

B. E. Chemical Engineering 3rd Year 2nd Semester Examination, 2025

Chemical Reaction Engineering II

Time: Three Hours

Full Marks: 100

Use separate answer-scripts for Part-I and Part-II

Part – I (50 Marks)

All COs (Course objectives) are compulsory

Assume any missing data

All symbols have their usual meaning

Overall CO-wise marks distribution

CO1	CO2	CO3	CO4	CO5
10	40	10	30	10

PART-I[50 Marks]

CO1	CO2	CO3	CO4
5	20	10	15

CO1 [5 Marks]

1. i) Eley – Rideal mechanism is followed when
 (A) an adsorbed molecule reacts with another adsorbed molecule; (B) an adsorbed molecule reacts with a molecule in gas phase; (C) none of (A) and (B)

(ii) “Make a series of runs in a packed bed reactor with fixed C_{A0} but with varying W or F_{A0} , in such a manner that a wide range of W/F_{A0} and X_{Aout} are obtained”.

For the determination of heterogeneous catalytic reactions, $A \rightarrow \text{Products}$, the above statement is correct in case of:

(A) Differential reactor; (B) Integral reactor; (C) none of (A) and (B).

(iii) For a first order catalytic reaction affected by independent deactivation, how does the internal effectiveness factor, η change with time?

(A) increases; (B) decreases; (C) remains unaffected

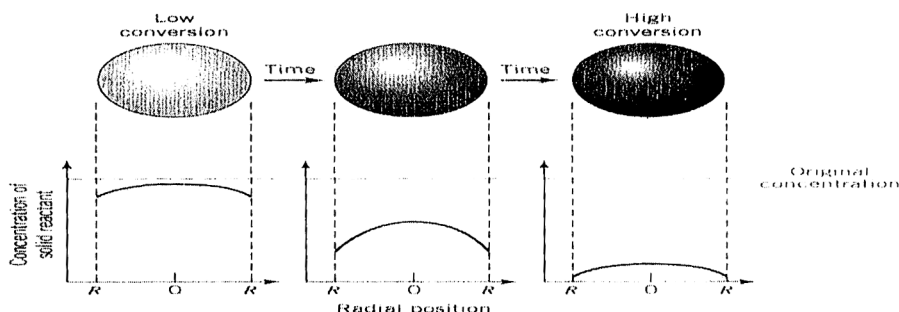
(iv) In case of competitive inhibition, what happens to the value of maximum reaction velocity, $r_{max} = k_3 C_{E0}$ of enzymatic reactions?

(A) decreases; (B) increases; (C) remains unaffected

(v) Out of progressive conversion model (PCM) and shrinking core model (SCM) which

1x5=5

one will fit the following conversion trajectory of the solid in a non-catalytic fluid-solid reaction?



CO2

Answer any two

[20 Marks]

2. A non-catalytic first order heterogeneous reaction involving a solid and a gaseous reactant is occurring in a 0.6m diameter and 9m high up-flow packed bed reactor. The bulk density and mass flow rate of solid are 2100kg/m^3 and 450kg/min respectively. From laboratory experiment, it has been established that 85% conversion of solid particles of size $85\text{-}105\mu\text{m}$ required 10 seconds. Solid hold-up, ϵ_s is 0.01. If the chemical reaction rate is controlling, calculate the average conversion of solid in the reactor if the size analysis and residence time distribution of solids in the reactor are as follows:

9+1

Particle size (μm)	Weight fraction	Residence time $= \frac{\theta}{\theta_s}$
55-65	0.50	0.60
65-75	0.50	0.80

Do you expect any change in the conversion if the solids flow downwards?

3. Reactant A, undergoing a first order reaction, is being converted by passing it through a bed of spherical catalyst solid pellets. The volumetric flow rate of reactant fluid is $1 \times 10^{-6} \text{ m}^3/\text{s}$. Both internal and external mass transfer resistance have to be considered. If the internal diameter of the reactor be 50mm, determine the length required for a conversion of 90%.

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Data: $S_g = 530 \text{ m}^2/\text{g}$, $k = 4.42 \times 10^{-10} \text{ m}^3/\text{m}^2\cdot\text{s}$; $D_e = 1.82 \times 10^{-8} \text{ m}^2/\text{s}$; $R = \text{radius of catalyst} = 3\text{mm}$, $\epsilon = 0.5$, $\rho_c = \text{density of particle} = 2800\text{kg/m}^3$, $a_c = 500\text{m}^{-1}$, $k_c = 5.99 \times 10^{-5} \text{ m/s}$.

4. a) Determine the amount of catalyst to achieve 30% conversion for a catalytic reaction $A \rightarrow 3R$ if the molar flow rate of reactant, A is 1000mol/h , $C_{A0} = 0.1\text{mol/L}$ and reaction rate constant is $95\text{L/h}\cdot\text{kg catalyst}$.

