GUJARAT TECHNOLOGICAL UNIVERSITY

CHEMICAL ENGINEERING (30)
CHEMICAL REACTOR ANALYSIS
SUBJECT CODE: 3713015
SEMESTER: I

Type of course: Chemical Engineering (Elective-I (b))

Course Outcomes:
At the end of the course, the student will be able to:
1. Evaluate heterogeneous reactor performance considering mass transfer limitations
2. Perform the energy balance and obtain concentration profiles in multiphase reactors.
3. Estimate the performance of multiphase reactors under non-isothermal conditions

Teaching and Examination Scheme:

Teaching Scheme			Credits	Examination Marks				Total Marks
L	T	P	C	Theory Marks		Practical Marks		
				ESE(E)	PA (M)	PA (V)	PA (I)	
3	0	2	4	70	30	30	20	150

Contents:

Sr. No.	Content	Hrs	% weightage
1	**Unit-I:** Chemical factor affecting the choice of the reactor, fundamental mass, energy and momentum balance, Model for a semi-batch reactor, optimum operation policies and control strategies, optimal batch operation time, optimal temperature policies, stability of operation and transient behavior for mixed flow reactor. Transient CSTR analysis, Hot spot equation; Optimization using Lagrange multiplier, Pontryagin's maximum principle.	6	15
2	**Unit-II:** Fixed bed catalytic reactor: The importance and scale of fixed bed catalytic processes, factors in preliminary design, modeling of fixed bed reactor. Pseudo-homogeneous model, the multibed adiabatic reactor, auto-thermal operation, non-steady-state model with axial mixing, two dimensional pseudo-homogeneous models, heterogeneous models, global and intrinsic rates, Mechanism of catalytic reactions, Engineering properties of catalysts - BET surface area, pore volume, pore size, pore size distribution, one dimensional and two dimensional model equation.	8	15
3	**Unit-III:**	8	20

	Multiphase flow reactor: Types of multiphase flow reactors, packed columns, plate columns, empty columns, stirred vessel reactors.Development of rate equations for solid catalyzed fluid phase reactions; Estimation of kinetic parameters. External mass and heat transfer in catalyst particles. Stability and selectivity, Packed bed reactor, slurry reactor; Trickle bed reactor and fluidized bed reactor. Intra-particle heat and mass transfer - Wheelers parallel pore model, random pore model of Wakao and Smith. deactivation of catalyst, Ideal and non-ideal flow in reactors.		
4	**Unit-IV:** Design model for multiphase flow reactors, gas and liquid phase in completely mixed and plug flow, gas phase in plug flow and liquid phase in completely mixed flow, effective diffusion model, two zone model, specific design aspects, packed absorber, two-phase fixed bed reactor, plate column, spray tower, bubble reactor, stirred vessel reactor.Computer - aided reactor design.	14	20
5	**Unit-V:** Temperature effects in reactor: Introduction, well mixed system with steady feed, the stability and start-up of CSTR, limit cycles and oscillatory reactions, the plug flow reactors, tubular reactor, diffusion control, prorogation of reaction zone.	16	30

List of Practicals:

1. Differential and integral method of analysis for kinetics in CSTR
2. Study of saponification reaction in batch reactor to find the kinetic rate constant.
3. Performance study of CSTR
4. Performance study of PFR and location of hot-spot
5. Modeling and simulation of Batch, PFR, and CSTR using CFD software
6. Modeling and simulation of packed bed reactor using CFD software
7. Modeling and simulation of multi-phase reactor using CFD software
8. Transient CSTR analysis for finding kinetics of reaction.
9. Study of temperature effects in hydrodealkylation process plant
10. Evaluation of kinetics of aromatic reaction in micro-reactor
11. Study of light-off behaviour in vehicular exhaust using PFR model
12. Modelling of Platforming reactions/Oxidative coupling of methane

References:

1. Froment G. F. and K.B.Bischoff, " Chemical Reactor Analysis and Design", John Wiley & Sons
2. Denbigh K. G. and J.C. Turner, " Chemical Reactor and Theory – an Introduction", 3rd edition Cambridge University Press.
3. Bruce Nauman, " Chemical Reactor Design", John Wiley & Sons
4. Elements of Chemical Reaction Engineering by H. Scott Fogler
5. Chemical Engineering Kinetics by J. M. Smith.
6. Chemical Reactor Design and Operation by K. R. Westerterp, W. P. M. Van Swaaij and A. A. C.M. Beenackers
7. Chemical Reactor Analysis and Design by G. F. Froment and K. B. Bischoff