

KATHMANDU UNIVERSITY
End Semester Examination [C]
November/December, 2023

Marks Scored:

Level : B.E.
Year : III

Course : CHEG 312
Semester : II

Exam Roll No. :

Time: 30 mins.

F. M. : 10

Registration No.:

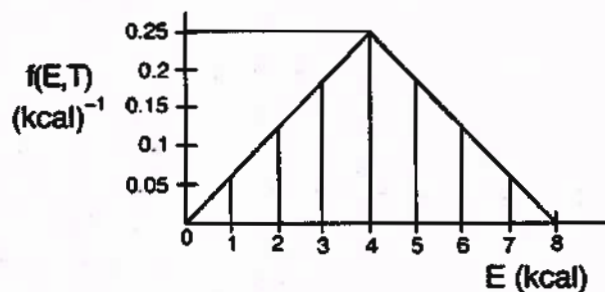
Date 30 NOV 2023

SECTION "A"

[20 Q. × 0.5 = 10 marks]

Encircle the most appropriate option of the given choices.

1. The following figure shows the energy distribution function at 300 K for the reaction $A + B \rightarrow C$.



What fraction of the collisions have energies between 3 and 5 kcal?

- a. 0.22 b. 0.45 c. 0.63 d. 0.8
2. For the energy distribution function given in question 1, what fraction of collisions have energies greater than 5 kcal?
a. 0.23 b. 0.28 c. 0.36 d. 0.42
3. For the elementary reaction $A \rightleftharpoons B$ with equilibrium constant K , what is the expression for equilibrium conversion?
a. $K / (1 - K)$ b. $K / (1 + K)$ c. $K / (1 + 2K)$ d. $K / (1 - 2K)$
4. For the reaction given in problem 3, what is the value of K if equilibrium conversion is 80%?
a. 1 b. 2 c. 3 d. 4
5. For the reaction $2A + B \rightarrow C$, which of the following is the correct rate law expression if the reaction is second order in A and overall first order?
a. $-r_A = kC_A^2$ b. $-r_A = kC_A^2/C_B$ c. $-r_A = kC_A$ d. $-r_A = kC_A/C_B$
6. For the elementary and reversible reaction $2A + B \rightleftharpoons C$, the correct rate law expression is
a. $-r_A = k_A^* [C_A^2 C_B - C_C / K_C]$ b. $-r_A = kC_A^2/C_B$
c. $-r_A = k_A^* [C_A C_B - C_C / K_C]$ d. $-r_A = k_A^* [C_A C_B - C_C^2 / K_C]$
7. The Thiele modulus for a 200 μm spherical catalyst is calculated to be 0.07 which suggests
a. Significant internal diffusion b. Significant external diffusion
c. Negligible internal diffusion d. Negligible external diffusion
8. For rapid reaction on the catalyst surface, the molar flux expression is given by
a. $W_{Az} = k_C * C_{A,b}$ b. $W_{Az} = k_C * (C_{A,b} - C_{A,b})$
c. $W_{Az} = D_{AB} * (C_{A,b} - C_{A,b})$ d. $W_{Az} = D_{AB} * (C_{A,b} - C_{A,b})^2$

