



# GUJARAT TECHNOLOGICAL UNIVERSITY

Program Name: Master of Engineering

Level: PG

Branch: Chemical Engineering

Subject Code: ME02030011

Subject Name : Advanced Reaction Engineering

w. e. f. Academic Year:	2024-25
Semester:	2
Category of the Course:	Professional Core Courses

<b>Prerequisite:</b>	Knowledge of Reaction engineering at Undergraduate Level
<b>Rationale:</b>	This subject deals with the heterogeneous reactions and non-ideal flow systems including performance of various types of reactors. The non-isothermal systems are introduced with its application. The catalyst systems are also be covered in this.

## Course Outcome:

After Completion of the Course, Student will able to:

No	Course Outcomes
01	Evaluate heterogeneous reactions and reactor performance
02	Apply computational and optimization techniques to reactor design and scale-up.
03	Estimate the performance of multiphase reactors under non-isothermal conditions
04	Understand non-ideal flow and reactor models

## Teaching and Examination Scheme:

Teaching Scheme (in Hours)			Total Credits L+T+ (PR/2)	Assessment Pattern and Marks				Total Marks
L	T	PR		C	Theory		Tutorial / Practical	
			ESE (E)		PA / CA (M)	PA/CA (I)	ESE (V)	
3	0	2	4	70	30	20	30	150

## Course Content:

Unit No.	Content	No. of Hours	% of Weightage
1.	<b>Introduction:</b> Overview of Reaction Engineering & challenges, Reactor Design Equations for ideal Reactors, Advantage Disadvantage and selection criteria of ideal reactors, Non-ideal Flow reactors.	5	10



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2.	<b>Plug Flow Reactors:</b> Plug Flow Recycle Reactors design equation, Advantages of plug flow recycle reactor, Effect of Pressure Drop on performance of Plug Flow vessels, Effect of Condensing gas on Reactor design, Design of fixed bed catalytic reactor.	7	16
3.	<b>CSTR:</b> Multiple Reactions, finding number of independent reactions and independent set, Polymerization reaction in a CSTR, Energy Balance for stirred vessels, Stability of Steady States in CSTR, Plotting Liapunov Contours, Understanding Multiple steady states in a CSTR.	8	18
4.	<b>Semi Batch Reactors:</b> Semi batch reactor operation, Heat Effects in reversible exothermic reactions, Need for Multi-staging, Optimal Design of Reactors for Reversible exothermic reactions.	7	16
5.	<b>Advanced Reaction Kinetics:</b> Complex reaction mechanisms (parallel, series, autocatalytic). Non-elementary reactions and enzyme kinetics. Chain reactions and polymerization kinetics. Reaction kinetics for multiphase systems. Adsorption isotherms (Langmuir, BET models). High-Temperature Kinetics (e.g. Combustion, Pyrolysis and Gasification reaction kinetics), Kinetic of photocatalytic reactions.	9	20
6.	<b>Design of Industrial Reactors:</b> Bubble column reactors, Loop reactors, Agitated vessel type batch reactor, Gas- liquid reactors involving Gas induction type agitator with spiral baffle jacket, Sulfonation reactor by using SO <sub>3</sub> as a sulfonating agent, Trickle bed reactor.	9	20
<b>Total</b>		<b>45</b>	<b>100</b>

## Suggested Specification Table with Marks (Theory):

Distribution of Theory Marks					
R Level	U Level	A Level	N Level	E Level	C Level
5	25	15	10	10	5

Where R: Remember; U: Understanding; A: Application, N: Analyze and E: Evaluate C: Create (as per Revised Bloom's Taxonomy)

## References/Suggested Learning Resources:

(a) Books:



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- K.G. Denbigh: Chemical Reactor Theory, Cambridge University Press, Second Edition, 1971
- J.M. Smith: Chemical Engineering Kinetics, Mcgraw Hill, Third Edition, 1981
- Keith J. Laidler and John H. Meiser: Reaction Kinetics: Principles and Applications in Organic and Biological Chemistry", Pearson, Third Edition, 1987
- Levenspiel O., Chemical Reaction Engineering, Wiley, 1998
- Foggler, H.S., Elements of Chemical Reaction Engineering, Prentice Hall of India, 2008
- Fromment G.F. and Bischoff K.B., Chemical Reactor Analysis and Design, John Wiley, 2010

**(b) Open source software and website:**

- DWSIM (Industrial reaction modeling, Thermodynamic property estimation, Process optimization.)
- OpenFOAM (Reactor modeling, multiphase systems, Industrial chemical processes)
- CHEMKIN (Computational tools for reaction mechanism analysis)
- Kinetics Database Resources (NIST Chemical Kinetics Database)
- ASCEND (Dynamic and steady-state reactor modeling)

**Suggested Course Practical List:**

- To study RTD in PFR, CSTR and CSTR in series.
- To compare conversion in CSTR and PFR.
- To compare catalytic and non-catalytic reaction conversion.
- To study the performance of quench bed reactor.
- To determine kinetic data and rate equation for esterification reaction.
- To determine kinetic data and rate of reaction for fermentation reaction.
- To verify performance of the Plug flow reactor.
- Design of quench bed reactor for synthesis of ammonia.
- Design of reactor of DCDA (Double Contact Double Absorption) process of sulfuric acid.
- Design of Ammonia oxidation reactor of Nitric Acid plant.



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## List of Laboratory/Learning Resources Required:

- Fluidized Bed Reactor
- Fixed Bed Reactor
- Microwave Reactor
- Autoclave Reactor
- Gas Chromatography Mass Spectrometry (GC/MS)
- High-Performance Liquid Chromatography (HPLC)
- Fourier Transform Infrared Spectroscopy (FTIR)
- UV-Vis Spectrophotometer for reaction kinetics in photochemical studies
- Flow calorimeters for studying reaction heat
- Thermogravimetric Analyzer and Derivative Thermogravimetric Analyzer (TGA/DTG)

## Suggested Activities for Students:

- Design a scale-up strategy for a lab-scale reaction to an industrial pilot plant.
- Work on real-world reaction engineering projects.
- Synthesize and characterize a catalyst

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