GUJARAT TECHNOLOGICAL UNIVERSITY

Bachelor of Engineering
Subject Code: 3160506
Semester – VI
Subject Name: Chemical Reaction Engineering 1

Type of course: Professional core

Prerequisite:
Basic knowledge of material and energy balances in chemical engineering applications, laws of thermodynamics.

Rationale:
The course is intended to familiarize the students with concepts of reaction rate, derivation of rate expressions from reaction mechanism, ideal reactor types, integral method of analysis, differential method of analysis, principles of chemical reactor analysis and design, experimental determination of rate equations, design of batch and continuous reactors, how to choose the most appropriate reactor for a given feed, optimization of selectivity in multiple reactions, consideration of temperature and pressure effects, etc.

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)	
3	0	2	4	70	30	30	20	150

Content:

Sr. No.	Content	Total Hrs
1	**Overview of chemical reaction engineering**, Classification of reactions, Variables affecting rate, Definition of reaction rate, single and multiple reactions, Elementary and non-elementary reactions, molecularity and order of reaction, extent of reactions, conversion, Selectivity, Reaction rate fundamentals - elementary reaction sequences, steady state approximation and rate limiting step theory	7
2	**Kinetics:** Constant volume and variable volume batch, CSTR and PFR reactor data, data collection & plotting, linearization of rate equations. Analysis of total pressure data obtained from a constant-volume batch reactor, Integral and differential methods of analysis of data, Autocatalytic reactions, Reversible reactions, and Bio-chemical reactions.	8
3	**Homogeneous Single Reactions:** Performance equations for ideal batch, Plug flow, Back-mix flow and semi batch reactors for isothermal condition, Size comparison of single reactors, Multiple-reactor systems, Recycle reactor, Optimum recycle operations	8
4.	**Multiple Reactions:** Parallel reactions of different orders, Yield and selectivity, Product distribution and design for single and multiple-reactors, Series reactions: first-order reactions and zero-order reactions, Mixed series parallel complex reactions,	8

5.	**Temperature Effects for Single and Multiple Reactions:** Thermal stability of reactors and optimal temperature progression for first order reversible reactions, Adiabatic and heat regulated reactions, Design of non-isothermal reactors, Effect of temperature on product distribution for series and parallel reactions.	**7**
6.	RTD theory and analysis of non-ideal reactors	**7**

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
14	26	23	7		

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, Wiley-India Pvt. Ltd.
2. H. Scott Fogler, Elements of Chemical Reaction Engineering, 4th Edition, Prentice Hall of India Pvt. Ltd
3. Froment, G.B., and K.B. Bischoff, 1990, Chemical Reactor Analysis and Design, 2nd Ed., Wiley, New York
4. Smith, J.M., 1981, Chemical Engineering Kinetics, 3rd Ed., McGraw-Hill, New York.
5. L. D. Schmidt, the Engineering of Chemical Reactions, Oxford Press.
6. Carberry, J.J., 1976, Chemical and Catalytic Reaction Engineering, McGraw-Hill, New York.

Course Outcomes: At the end of the course, the students will be able to

Sr. No.	CO statement	Marks % weightage
CO-1	To classify reactions based on reaction mechanisms and reaction rates and reactors based on flow patterns	10
CO-2	To determine kinetics of single and multiple homogeneous reactions	20
CO-3	To choose an appropriate reactor type and operating conditions to achieve a desired output such as reactant conversion, selectivity and yield.	25
CO-4	To formulate a set of consistent material and energy balance equations to describe operation of batch, semi-continuous and continuous reactor systems with single or multiple reactions	25
CO-5	To summarize the effect of temperature and pressure on equilibrium conversion and choice of reactors.	10

List of Open Source Software/learning website:

Preparation of power-point slides, which include videos, animations, Pictures, graphics for better understanding theory – The faculty will allocate chapters/ parts of chapters to groups of students so that the entire syllabus of Chemical Reaction engineering -1 is covered.

Suggested list of experiments to be performed (8 to 10 experiments are to be given)

The analysis will include various experiments with the objective of sample preparation, measurement of concentration, prediction of kinetics and modeling of kinetics data. Learning outcomes: Students will (a) Familiarize with suitable measurement techniques and devices to measure concentration and temperature (b) Learn to employ various methods to determine the kinetics of reactions. (c) Quantify the effect of non-ideality of flow in chemical reactors. (d) Calculate the effects of mass transfer on chemical reactions, (e) Predict errors in experimentation and compare experimental data with models

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
9	To study and analyze Residence Time Distribution (RTD) of a straight tubular flow reactor without helical coils and as a helical coil
10	To study and analyze Residence Time Distribution (RTD) for single tank reactor, two tanks in series and three tanks in series.
11	To analyze Residence Time Distribution (RTD) of packed bed reactor and prediction of extent of dispersion.
12	To study and analyze Kinetics of Dye degradation using Microwaves.

13	To study and interpret Kinetics of Bio-diesel synthesis from vegetable oils by Transesterification
14	To study Multiphase reaction: Effect in mass transfer limited reaction.
15	To study Oscillating reactions, pattern formation and reduced order modeling
16	To conduct Kinetic study of any biochemical reaction

List of Open Source Software/learning website: Software:

Students can refer to video lectures available on the websites including NPTEL, Students can refer to the CDs which are available with some reference books for the solution of problems using software. Students can develop their own programs for the solutions of problems.

Open Source Software/learning website:

1. Students can refer to video lectures available on the websites including NPTEL.
2. Students can perform experiments on Virtual lab by IIT Bombay.
3. FOSSEE –DWSIM https://dwsim.fossee.in/