

B. Chemical Engineering 3rd Year 2nd Semester Examination, 2022

Chemical Reaction Engineering II

Time: Three Hours

Full Marks: 100

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

All COs (Course objectives) are compulsory

Assume any missing data

All symbols have their usual meaning

CO-wise marks distribution

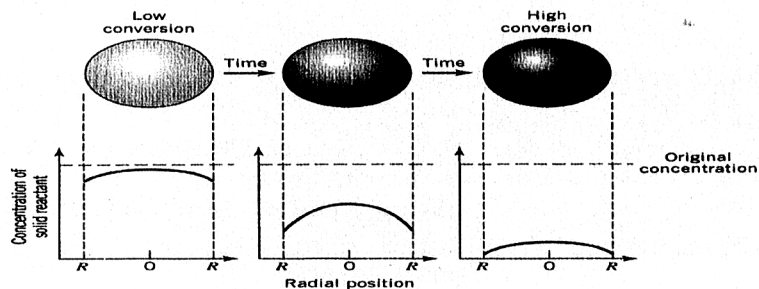
CO1	CO2	CO3	CO4	CO5
5	30	10	45	10

PART-I [50 Marks]

CO1 [5 Marks]

Answer any one

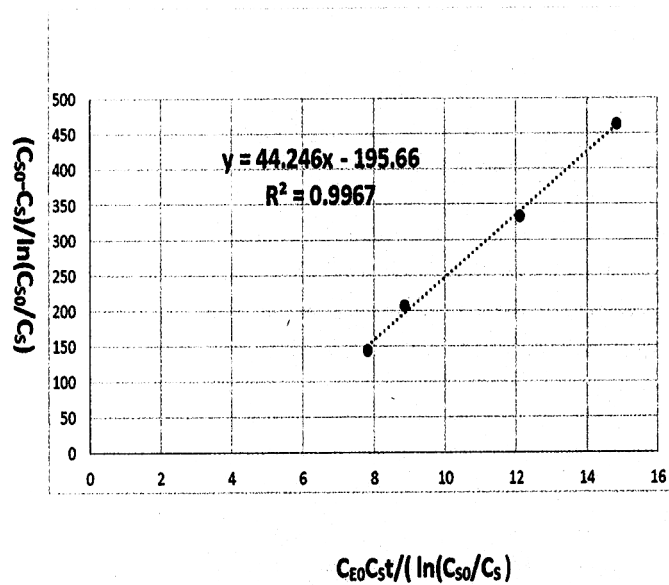
1. A) Out of progressive conversion model (PCM) and shrinking core model (SCM) which one will fit the following conversion trajectory of the solid in a non-catalytic fluid-solid reaction? [1]



- B) If the internal mass transfer resistance strongly dominates a catalytic reaction having true values of activation energy and order of 30kJ/mol and 2.0 respectively, what would be the apparent values of activation energy and order? Justify your answer. [2]

- C) For an enzymatic reaction conducted in a batch reactor, the following plot has been obtained.

[Turn over



C_5 and C_{50} are in mol/m^3 , C_{E0} is in g/m^3 and time is in hour
 What is the value of Michaelis-Menten constant? [1]

D) For a first order catalytic reaction using batch solid and continuous flow of fluid in presence of independent catalyst deactivation the following equation is valid

$$\frac{C_{A0}}{C_A} = 1 + k' e^{-k_d \tau'}$$

What are k' and τ' ? [1]

2. a) Define the following terms with respect to characteristics of a catalyst: [3x1=3]

i) Activity, ii Selectivity, and iii) Stability.

