

KATHMANDU UNIVERSITY
End Semester Examination
July/August, 2024

Marks Scored:

Level : B.E.

Year : III

Exam Roll No. :

Time: 30 mins.

Course : CHEG 312

Semester : II

F. M. : 10

Date :

08 AUG 2024

Registration No.:

SECTION "A"

[20 Q. × 0.5 = 10 marks]

Choose and encircle in the most appropriate option from each set of choices

- For the reaction $A + B \rightarrow C$, if doubling the concentration of A doubles the rate of the reaction while doubling the concentration of B has no effect, what is the order of the reaction with respect to A and B?
 - Zero order in A, first order in B
 - First order in A, zero order in B
 - First order in both A and B
 - Second order in A, zero order in B
- In a batch reactor, the conversion of a reactant A follows first-order kinetics. If the initial concentration of A is 2 mol/L and the rate constant is 0.5 hr^{-1} , what is the concentration of A after 2 hours?
 - 0.5 mol/L
 - 0.74 mol/L
 - 1.22 mol/L
 - 2.43 mol/L
- Which of the following is a characteristic of an ideal plug flow reactor (PFR)?
 - Complete back-mixing
 - Axial mixing
 - No radial mixing
 - Constant residence time for all molecules
- The Langmuir adsorption isotherm is applicable to:
 - Monolayer adsorption
 - Multilayer adsorption
 - Chemisorption
 - Physisorption
- In enzyme kinetics, competitive inhibition:
 - Increases K_m and decreases V_{max}
 - Increases K_m and has no effect on V_{max}
 - Decreases K_m and has no effect on V_{max}
 - Has no effect on K_m and decreases V_{max}
- Pick the correct statement about Thiele modulus
 - Measures the ratio of internal diffusion rate to external diffusion rate
 - Measures the ratio of internal diffusion to surface reaction rate
 - Measures the effect of catalyst particle diameter on the reaction rate
 - Measures the ratio of surface reaction rate to internal diffusion rate
- Bulk diffusion in catalyst pore _____ with increase in pressure:
 - Increases
 - Decreases
 - Remain unchanged
 - Increases exponentially

8. For a first order decay law the catalyst activity is equal to zero in:
- Infinite time
 - At the beginning of the reaction
 - At halfway through the reaction
 - Never reaches zero
9. The Weisz-Prater criterion value of greater than 1 suggests:
- No internal diffusion limitation
 - Some internal diffusion limitation
 - Severe internal diffusion limitation
 - The criterion does not provide information on internal diffusion limitation
10. The Weisz-Prater and Mear's criterion help determine if:
- Internal diffusion and mass transfer from bulk to catalyst surface is the rate limiting step
 - Internal diffusion or catalytic surface reaction is the rate limiting step
 - The catalytic reaction rate
 - Helps measure the activation energy for a catalytic reaction mechanism
11. For a first order reaction $A \rightarrow$ products, what is the conversion expression for batch reactor?
- $X(t) = 1 - \exp(-kt)$
 - $X(t) = 1 - 2\exp(-2t)$
 - $X(t) = 1 - \exp(-kt)$
 - $X(t) = 1 + \exp(-2kt)$
12. For the gas phase reaction $A(g) \rightarrow 3B(g)$ obeys zeroth-order kinetics with $r = 0.25$ moles/liter·hr at 200 C. Starting with pure A at 2 atm, calculate the initial concentration of A.
- 0.0212 mol/L
 - 0.0516 mol/L
 - 0.000233 mol/cm³
 - 0.000267 mol/cm³
13. For the elementary and reversible reaction $2A + B \rightleftharpoons C$ the correct rate law expression is:
- $-r_A = k_A * [C_A^2 C_B - C_C / K_C]$
 - $-r_A = k_C A^2 / C_B$
 - $-r_A = k_A * [C_A C_B - C_C / K_C]$
 - $r_A = k_A * [C_A^2 C_B - C_C / K_C]$
14. For rapid reaction on the catalyst surface the molar flux expression is given by:
- $W_{Az} = k_C * C_{Ab}$
 - $W_{Az} = k_C * (C_{Ab} - C_{As})$
 - $W_{Az} = D_{AB} * (C_{Ab} - C_{As})$
 - $W_{Az} = D_{AB} * (C_{Ab} - C_{As})^2$
15. The presence of a long tail in the residence time distribution curve of a packed bed reactor is an indication of:
- Ideal plug flow
 - Channeling
 - Dead zone
 - Bypass
16. For the water gas shift reaction ($H_2O + CO \rightleftharpoons CO_2 + H_2$) at 1000 K and 10 atm with an equilibrium constant of 1, what is the equilibrium conversion? Assume an equimolar feed of water and carbon monoxide.
- 0.385
 - 0.484
 - 0.555
 - 0.692
17. For the water gas shift reaction given in the previous problem what is the equilibrium concentration of carbon monoxide in mol/dm³? $R = 0.082 \text{ dm}^3 \cdot \text{atm} / \text{mol} \cdot \text{K}$
- 0.0235
 - 0.0375
 - 0.0545
 - 0.0625

