GUJARAT TECHNOLOGICAL UNIVERSITY

CHEMICAL ENGINEERING (05)
CHEMICAL REACTION ENGINEERING – I
SUBJECT CODE: 2160506
B.E. 6th SEMESTER

Type of course: Chemical Engineering

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

Rationale: This subject introduces 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
L	T	P	C	Theory Marks			Practical Marks			
				ESE (E)	PA (M)		ESE (V)		PA (I)	
					PA	ALA	ESE	OEP		
3	0	3	6	70	20	10	20	10	20	150

Content:

Sr. No.	Content	Total Hrs	% Weightage
1	**Introduction to Reaction Engineering:** Classification of reactions, definitions of reactions rate, variables affecting reaction rate, speed of chemical reactions.	4	**7**
2	**Kinetics of homogenous reactions:** Simple reactor types, the rate equation, concentration dependent term of rate equation. Molecularity and order of reaction. Rate constant *k*, representation of an elementary and nonelementary reaction. Kinetic models for nonelementary 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. Predictability of reaction rate from theory.	8	15
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.	12	23
4	**Introduction to reactor design & Ideal reactors for single reaction:** Mass and energy balances around a volume element. Ideal batch reactor, steady-state mixed flow reactor, steady-state plug-flow reactor, holding and	8	15

	space time for flow reactors, space-time and space velocity. Introduction to semi batch reactor.		
5	**Design of reactor for single reactions:** Size comparison of single reactors, multiple reactor systems, recycle reactor and autocatalytic reactions.	4	7
6	**Design for parallel reactions:** Introduction to multiple reactions, qualitative and quantitative treatment of product distribution and of reactor size, the selectivity.	4	7
7	**Potpourri of multiple reactors:** Irreversible first order reactions in series. Quantitative treatment, for plug flow or batch reactor and mixed flow reactor, their performance characteristics, kinetic studies and design. First order followed by zero order reaction, zero order followed by first order reaction, successive irreversible reactions of different orders, reversible reactions, irreversible series-parallel reactions.	7	13
8	**Temperature and pressure effects:** Single Reactions: Calculations of heats of reaction and equilibrium constants from thermodynamics, equilibrium conversion, general graphical design procedure. Optimum temperature progression, Energy balances equations in adiabatic and non-adiabatic case. Exothermic reaction in mixed flow, Rules for choice of reactors and optimum operation of rectors. Multiple Reactions: Product distribution and temperature.	7	13

Suggested Specification table with Marks (Theory):

Distribution of Theory Marks					
R Level	U Level	A Level	N Level	E Level	C Level
10	25	21	7	7	0

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. J.M. Smith, Chemical Engineering Kinetics, 2nd edition, McGraw-Hill.
4. L. D. Schmidt, the Engineering of Chemical Reactions, Oxford Press.

Course Outcome:

After learning the course the students should be able to:

- Build basic knowledge of classification of reactions.
- Understand kinetics of competing reactions and their influence on product yield and selectivity.

- Understand fundamentals of kinetics including definitions of rate and forms of rate expressions and relationships between moles, concentration, extent of reaction and conversion.
- Derive batch, CSTR, and PFR performance equations from general material balances.
- Do size and performance calculations on isothermal plug, mixed, and batch reactors for a homogeneous and heterogeneous reaction from given rate data or a rate expression.
- Develop skills to choose the right reactor among single, multiple, recycle reactors etc.
- Understand and apply the concepts of heat capacity, latent heat, heat of reaction, heat of combustion, and heat of formation.

List of Experiments:

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

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.**

Open Ended Project Fields:

- Non working models of batch, plug and mixed flow reactors.
- Designing reactors for exemplary reactions.
- Analyzing reactor data for higher order reactions.
- Studies related to advancements in reaction kinetics.

List of Open Source Software/learning website:

- NPTEL lecture series
- Literature available on Chemical Reaction Engineering.
- MIT Open course lecture on Chemical Reaction Engineering.

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.