by the differential method of analysis.
7	To determine the kinetics of the reaction between n- butyl acetate and sodium hydroxide at room temperature by the integral method of analysis.
8	To determine the kinetics of the reaction between n- butyl acetate and sodium hydroxide at room temperature by the differential method of analysis

Major Equipments:
Nil

Open Ended Project fields:-
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:

- Carry out different liquid reaction to determine its kinetics.
- To determine mass transfer coefficient with and without reaction.
- To study various types of contacting patterns of fluids.

List of Open Source Software/learning website:

1) Literature available in any laboratory manual of Chemical Reaction Engineering.
2) NPTEL
3) Website: academia.edu for Laboratory view based e-learning portal for virtual reaction engineering laboratory

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.