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. For the reaction $N_2 + 3H_2 \rightarrow 2NH_3$, the heat of formation of ammonia is -11020 cal/mol. What is the standard heat of reaction?
- 11020 cal/mol
 - 11020 cal/mol
 - 22040 cal/mol
 - 22040 cal/mol
11. For the reaction in question 10, the heat capacity of H_2 , N_2 and NH_3 are given to be 6.992, 6.984 and 8.92 cal/mol.K respectively. What is the heat of reaction at 150 °C?
- 22419 cal/mol
 - 23228 cal/mol
 - 23305 cal/mol
 - 24101 cal/mol
12. For an enzymatic biological reaction, the doubling of the amount of enzyme will affect what parameter of the M-M reaction kinetics?
- Concentration of the substrate
 - Michaelis constant
 - Turnover number
 - Maximum specific growth reaction rate
13. For a catalytic reaction $A \rightarrow B$, if a catalyst deactivation follows a first order decay law and is independent of the concentrations of both A and B, the catalyst activity
- Increases logarithmically with time
 - Decreases logarithmically with time
 - Decreases exponentially with time
 - Increases linearly with time
14. 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
15. Which of the following will give maximum gas conversion?
- Fixed bed reactor
 - Fluidized bed reactor
 - Semi- fluidized bed reactor
 - Plug flow catalytic reactor
16. With increase in pressure, bulk diffusion in catalyst pore..... pressure.
- Increases
 - Increases exponentially
 - Decreases
 - Remain unchanged
17. The conversion for an isothermal irreversible reaction in an ideal PFR willwith decrease in space time
- Decrease
 - Increase
 - Remain unchanged
 - Decrease logarithmically
18. One of the following is not the type of catalyst deactivation
- Sintering
 - Coking
 - Poisoning
 - Filtering
19. What is the solution for the zero order catalyst decay?
- $a = 1 - \beta t$
 - $a = e^{-\beta t}$
 - $a = 1/(1 + \beta t)$
 - $a = A_0 t^\beta$
20. In competitive enzyme inhibition, _____
- Both the y-intercept and slope increases with increasing inhibitor concentration
 - The y-intercept increases while the slope remains fixed with increasing inhibitor concentration
 - The y-intercept remains fixed while the slope increases with increasing inhibitor concentration
 - Both the y-intercept and slope increases even with constant inhibitor concentration

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F. M. : 40

SECTION "B"

Attempt ALL questions.

1. The irreversible elementary gas phase reaction $A + B \rightarrow C + D$ is carried out isothermally at 305 K in a PBR with 100 kg of catalyst. The entering pressure is 20 atm and the exit pressure is 2 atm. The feed is equimolar in A and B with $F_{A0} = 10$ mol/min. Currently, 80% conversion is achieved.

- a. Calculate the value for the rate constant k . [5]
- b. Suppose the flow is in turbulent region for which $\alpha \sim 1/D_p$, where D_p is the catalyst size. What would be the new conversion if the catalyst size were doubled and everything else remained constant? [3]

Given,

$$R = 0.082 \text{ dm}^3 \cdot \text{atm} / \text{mol} \cdot \text{K}$$

$$\frac{dy}{dW} = -\frac{\alpha}{2y} (1 + \varepsilon X) \quad \text{where } y = P / P_0$$

$$v = v_0 (1 + \varepsilon X) \frac{T P_0}{T_0 P}$$

2. Experimental data for the gas phase catalytic reaction $A + B \rightarrow C$ is given below. The limiting step is known to be irreversible so that the overall reaction is irreversible. The reaction was carried out in a differential reactor to which A, B and C were all fed

S.N.	P_A (atm)	P_B (atm)	P_C (atm)	Reaction rate (mol/gcat.s)
1	1	1	2	0.114
2	1	10	2	1.14
3	10	1	2	0.18
4	1	20	2	2.273
5	1	20	10	0.926
6	20	1	2	0.186
7	0.1	1	2	0.0243

- a. Suggest a rate law consistent with the experimental data with reasoning. [3]
- b. Suggest a mechanism and derive the rate law. [4]

3. The gas phase exothermic elementary reaction $A \rightarrow B + C$ is carried out in a moving bed reactor. The excess heat is removed by a heat exchanger jacketing the reactor. The flow rate of the coolant in the exchanger is sufficiently high that the ambient temperature is constant at 50 °C. Pure A enters the reactor at a rate of 5.42 mol/s at a concentration of 0.27 mol/dm³. Both the solid catalyst and the reactant enter the reactor at a temperature of 450 K and the heat transfer coefficient between the catalyst and gas is virtually infinite. The heat capacity of the solid catalyst is 100 J/kg cat.K. The catalyst charge rate is 17 kg/s. There is 50 kg of catalyst in the bed and the catalyst decay is first order in activity with

$$k_d(s^{-1}) = 0.01 \exp\left[7000 \left(\frac{1}{450} - \frac{1}{T}\right)\right]$$