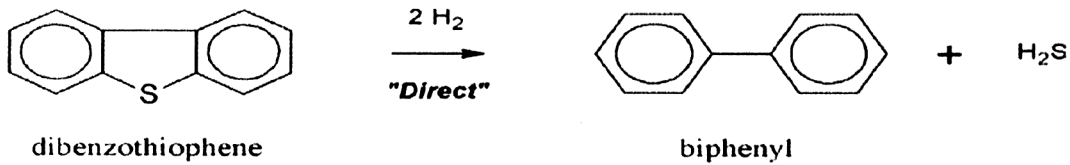
b) What is bi-functional catalyst? Give one example. [2]

CO4 [45 Marks]

Answer any three questions

3. The catalytic cracking of gas oil A follows 2nd order reaction in a conveyer moving bed reactor. Due to formation of coke independent deactivation occurs. $r_A = 0.6 \frac{\text{dm}^3}{(\text{g Cat.}) \cdot \text{mol} \cdot \text{min}} C_A^2$; $k_d = 0.72 \text{min}^{-1}$. The reactor contains 20kg of catalyst moving at a rate of 10kg/min. The gas oil is fed at a rate of 50 mol/min at a concentration of $0.1 \text{mol}/\text{dm}^3$. Determine the conversion that can be achieved in this reactor. [15]

4. The catalytic hydro-desulfurization of dibenzothiophene (DBT) of diesel is as follows:



Correlate the conversion of DBT with respect to axial length of a trickle bed reactor when a) the reaction is of pseudo-first order with respect to hydrogen concentration due to high concentration of DBT (1000ppm) in feed diesel, if the liquid is saturated with hydrogen; b) the reaction is of pseudo-first order with respect to the concentration of DBT as its concentration is low. [7.5+7.5]

5. A fluidized bed reactor operates in bubbling regime. Dense phase is well mixed. Reaction occurs mainly in dense phase. The bubble moves in plug flow. If $\rho_d=0.01\text{kg/L}$, $k_m a_v=0.6\text{s}^{-1}$; $k=50 \frac{\text{L}}{\text{kg.s}}$; $u_b=0.1\text{m/s}$; $z=L=0.4\text{m}$; $\epsilon_d=0.8$ determine the conversion. [15]

6. The reduction of iron ore of particle diameter of 10 mm and density of 4.6 gm/cm^3 by pure hydrogen gas can be represented as $4\text{H}_2 + \text{Fe}_3\text{O}_4 \rightarrow 4\text{H}_2\text{O} + 3\text{Fe}$. With no water vapor present, the process follows shrinking-core model well. The first order rate constant is given by $k'' = 1.93 \times 10^5 e^{-12078/T}$, cm/s. Calculate the time needed for complete conversion of a particle of oxide at a temperature of 600°C and at a pressure of 1 atm by neglecting gas film resistance. Take $D_e = 0.03 \text{ cm}^2/\text{s}$, the diffusion coefficient for hydrogen penetration. [15]

7. The catalytic reaction $A \rightarrow 3R$ is carried out in a packed bed reactor at 3.5 atm and 115°C . It is desired to treat 1500 mol/h pure A to achieve 32% conversion. The following rate-concentration data are available:

C_A , mol/liter	0.04	0.06	0.075	0.09
$-r'_A$, mol A/kg cat.h	3.5	5.7	7.2	8.8

Find out the amount of catalyst needed for this reaction. [15]

8. The following data of the gaseous second order reaction $A \rightarrow R$ are obtained in experimental catalytic packed bed reactor with $C_{A0} = 60 \text{ mol/m}^3$ and $v_0 = 3 \text{ liter/min}$.

W , gm catalyst	0.50	1.0	2.5
C_A , mol/m ³	30	20	10

Find the rate constant and the rate equation for this reaction. [15]

PART-II [50 Marks]**CO2 [30 Marks]****Answer any three questions**

1. 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:

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?

[10]

2. For cylindrical catalysts, determine the expression for effectiveness factor if the reaction is of 1st order. You can use the following mathematical information.