4.b) Catalytic conversion of gas oil following second order kinetics is being conducted

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with a reaction rate constant of $0.6 \frac{dm^6}{(g \text{ cat})-mol-min}$ in a packed bed reactor. Simultaneously the catalyst is getting deactivated following first order independent deactivation kinetics with a rate constant of $0.7 min^{-1}$. The reaction volume can be considered to be constant. The amount of catalyst is 20kg and flows through at a rate of 10kg/min. The molar flow rate of gas oil is 25mol/min with a concentration of $0.1 mol/dm^6$. Determine the conversion in the bed. 5.a) For a fluidized bed reactor in which a first order reaction is being conducted, show that $\ln \frac{C_b}{C_{bf}} = -\frac{1}{u_b} [\frac{1}{k_m a_v} + \frac{1}{\epsilon_d \rho_d k'}]^{-1} Z$ stating the significance of all variables involved in the correlation. 5b) For an adiabatic packed bed reactor, show that: $T - T_f = \frac{F(-\Delta H)}{F_T C_P} (X - X_f)$ State the significance of all parameters:	7 5 5
CO3 10	
6.a) An enzymatic reaction $S + E \rightarrow P + E$ follows Michaelis -Menten kinetics and hence $-\frac{dC_S}{dt} = \frac{dC_P}{dt} = r = \frac{r_{max} C_S}{K_M + C_S}$. What are r_{max} and K_M? What change in the rate equation would you expect if a compound B competitively inhibits the reaction? 6.b) The following plot is for a continuous stirred tank bioreactor with D and C_{SS}, expressed in units of h^{-1} and g/L respectively. What are the values of μ_{max} and K_S? Plot of 1/D versus 1/ C_{SS} $y = 6.5274x + 3.3245$ $R^2 = 0.9872$ 6. c) If a microorganism in a $5m^3$ continuous stirred tank bioreactor under steady state follows Monod type kinetics with $\mu_{max} = 0.3 h^{-1}$ and $K_S = 0.2 \frac{g}{L}$, what flow rate must	2 2 5

be maintained at inlet and outlet to keep the substrate concentration of 1.5g/L in the outlet stream? 7. If a slurry reactor is operated under reaction kinetics controlled regime, what change would you expect in the slope of $\frac{C_i}{r_i}$ versus $\frac{1}{m}$ plot with change in particle size of catalyst?	1
CO4 Answer any one 15	
8. a) A catalytic reaction, $P(l) + qQ(g) \rightarrow R(l) + S(g)$ is occurring in a trickle bed reactor. The liquid phase is always saturated with Q. The concentration of P is low and the reaction follows pseudo-first order kinetics with respect to the concentration of P. Considering the superficial liquid velocity, reaction rate constant, volumetric coefficient for liquid to catalyst surface mass transfer of P and effectiveness factor to be u_l; k_p'; $(k_c a_c)_p$ and η respectively. Correlate the conversion of P as a function of reactor length if the dispersion in the bed can be neglected. 8.b) A 4L slurry reactor is used for the reaction of Liquid reactant, A with a gaseous reactant, B. The resistance associated with mass transfer from gas-liquid interface to bulk liquid is 0.08 min. The combined resistance of liquid to solid surface mass transfer and reaction is 0.21 min-g/L. Determine the catalyst loading for 50% conversion at a 0.7mol/min feed rate of A. The interface concentration of B is 0.014mol/L. 9. a) Thiophene in gas oil is hydrogenated($C_4H_4S + 4H_2 \rightarrow C_4H_{10} + H_2S$) in a trickle bed reactor. Both gas oil and hydrogen are co-fed from the top of the reactor and flows downwards in co-current mode. The liquid phase is always saturated with hydrogen. The reaction rate can be considered to be controlling. The dispersion in the bed can be neglected. The thiophene concentration is large with respect to that of hydrogen and the reaction can be treated to be of pseudo-first order with respect to hydrogen concentration. Determine the reactor length for 80% conversion of thiophene with the following data: $C_{Th,in} = 1000ppm, C_{H_2g} = \frac{1.03 \times 10^{-3} kmol}{L}$; superficial liquid velocity = 0.05m/s $k_{H_2}' = 0.11 \frac{L}{kg.s}$; $(k_c a_c)_{H_2} = 0.5 s^{-1}$; $H_{H_2} = 50$ (where, $C_{H_{2L}} = \frac{C_{H_{2g}}}{H_{H_2}}$); $\rho_b = 0.96 kg/L$ 9.b) For a slurry reactor in which a gas phase reactant reacts with a liquid phase one in presence of solid catalysts, the following steps are involved:	8 7 10 5

1. Mass transfer from the bulk concentration in the gas bubble to the bubble-liquid interface
2. Mass transfer from the bubble interface to the bulk liquid phase
3. Diffusion from the bulk liquid to the external surface of the solid
4. Internal diffusion of the solid reactant in the porous catalyst
5. Reaction within the porous catalyst

Correlate the gas-liquid interface concentration of gas phase reactant and reaction rate with catalyst loading. Define all types of resistances prevailing in the system and their significance. State the steps to determine the controlling step in the system.

