Ref. No.: Ex/PG/CHE/PC/T/112/2025

M.E. CHEMICAL ENGINEERING FIRST YEAR FIRST SEMESTER EXAM 2025

ADVANCED CHEMICAL ENGINEERING KINETICS AND REACTOR DESIGN

Full Marks 100

Time: 3 Hours

Use separate Answer Scripts

All symbols have usual meaning; assume any missing data/information

Part –I

Marks:70

CO1 Answer any two questions **[2x 15= 30 Marks]**	
1. a) Write all the steps involved in a heterogeneous chemical reaction deploying porous catalyst. How would you consider surface reaction as the rate limiting step?	[4]
1.(b) Explain using relevant equations the dual site Langmuir – Hinshelwood mechanism for heterogeneous catalytic reaction.	[5]
1(c). For isomerization of n-butane to isobutane over a solid (heterogeneous)catalyst; considering negligible resistance to mass transfer(surface reaction step is the rate limiting or controlling step following a single site Langmuir – Hinshelwood (LH) mechanism); derive the reaction rate equation; also show the plot for the calculation of heterogeneous rate constant, k and adsorption equilibrium constant.	[6]
2. (a) Write a general decay rate equation for catalyst deactivation.	[4]
2.(b) Briefly elucidate the mechanism of catalyst deactivation by (i) poisoning and (ii) coking	[5]
2.(c) (iii) For production of green fuel, a first-order heterogeneous catalytic reaction ($P \rightarrow Q$) is conducted isothermally in a batch reactor on a solid catalyst that is decaying as a result of aging. Derive an equation for conversion as a function of time.	[6]
3.(a) Consider the occurrence of a first order isomerization reaction $A \rightarrow B$ in a catalytic packed bed reactor. Neglecting any radial variation in concentration and assuming the reactor is operated at steady state, find the conversion of A at the reactor exit (neglecting axial dispersion/diffusion) in terms of bulk density of the catalyst bed, k'', S_a, overall effectiveness factor, reactor length, and superficial velocity.	[11]
3.(b) 'In a catalytic packed bed reactor, a low conversion of reactant is observed at both large and small particle sizes of the porous catalyst, while the optimal conversion being achieved in between". Elucidate the statement using a representative plot.	[4]
CO2 **Answer any two questions** **[2x 10= 20 Marks]**	
4. Consider an isothermal shifting order gas phase ($1 >> \varepsilon X$) chemical reaction:	[5+5]

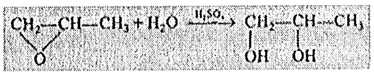
[Turn over

$-r_A^{/} = \frac{k_1^{/} C_A}{1 + k_2^{/} C_A}$ The reaction is conducted in a catalytic PBR. Find an expression relating catalyst weight and conversion of the reactant (considering pressure drop effect) under the following conditions: (a) At high C_A (or $k_2^{/} C_A >> 1$) and (b) At low C_A (or $k_2^{/} C_A << 1$)	
5. Derive the steady state conversion/design equation of a (a) Circulating Fluidized Bed (CFB) Reactor and (b) Moving Bed Reactor considering catalyst deactivation.	**[5+5]**
6. (a) Identify two reasons each for non-ideal behaviour of a packed bed reactor and a CSTR. 6.(b) For a non-ideal CSTR, determine the number of ideal tanks, n, in series that will give approximately the same RTD as the nonideal reactor employing tanks-in-series (T-I-S) model. Hence, find the conversion for a first order reaction as per the model.	**[2+8]**
CO3 **Answer <u>any one</u> between Q.7 and Q.8** **[10 Marks]**	
7. a) A fully turbulent, baffled stirred vessel is to be scaled up by a factor of 512 in volume while maintaining constant power per unit volume. Determine the effects of the scale up on the impeller speed and mixing time.	[6]
7. b) How can 'scale-up of packed bed reactor under constant pressure drop' be achieved? what are the possible limitations of such 'scale-up' strategy?	[4]
8.(a) 'In a tubular catalytic packed bed reactor, it is not always recommended to increase the reactor diameter to decrease the pressure drop for a specified mass flow rate of the feed'. Justify the statement.	[3]
8. (b) For tubular reactors operating with constant physical properties under fully turbulent flow, keeping the mean residence time and pressure drop constant, express the 'scaling factor' for diameter, length, superficial velocity in terms of throughput scale-up factor "S".	[7]
CO4 **Answer <u>any one</u> between Q.9 and Q.10** **[10 Marks]**	

9. (a)Defining steady state multiplicity, elucidate the 'ignition', 'extinction' and 'unstable steady state' temperatures using pertinent plots. **[4]**

9.(b) For a first order irreversible reaction, for which the concentrations of the reacting species are weak functions of temperature; elucidate the construction of the stability diagram to show the regions of stable and unstable operation of a CSTR. What is critical temperature difference? **[5+1]**

10. The hydrolysis of propylene oxide to Propylene glycol:



$$\underset{\diagdown\, O \,\diagup}{CH_2—CH}—CH_3 + H_2O \xrightarrow{H_2SO_4} \underset{OH}{\underset{|}{CH_2}}—\underset{OH}{\underset{|}{CH}}—CH_3$$