Generalized Bessel's equation:

$$x^2 \frac{d^2 y}{dx^2} + x(a + 2bx^r) \frac{dy}{dx} + [c + dx^{2s} - b(1 - a - r)x^r + b^2 x^{2r}] y = 0$$

$$y = x^{\left(\frac{1-a}{2}\right)} e^{-\left(\frac{bx^r}{r}\right)} \left[AZ_p\left(\frac{\sqrt{|d|}}{s} x^s\right) + BZ_{-p}\left(\frac{\sqrt{|d|}}{s} x^s\right) \right]$$

$$p = \frac{1}{s} \sqrt{\left(\frac{1-a}{2}\right)^2 - c}$$

If $\frac{\sqrt{d}}{s}$ is imaginary and p is zero or integer, $Z_p = I_n$; $Z_{-p} = K_n$.

$$K_0(0) \rightarrow \infty \text{ and } \frac{d}{dx} x^{-p} Z_p(\alpha x) = \alpha x^{-p} Z_{p+1}(\alpha x)$$

[10]

3. The elementary irreversible 1st order gas-phase catalytic reaction $A \rightarrow B$ is carried out isothermally in a batch reactor. The catalytic deactivation follows a first order decay law and is

independent of the concentration of both A and B.

a) Derive the equations to predict the time trajectories of catalyst activity and conversion.

b) Calculate the catalytic activity and conversion after 10 minutes at 300K.

Additional information:

$$C_{A0} = 1 \frac{\text{mol}}{\text{L}}; V = 1\text{L}; W = 1\text{kg}; k_d = 0.1\text{min}^{-1}; k' = 0.1\text{L}(\text{kg Cat} - \text{min})^{-1}\text{at } 300\text{K};$$

$$\frac{E_d}{R} = 2000\text{K}; \frac{E_A}{R} = 500\text{K} \quad [10]$$

4. Two small samples of solids are roasted isothermally in a constant environment in air stream. The following data is obtained:

R, mm	Time, h	X _B
2	1	0.578
1	1	0.875

Assume that the reaction follows the SCM. a) Find the rate controlling mechanism and rate equation.

b) Determine the time needed for complete conversion of the solid of size R = 1 mm, all other parameters remain unchanged. [10]

5. The data obtained for a first order solid catalyzed gas phase reaction, in absence of pore diffusion resistance, as follow: Rate of the reaction ($-r_A^m$) = 10^{-6} mol/(s·cm³ catalyst) with $C_A = 1.81 \times 10^{-5}$ mol/cm³ at 1 atm and 400°C. Determine the largest size of catalyst pellet that should be used to ensure negligible pore diffusion for this reaction. The effective diffusivity of A in catalyst pellet = 10^{-3} cm²/s. [10]

6. Substrate A and enzyme E flow through a MFR (V = 10 liter). Find a rate equation to represent the action of enzyme on the substrate using the following data:

Parameters	Run 1	Run 2	Run 3	Run 4
C_{A0} , mol/liter	0.2	0.3	0.4	0.6
C_A , mol/liter	0.05	0.15	0.25	0.5
v , liter/h	3	6	7	12

The concentration of enzyme is fixed for each run, $C_{E0} = 0.02$ mol/liter. [10]

CO3 [10 marks]

Answer any two questions

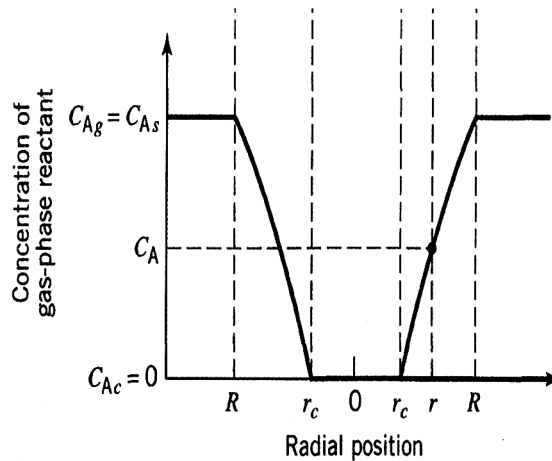
7. a) For the determination of rate equation of the enzymatic hydrolysis of A, some experiments were conducted in a CSTR with and without a component B. When C_S is plotted against $(C_{E0}C_S T / (C_{S0} - C_S))$, the following correlations are obtained