For awareness only

CO1: **Define** and **describe** non-catalytic and catalytic heterogeneous reaction kinetics **K1 and K2**

CO2 **Develop** rate equations for different types of heterogeneous reactions **K3**

CO3 **Solve** the rate equations for heterogeneous reactions and **analyze** the controlling steps **K3&K4**

CO4 **Formulate** design equations for heterogeneous reactors and **predict** their performance **K5& K6**

CO 5 **Explain** steady state multiplicity in CSTRs **K6**

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Use separate answer-scripts for Part-I and Part-II

PART-II [50 Marks]

Assume any missing dataAll symbols have their usual meaning

CO1	CO2	CO4	CO5
5	20	15	10

CO1: Answer <u>Q.No.1</u>	Marks
1.a) Write all the steps involved in a heterogeneous chemical reaction deploying porous catalyst. When can you consider surface reaction as the rate limiting step?	[2.5]
1.(b) How do you define “activity” of a catalyst? Write a general decay rate equation mentioning the pertinent terms.	[2.5]
CO2: Answer any <u>Two questions</u>	Marks
2. (a) A pure carbon (C) particle 0.010 m in diameter is to be burned in 21% oxygen at 850°C. Density of C particle =2000kg/m ³ . Reaction rate constant for the pure carbon combustion, k=2.5 m ³ /kmol.s. The gas film diffusion may be neglected since a considerably high gas velocity is maintained during combustion. Find the time required for complete combustion of the carbon particle, assuming chemical reaction is the controlling step.	[5]
2.(b) A packed bed reactor converts A to R by a first-order catalytic reaction, $A \rightarrow R$. With 9-mm pellets the reactor operates in the strong pore diffusion resistance regime and gives 63.2% conversion. If these pellets were replaced by 18-mm pellets how would this affect the conversion?	[5]
3. Consider a chemical reaction $R \Rightarrow \text{Product}$ being conducted in a heterogeneous catalytic continuous flow expanded bed reactor where the solid (catalyst) fraction ‘ ψ ’ varies with catalyst bed	[10]

height 'y'. U_0 = superficial gas velocity, A= cross-sectional area of the reactor; H= Total Reactor height. Derive the steady state design equation to find conversion (X_R). 4. A first-order reaction $R \rightarrow S, \Delta H_r = 0$ is being conducted at 1 atm and 609 K in a Mixed Flow (Basket-Type) Reactor with 0.01kg of 0.0012 m catalyst particles at a feed rate of $4 \times 10^{-6} \text{ m}^3/\text{s}$ of pure R. Under these conditions, 80% conversion of R can be achieved. It is envisaged to design a high capacity commercial-sized reactor with 80% conversion at the above conditions. The choice is between a fluidized bed (approximated as MFR) with 0.001 m particles and a PBR with 0.015 m particles. Which reactor type should be selected to minimize the catalyst amount?	[10]
CO4: Answer <u>Q.No.5(a)</u> and any <u>one</u> between 5.(b) and 5.(c)	Marks
5. (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'. Elucidate the statement with respect to overall reactor performance for an exothermic reversible reaction . 5.(b) Consider an isothermal shifting order gas phase ($1 \gg \epsilon X$) chemical reaction: $-r'_A = \frac{k'_1 C_A}{1 + k'_2 C_A}$ 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: (i) At high C_A (or $k'_2 C_A \gg 1$) and (ii) At low C_A (or $k'_2 C_A \ll 1$) 5.(c) Consider that a catalytic PBR is operated under isothermal condition, assuming $1 \gg \epsilon X$; for a third order isothermal reaction $3 R \rightarrow Q$. Find an expression relating catalyst weight and conversion of the reactant and find the pressure profile; i.e. the total pressure (P) as a function of catalyst weight (W_c). Hence, show the nature of the plots of (i) Pressure as function of catalyst weight; (ii) reactant conversion as function of catalyst weight. The pressure drop in the catalytic PBR may be computed using Ergun Equation: $\frac{dP}{dy} = \frac{-G}{\rho g_c d} \frac{(1-\psi)}{\psi^3} \left[\frac{150(1-\psi)\mu}{d} + 1.75G \right]$	[5] [5+5] [5+5]
CO5: Answer any <u>One question</u>	Marks
6.(a) Briefly explain the method of finding the conversion –temperature plot for a reversible exothermic 1st order reaction, assuming that the required thermodynamic data are known. Hence,	[4]

graphically find the equilibrium conversion and corresponding reaction temperature.	
6. (b) Briefly explain (graphically) the optimum temperature progression for a reversible exothermic reaction.	[3]
6.(c) Explain the graphical method of finding the volume of an adiabatic plug flow reactor (PFR) in case of reversible first-order exothermic reaction.	[3]
7. For a plug flow reactor(PFR)/tubular reactor, in which heat is either added or removed through the cylindrical walls of the tubular reactor, assuming that there are no radial gradients in the reactor, carry out a steady-state energy balance to derive the energy balance equation for finding the temperature profile in the reactor. Define clearly all pertinent terms in the equations. Also, show the energy balance equation for a packed bed reactor (PBR).	[10]