Also given,

$$k(s^{-1}) = 0.33 \exp\left[3777 \left(\frac{1}{450} - \frac{1}{T}\right)\right]$$

$$\frac{U_a}{\rho_b} = \frac{0.8 \text{ J}}{\text{s. kg cat. K}}$$

$$C_{pA} = 40 \text{ J/mol.K}$$

$$C_{pB} = 25 \text{ J/mol.K}$$

$$C_{pC} = 15 \text{ cal/mol.K}$$

$$\Delta H_{rxn}^o = -80 \frac{\text{kJ}}{\text{mol}} A$$

The energy balance equation is given by

$$\frac{dT}{dV} = \frac{U_a(T_a - T) + [\Delta H_{rxn}(T_r) + \Delta C_p(T - T_r)].r_A}{U_s C_{p,cat} + \sum_{i=1}^n \theta_i C_{p,i} F_{A0}}$$

Write the complete algorithm in order of the CRE pyramid to plot conversion and temperature change along the weight of the catalyst. Please simplify the expressions to the extent possible with the values provided above for full points. [6]

4. Cell growth is taking place in a CSTR. The following cell growth rate for the system is given,

$$r_g = \frac{\mu_{max} C_s C_c}{K_s + C_s \left(1 + \frac{C_s}{K_I}\right)}$$

Where, $\mu_{max} = 1.5 \text{ h}^{-1}$, $K_s = 1 \text{ g/dm}^3$, $K_I = 50 \text{ g/dm}^3$, $C_{s0} = 30 \text{ g/dm}^3$, $Y_{c/s} = 0.08$, $C_{c0} = 0.5 \text{ g/dm}^3$, $V = 500 \text{ dm}^3$ and $D = 0.75 \text{ h}^{-1}$.

- Derive the equation for D as a function of C_s and C_c . [4]
- From the equations derived above, find the volumetric flow rate for which cell production is maximum. [3]
- If $C_{c0} = 0$, what is the volumetric flow rate for which cell production is maximum. Also, find the washout rate. [3]

For c and d, it will be better to guess a value for C_s , then calculate D and C_c and move accordingly instead of trying to solve differential equations. To save time, C_s values will fall between 2 and 3 g/dm³.

5. An RTD analysis was carried out on a liquid phase reactor. Analyze the following data.

t (s)	0	150	175	200	225	240	250
C x 10 ³ (g/m ³)	0	0	1	3	7.4	9.4	9.1
t (s)	275	300	325	350	375	400	450
C x 10 ³ (g/m ³)	8.2	5.0	2.5	1.2	0.5	0.2	0

- Find the E(t) values for these data. Take the area under the curve for C (t) to be 0.965 gm.s/dm³ to save time for calculation. [3]
- What is the mean residence time? [2]
- The hydrolysis of t-isobutyl chloride (first order rate) was carried out in this reactor. The specific reaction rate is 0.0115 s⁻¹. What conversions do the segregation model predict? [4]

Useful equations:

1. Simpson's 2 point rule

$$\int_{X_0}^{X_1} f(X) dX = \frac{h}{2} [f(X_0) + f(X_1)] \quad h = X_1 - X_0$$

2. Simpson's 3 point rule

$$\int_{X_0}^{X_2} f(X) dX = \frac{h}{3} [f(X_0) + 4f(X_1) + f(X_2)] \quad h = \frac{X_2 - X_0}{2}$$

3. Simpson's 4 point rule

$$\int_{X_0}^{X_3} f(X) dX = \frac{3}{8} h [f(X_0) + 3f(X_1) + 3f(X_2) + f(X_3)] \quad h = \frac{X_3 - X_0}{3}$$

4. Simpson's 5 point rule

$$\int_{X_0}^{X_4} f(X) dX = \frac{h}{3} [f(X_0) + 4f(X_1) + 2f(X_2) + 4f(X_3) + f(X_4)] \quad h = \frac{X_4 - X_0}{4}$$

5. Simpson's N + 1 points, where N is even

$$\int_{X_0}^{X_N} f(X) dX = \frac{h}{3} [f(X_0) + 4f(X_1) + 2f(X_2) + \dots + f(X_N)] \quad h = \frac{X_N - X_0}{N}$$