18. For an enzymatic biological reaction the doubling of the amount of enzyme will affect what parameter of the M-M reaction kinetics?
- a. Concentration of the substrate
 - b. Michaelis constant
 - c. Turnover number
 - d. Maximum specific growth reaction rate
19. For the reaction $3A \rightarrow B$, pure gas A is fed to the reactor at constant temperature and pressure. The concentration of A is given by,
- a. $C_A = C_{A0}*(1 - X)$
 - b. $C_A = C_{A0}*(1 - X) / (1 - 2X)$
 - c. $C_A = C_{A0}*(1 - X) / (1 - 0.67X)$
 - d. $C_A = C_{A0}*(1 - X) / (1 + 2.5X)$
20. The specific reaction rate for a certain reaction is 31.1 h^{-1} at 360 K. If the activation energy for the reaction is 65.7 kJ/mol, what is the specific reaction rate at 338.6 K?
- a. 31.1 h^{-1}
 - b. 31.76 h^{-1}
 - c. 14.76 h^{-1}
 - d. 7.76 h^{-1}

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F. M. : 40

SECTION "B"
[40 marks]

Attempt ALL questions.

1. The following complex gas-phase reactions follow the elementary rate laws
- | | | |
|-------------------------|--------------------------------|---|
| $A + 2B \rightarrow C$ | $-r_{1A} = k_{1A} C_A C_B^2$ | $\Delta H_{rxn1B} = -15 \text{ kcal/mol B}$ |
| $2A + 3C \rightarrow D$ | $-r_{2C} = k_{2C} C_A^2 C_C^3$ | $\Delta H_{rxn1B} = -10 \text{ kcal/mol A}$ |

and take place in a PFR. The feed is stoichiometric for reaction (1) in A and B with $F_{A0} = 5 \text{ mol/min}$. The reactor volume is 10 dm^3 and the total entering concentration is $C_{T0} = 0.2 \text{ mol/dm}^3$. The entering pressure is 100 atm and the entering temperature is 300 K . The coolant flow rate is 50 mol/min and the entering coolant fluid has a heat capacity of $C_{p,cool} = 10 \text{ cal/mol.K}$ and enters at a temperature of 325 K . The following information is provided.

$$k_{1A} = 40 \left(\frac{\text{dm}^3}{\text{mol}} \right)^2 / \text{min} \text{ at } 300\text{K} \text{ with } E_1 = 8,000 \text{ cal/mol}$$

$$k_{2C} = 2 \left(\frac{\text{dm}^3}{\text{mol}} \right)^4 / \text{min} \text{ at } 300\text{K} \text{ with } E_2 = 12,000 \text{ cal/mol}$$

$$C_{pA} = 10 \text{ cal/mol/K}$$

$$Ua = 80 \frac{\text{cal}}{\text{min} \cdot \text{K}}$$

$$C_{pB} = 12 \text{ cal/mol/K}$$

$$T_{a0} = 325 \text{ K}$$

$$C_{pC} = 14 \text{ cal/mol/K}$$

$$\dot{m} = 50 \text{ mol/min}$$

$$C_{pD} = 16 \text{ cal/mol/K}$$

$$C_{p,cool} = 10 \text{ cal/mol/K}$$

$$\frac{dT}{dV} = \frac{\sum_{i=1}^q -r_{ij} [-\Delta H_{rxn ij}(T)] - Ua(T - T_a)}{\sum_{j=1}^m F_j C_{p,j}}$$

For the case of constant coolant temperature, write the complete algorithm to solve the problem in the sequence of CRE pyramid. Simplify equations where possible. [8]

P.T.O.

