GUJARAT TECHNOLOGICAL UNIVERSITY

Program Name: Bachelor of Engineering
Level: UG
Branch: Chemical Engineering
Subject Code: BE05000111
Subject Name: Chemical Reaction Engineering-I

w.e.f. Academic Year:	2024-25
Semester:	5
Category of the Course:	Professional Core Courses

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.

Course Outcome:

After Completion of the Course, Students will be able to:

No	Course Outcomes	% of Weightage
01	Classify type of reaction, develop mechanism and rate expression of single and multiple homogeneous reactions	25
02	Select and design suitable ideal reactor for single and multiple homogeneous reactions	30
03	Optimize reactor arrangement and reaction conditions for maximum desired product formation for multiple reactors and multiple reactions for sustainable raw material and energy consumption	30
04	Evaluate temperature, heat of reaction, and equilibrium effects to design energy-efficient, thermally stable reactor systems	15

Teaching and Examination Scheme:

Teaching / Learning Scheme (in Hours per semester)					Total Credits = TH/30	Assessment Pattern and Marks					Total Marks
						Theory		Tutorial / Practical			
L	T	P	PBL*	TH	04	ESE (E)	PA (M)	PA/ (I)	TW/ SL (I)	ESE (V)	
45	0	30	15	90	03	70	30	20	30	50	200

• Problem Based Learning (PBL) aims to accommodate learning beyond syllabus as per clause 9.4 of NBA manual.

Where L = Lecture, T= Tutorial, P= Practical, TW/SL = Term-Work / Self-Learning, TH = Total Hours, PA = Progressive Assessment, ESE = End-Semester Examination

Course Content:

Unit No.	Content	No. of Hours	% of Weightage
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	6	13
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.	9	20

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	12	27
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 for improved efficiency and reduced environmental impact.	12	27
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 reaction for emphasizing efficient heat management and sustainable reactor operation.	6	13

Sustainability alignment: This course addresses the different weightage of SDG 12 (Responsible Consumption and Production) and SDG 13 (Climate Action) by applications of Chemical Reaction Engineering knowledge essential for industrial operations.

Suggested Specification table with Marks (Theory):

Distribution of Theory Marks					
R Level	**U Level**	**A Level**	**N Level**	**E Level**	**C Level**
10	20	30	30	10	---

Legends: R: Remembrance; U: Understanding; A: Application, N: Analyze; E: Evaluate and 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.

List of Experiments:

1. To prepare a calibration chart for NaOH solution.
2. To measure the kinetics of a reaction between ethyl acetate and sodium hydroxide under condition of equimolal concentration at room temperature using integral method of analysis.
3. To determine the kinetics of the reaction between excess ethyl acetate and sodium hydroxide at room temperature by the differential method of analysis.
4. To determine the activation energy of the reaction between ethyl acetate and sodium hydroxide using Arrhenius Equation.
5. Verify the performance equation of PFR and predict conversion using known rate expression.
6. Study characteristics of CSTR and predict conversion using known rate expression.
7. Compare performance of reactors in series. For example, PFR + CSTR
8. Compare performance of single CSTR and multiple CSTR in series.
9. Compare performance of PFR and PFR with recycle.
10. Study experiment..Prepare Optimal Temperature Progression Curve for any one system using Excel. And carry out reactor design for musti stage adiabatic reaction (any one such application).

Major Equipment:

Batch Reactor, CSTR, PFR, CSTR in series, multiple reactors in series, Conductivity meter,

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/

List of suggested activities for Problem Based Learning:

Sr. No.	Description	No. of hours	Total Hrs.
1	**Assignment writing.** Numerical based assignment is preferable.	5 assignments of 1h each.	5
2	Discussion on research paper based on relevant subject. Summarize research paper and evaluation critical parameters	2 research papers can be included. Each one has 5h	10
3	Complex problem solving of real world problem	Study of the problem and solution finding using reaction engineering knowledge	5
4	Industrial exposure to observe and provide tentative solutions on environment/ health/ any other issue	Duration (5h) for industrial exposure Problem identification and tentative solution (5h)	10
Max. Hours to be allotted			15

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