There is a glass-lined CSTR of 300-gal capacity. **[10]**

Feed rate of propylene oxide (P.O.) to the reactor is 2500 lb/h (43.04 lb mol/h). The feed stream consists of (1) an equi-volumetric mixture of propylene oxide (46.62 ft^3/h) and methanol (46.62 ft^3/h), and (2) water containing 0.1 wt % H_2SO_4. The volumetric flow rate of water is 233.1 ft^3/h, which is 2.5 times the Methanol-P.O. flow rate. The corresponding molar feed rates of methanol and water are 71.87 and 802.8 lb mol/h, respectively. The volume reduction in water-propylene oxide-methanol mixture upon mixing may be neglected. The temperature of each feed stream is 58°F prior to mixing, but there is an immediate 17°F temperature rise upon mixing due to heat of mixing.

The reaction is first-order in propylene oxide concentration and apparent zero-order in excess of water: $A + B \Rightarrow C$

A is propylene oxide ($C_{p_A} = 35$ Btu/lb mol. °F)
B is water ($C_{p_B} = 18$ Btu/lb mol · °F)
C is propylene glycol ($C_{p_C} = 46$ Btu/lb mol. °F)
M is methanol ($C_{p_M} = 19.5$ Btu/lb mol · °F)

with the specific reaction rate:

$k = Ae^{-E/RT} = 16.96 \times 10^{12}(e^{-32,400/RT})\ h^{-1}$ The units of E are Btu/lb mol.

$$H^{\circ}_{Rx}(68°F) = -226,000 - (-123,000) - (-66,600)$$
$$= -36,400 \text{ Btu/lb mol propylene oxide}$$

The operating temperature cannot exceed 125°F, or too much oxide would be lost by vaporization through the vent system. Can the CSTR be used if it is operated adiabatically? what will be the conversion of PO to glycol?

For awareness only

CO1: Determine the Kinetics of Homogeneous and Heterogeneous Catalytic Reactions (K4)
CO2: Develop the Performance and design equations for two-phase and Multi-phase Reactors (K5)
CO3: Describe the methods of Optimization and Scale up of Reactors
CO4: Assess and Judge the Criteria of Control, Multiplicity and Bifurcation Behaviour and parametric Sensitivity of Reactors (K6)

Ref. Ex/PG/CHE/PC/T/112/2025

M.E. Chemical Engineering - First Year - First Semester 2025

Advanced Chemical Engineering Kinetics and Reactor Design (PG/CHE/PC/T/112)

(Subject code: (PG/CHE/PC/T/112))

FullMarks100

All symbols have usual meaning; Assume any missing data/information

Time: 3 Hours

Questions from all COs must be attempted

CO1 Determine the Kinetics of Homogeneous and Heterogeneous Catalytic Reactions K4

CO2 Develop the Performance and design equations for two-phase and Multi-phase Reactors K5

CO3 Describe the methods of Optimization and Scale up of Reactors

CO4 Assess and Judge the Criteria of Control, Multiplicity and Bifurcation Behaviour and parametric Sensitivity of Reactors K6

Part-II

Marks 30

CO1+CO2 **Answer any one from 1, 2 and 3** **Marks: 10**	
1. The catalytic reaction, $A(g) + 3B(l) \rightarrow C(g) + D(l)$occurs in an isothermal trickle bed reactor. The concentration of B is very high and the rate of reaction is of pseudo first order with respect to A. If the liquid is saturated with A, correlate the conversion of B with the length of reactor.	**10**
2. A reaction $A(l) + B(g) \rightarrow C(l)$ occurs in a 2m^3 slurry reactor using 60μm.catalysts. The molar flow rate of A is 0.7kmol/min. The concentration of B at the gas-liquid interface, $C_{Bi} = 0.014 kmol/m^3$. The catalyst loading required for 30% conversion is 3.95kg/ m^3. The value of bubble phase resistance, $r_b = 0.08 min$. What is the value of combined resistance, r_{cr}, due to reaction and liquid to solid surface mass transfer? If the value of r_{cr} for 40μm catalysts be 0.14min-kg/ m^3 which step is controlling?	**10**
3. For a bubble reactor, correlate $N_A = -D_A \left.\frac{dC_A}{dy}\right\|_{y=0}$ with the bulk and interfacial concentration of reactant, A, and the Hatta number. A reaction aA(g) + bB(l) → cC(l) + dD(g) is occurring in a	**10**

bubble reactor. The volumetric flow rate of liquid feed is L and the molar flow rate of gas phase is F. Correlate the required axial length with F, L, partial pressure of A, liquid phase concentration of A at the outlet, Hatta number and other important parameters, H, gas hold-up, ε, bubble diameter, d_p, D_A and k_l.