2. An irreversible liquid phase elementary reaction $A + B \rightarrow R$ is conducted in an adiabatic reactor. The reactants are fed in equimolar concentrations at 27 °C and 0.02 m³/s. Calculate
- The PFR volume to achieve 85% conversion. [4]
 - The maximum input feed temperature allowed if output temperature is not to exceed 550 K. [2]

The following data is provided.

$$k = 1.93 \times 10^5 e^{-(10,000/RT)}$$

$$H_A^0(273 \text{ K}) = -20 \text{ kcal/mol}$$

$$E = 10 \text{ (kcal/mol)}$$

$$H_B^0(273 \text{ K}) = -15 \text{ kcal/mol}$$

$$C_{A0} = 0.1 \text{ (kmol/m}^3\text{)}$$

$$H_R^0(273 \text{ K}) = -41 \text{ kcal/mol}$$

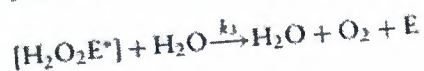
$$C_{PA} = C_{PB} = 15 \text{ cal/mol K}$$

$$C_{PR} = 30 \text{ cal/mol K}$$

The energy balance equation is given by,

$$T = T_{i,0} - \frac{\Delta H_{rxn}(T) \cdot X_A}{\sum_{i=1}^n \Theta_i C_{p,i}}$$

3. Decomposition of H₂O₂ occurred in the presence of an enzyme E in a batch reactor and the corresponding concentrations are presented in the table below.



t (min)	0	10	20	50	100
[H ₂ O ₂] (mol/L)	0.02	0.0177	0.0158	0.0106	0.005

Using enzymatic kinetic model

- Derive the reaction rate $-r_s = \frac{V_{max}[\text{H}_2\text{O}_2]}{K_M + [\text{H}_2\text{O}_2]}$ [5]
- Calculate the Michaelis constant and the maximum rate [3]
- Calculate the time needed to reach 95% conversion if the enzyme concentration is tripled. [2]

4. The third order liquid phase reaction $A \rightarrow B$ was carried out in a reactor that the following RTD

$$E(t) = 0 \text{ for } t < 1 \text{ min}$$

$$E(t) = 1 \text{ for } 1 \leq t \leq 2 \text{ min}$$

$$E(t) = 0 \text{ for } t > 2 \text{ min}$$

The entering concentration of A is 2 mol/dm^3 .

- a. What is the conversion predicted by PFR, LFR and the segregated model. [6]
 b. Suppose the reaction is carried out adiabatically with entering temperature of 305 K. Write the algorithm for calculating conversion by segregation model. [2]
5. When the impurity cumene hydroperoxide (CHP) is present in trace amounts in a cumene feed stream, it can deactivate the silica-alumina catalyst over which cumene (C) is cracked to form benzene (B) and propylene (P). The following data were taken from the reactor operating at 1 atm and 420°C when the feed consists of cumene (99.92%) and trace (0.08 mol%) of CHP.

Benzene mol fraction in exit stream	0.02	0.0162	0.0131	0.0106	0.0085	0.0056	0.0037	0.0024
t (s)	0	50	100	150	200	300	400	500

- a. If the decay is first order, calculate the decay constant from the above data. [3]
 b. The reaction is first order with respect to partial pressure of cumene. The specific reaction rate with respect to cumene is $k = 3800 \text{ mol/kg fresh cat.s.atm}$ and the molar flow rate of cumene (99.92% C, balance CHP) is 200 mol/min. The entering concentration is 0.06 kmol/m^3 and the catalyst weight is 100 kg and the velocity of solids is 1 kg/min. What conversion can be achieved in a moving bed reactor? Take decay constant as 0.00427 s^{-1} if you did not solve part a. Take ϵ as 1 to make calculation easier. [5]