Without B	$C_S = 20(C_{E0}C_S T / (C_{S0} - C_S)) - 200$	Slope=20 Intercept=-200
With B	$C_S = 13.992(C_{E0}C_S T / (C_{S0} - C_S)) - 200$	Slope=13.992 Intercept=-200

Write down the rate equation for the enzymatic reaction in absence of B. What is the role of B in the reaction? Justify your answer showing all derivations. **[3]**

7. b) At wash out condition, what is the value of biomass concentration in a continuous stirred tank bioreactor (CSTBR)? What is the relationship between μ and D for a CSTBR under steady state? **[1+1]**

8. a) The following figure represents the radial concentration profile of gaseous reactant, participating in a noncatalytic gas-solid reaction, across the spherical solid reactant.



$R =$ radius of the particle; $r_c =$ radius of unreacted core

Which resistance is controlling?

[1]

8. b) It has been observed that 60% conversion of reactant A is achieved during its hydrogenation in a 4m^3 slurry reactor using 5kg/m^3 loading of $60\mu\text{m}$ spherical catalyst. If the inlet molar flow rate of reactant A is 0.7kmol/min , value of r_{cr} is $0.21\text{min}\cdot\text{kg/m}^3$ and the interfacial concentration of hydrogen is 0.014kmol/m^3 , determine the value of bubble to liquid phase mass transfer resistance, r_b . If the overall reaction is internal mass transfer controlled, do you expect any change in the catalyst loading if the stirring rate is doubled? **[4]**

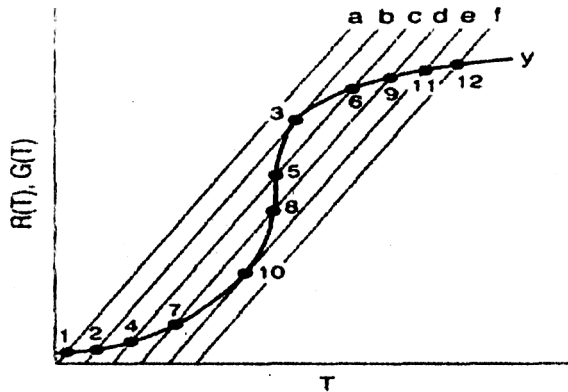
9. A catalytic reaction $A \rightarrow R$ is made in a packed bed employing a large recycle of product stream. Find the amount of catalyst that would be required for a feed rate of 300 kmol/h to achieve 45% conversion of A with $-r'_{A,out} = 0.60$ kmol/kg catalyst·h. [5]

10. Discuss Mears' and Weisz Prater criterions for rate controlling resistances for solid catalyst. [5]

CO 5 [10 Marks]

Answer any one question

11. a) What is meant by steady state multiplicity? With proper justification, sketch the ignition-extinction plot showing lower and upper steady state lines and locate the steady state points. Make a brief discussion about the stability of these steady states. Use the following figure:



11.b) What do you mean by runaway of a reactor? What is the upper limit of $(T^* - T_c)$ to avoid runaway? Justify with derivations. [4+6]

12. The elementary irreversible liquid-phase reaction $A \rightarrow B$ takes place in a CSTR with a heat exchanger. Pure A enters the reactor. $G(T)$ as a function of T is given below: [10]

$G(T)$, Cal/mol	0	3000	6000	20000	50000	65000	68000	70000	72000
T , Kelvin	300	325	350	375	400	425	450	475	500

Find the steady-state temperatures for the CSTR in a graph paper.

Given: $UA = 3600$ cal/min·K, $C_{p0} = 40$ cal/mol·K, $F_{A0} = 10$ mol/min, Ambient Temperature, $T_a = 27^\circ\text{C}$, Feed Temperature, $T_a = 27^\circ\text{C}$.

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**