CO1+CO4
Answer any two from Question no. 4, 5 and 6
Marks:20

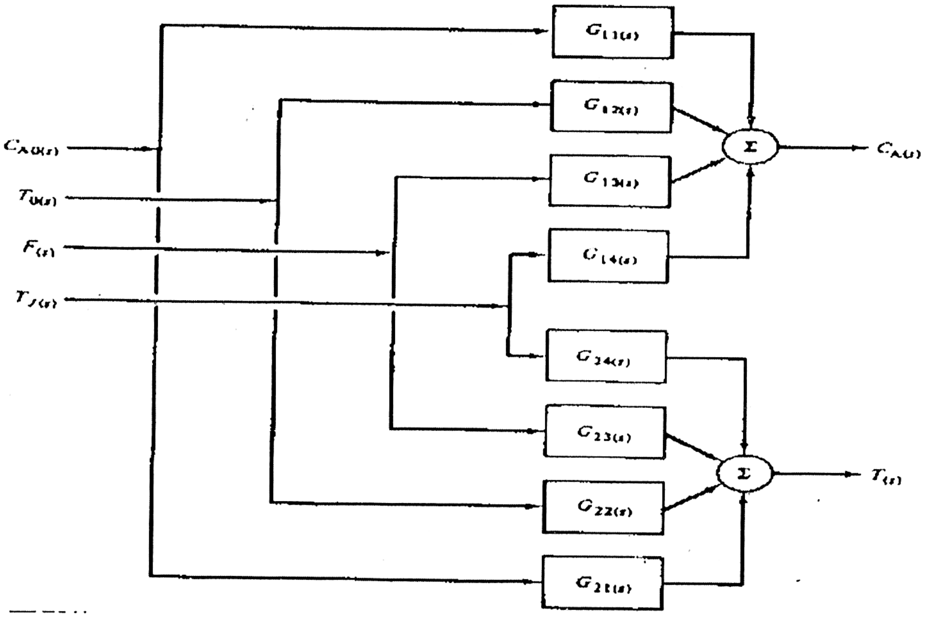
4. An irreversible 1st order reaction, $A \rightarrow B$ is carried out in an ideal CSTR. Write down the mole and energy balance equations in terms of perturbation variables using the concept of Taylor series expansion. The variation of heat of reaction, ΔH_r with temperature can be neglected. Determine the time dependence of concentration of A, i.e., $C_A(t)$, under isothermal condition using the principle of Laplace transformation when a step change in input concentration has been made from zero to C_{A0}. Defining steady state gain and open loop time constant of the process, determine their values if rate constant, $k = 1 min^{-1}$ and residence time, $\tau = 5\ min$. **10**

$$\boxed{\mathcal{L}[e^{-at}] = \frac{1}{s+a}}$$

5. For a jacketed CSTR undergoing a first order reaction, write down the system equations for concentration and temperature under the dynamic state in the following form: **10**

$$\frac{dC_A}{dt} = a_{11}C_A + a_{12}T + a_{13}C_{A0} + a_{14}T_0 + a_{15}F + a_{16}T_j$$
$$\frac{dT}{dt} = a_{21}C_A + a_{22}T + a_{23}C_{A0} + a_{24}T_0 + a_{25}F + a_{26}T_j$$

What is the significance of the following diagram? Determine $G_{11}, G_{12}, G_{13}, G_{14}, G_{15}, G_{16}$.



6. a) What do you mean by bifurcation with respect to steady state stability? For a reaction network, P and Q are the major reactant and product respectively. The dynamics of concentrations of P(C_p) and Q(C_q) are represented by the following equations: 7

$$\frac{dC_p}{dt} = X - YC_p + C_p^2C_q - C_p$$

$$\frac{dC_q}{dt} = YC_p - C_p^2C_q$$

X and Y are two non-zero constants. Determine the locus $(C_{ps}, C_{qs})$of steady state and the condition leading to bifurcation.

b) What do you mean by an autothermal reactor? Explain the operation of an autothermal reactor represented in the following figure: 3

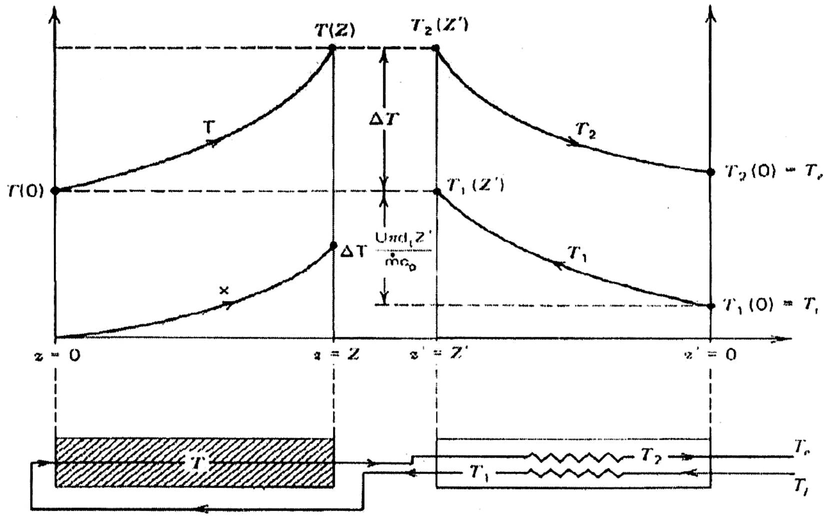


Figure 11