KATHMANDU UNIVERSITY
End Semester Examination
June/July, 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 : 0 7 JUL 2023

SECTION "A"

[20Q. × 0.5 = 10 marks]

Encircle the most appropriate option.

1. For an exothermic reaction, ________________.
   a. the equilibrium conversion increases with decreasing temperature
   b. the equilibrium conversion decreases with decreasing temperature
   c. the equilibrium conversion increases with increasing temperature
   d. the equilibrium conversion decreases with increasing temperature

2. The gas-phase reaction $B \rightarrow C$ obeys zeroth-order kinetics with $r = 0.15$ moles/liter·hr at 300 °C. Starting with pure B at 10 atm, calculate the initial concentration of B. Take $R = 0.082$ L·atm/mol·K.
   a. 0.212 mol/L b. 0.258 mol/L c. 2.33 mol/cm^3 d. 0.0267 mol/cm^3

3. For the problem in question 2, calculate the time it takes for 30% of B to react away in a constant volume batch reactor.
   a. 0.083 hr b. 0.271 hr c. 0.424 hr d. 0.698 hr

4. The equilibrium constant for the reaction $CH_3COOH + C_2H_5OH \leftrightarrow CH_3COOC_2H_5 + H_2O$ at 100 °C and 1 atm is 4.86. If initially there is one mole each of acetic acid and ethanol, what is the equilibrium conversion?
   a. 0.35 b. 0.48 c. 0.55 d. 0.69

5. For the problem in question 4, what is the equilibrium constant if the reaction is carried out at 298 K if the heat of reaction is -3640 J?
   a. 4.86 b. 6.53 c. 8.42 d. 9.79

6. The liquid phase reaction $A \leftrightarrow B$ is elementary and reversible. If equimolar amount of A and B are fed to the reaction, which one of the following is the correct rate expression in terms of conversion?
   a. $-r_A = k*C_{A0}*(1-X) / (K_c*X)$
   b. $-r_A = k*C_{A0}*[(1-X) - (X/K_c)]$
   c. $-r_A = k*C_{A0}*(1-X)^2$
   d. $-r_A = k*C_{A0}*[(1-X) - ((1+X)/K_c)]$

7. Rate law for the reaction $A + 2B \rightarrow C$ is found to be rate = k*[A][B]. If the concentration of reactant B is doubled while keeping the concentration of A constant, the rate of reaction will be __________.
   a. the same b. doubled c. quadrupled d. halved

8. One rule of thumb in developing a reaction mechanism using PSSH states that if a constant appears in the denominator, one of the reaction steps is probably__________.
   a. $A + A^* \rightarrow$ [Collison products]
   b. $A^* \rightarrow$ [Decomposition products]
   c. [Reactant] $\rightarrow A^* +$ [Other products]
   d. $A^* +$ [Reactant] $\rightarrow A +$ [Collision products]

9. In non-competitive enzyme inhibition, ___________________.
   a. both the y-intercept and slope increases with increasing inhibitor concentration
   b. the y-intercept increases while the slope remains fixed with increasing inhibitor concentration
   c. the y-intercept remains fixed while the slope increases with increasing inhibitor concentration
   d. both the y-intercept and slope increases even with constant inhibitor concentration

10. For the reaction 3A → 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. $C_A = C_{A0}*(1 - X) / (1 + 2.5X)$

11. For an enzymatic biological reaction, changing the amount of enzyme will affect _________ of the Michaelis-Menten equation.
   a. Turnover number
   b. Michaelis constant
   b. Concentration of the product
   d. Maximum specific growth rate of substrate

12. For a catalytic reaction A → B + C, the rate of catalyst decay is found to be first order in the activity and first order in the reactant concentration_______________.
   a. increases linearly with time
   b. increases logarithmically with time
   c. decreases logarithmically with time
   d. decreases exponentially with time

13. For a first order decay law, the catalyst activity is equal to zero in_______________.
   a. never reaches zero
   b. infinite time
   c. at the beginning of the reaction
   d. at halfway through the reaction

14. How would the rate of product formation change if the catalyst amount is doubled for a bioreaction following Michaelis-Menten kinetics?
   a. No change in rate
   b. The rate if halved
   c. The rate is doubled
   d. The rate if quadrupled

15. 1 mol of N_2 reacts with 3 moles of H_2 to form 2 moles of NH_3. If the feed mixture of N_2 and H_2 are in stoichiometric proportions and reaction occurs are 423 K, what is the equilibrium constant if the equilibrium conversion is known to be 21%?
   a. 0.0456
   b. 0.0676
   c. 0.0856
   d. 0.0966

16. 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. 21.76 h^{-1}
   c. 14.76 h^{-1}
   d. 7.76 h^{-1}

17. Which of the following is the solution for hyperbolic catalyst decay?
   a. $a = 1 - \beta t$
   b. $a = e^{-\beta t}$
   c. $a = 1/(1 + \beta t)$
   d. $a = A_0 t^{-\beta}$

18. Which of the following is **CORRECT** statement about Thiele modulus?
   a. Measures the ratio of internal diffusion rate to external diffusion rate.
   b. Measures the ratio of internal diffusion to surface reaction rate.
   c. Measures the effect of catalyst particle diameter on the reaction rate.
   d. Measures the ratio of surface reaction rate to internal diffusion rate.

19. Pore tortuosity is defined as______________.
    a. the ratio of volume of void space to the volume of the particle
    b. the ratio of actual distance a molecule travels between two points to the shortest distance between those two points
    c. time it takes for the molecules to travel from point A to B inside a catalyst particle
    d. the ratio of surface reaction to external diffusion rate

20. The Mear's criterion help determine if______________.
    a. mass transfer from bulk to catalyst surface is the rate limiting step
    b. internal diffusion is the rate limiting step
    c. catalytic surface reaction is the rate limiting step
    d. observed activation energy for a catalytic reaction mechanism is same as true activation energy

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F. M. : 40

SECTION "B"

[2Q. × 4 = 8 marks]

Attempt *ALL* questions.

1. The elementary irreversible organic liquid phase reaction A + B → C is carried out adiabatically in a flow reactor. An equal molar feed in A and B enters the reactor at 27 °C, and the volumetric flow rate is 2 dm^3/s and $C_{A0} = 0.1\ kmol/m^3$.
   a. Calculate the CSTR volume necessary to achieve 85% conversion. [2.5]
   b. What is the maximum inlet temperature one could have so that the boiling point of the liquid (550 K) would not be exceeded even for complete conversion? [1.5]

   The following information is given:

   $H_A^0\ (273) = -20$ kcal/mol
   $C_{pA} = 15$ cal/mol.K
   $k = 0.01\ dm^3/mol.s$ @ 300K

   $H_B^0\ (273) = -15$ kcal/mol
   $C_{pB} = 15$ cal/mol.K
   $E = 10{,}000$ cal/mol

   $H_C^0\ (273) = -41$ kcal/mol
   $C_{pC} = 30$ cal/mol.K

   The energy balance equation is given by

$$\frac{dE}{dt} = Q + W + \sum_{i=1}^{n} F_{A0}\Theta_i\, C_{p,i}(T_{io} - T) - \Delta H_{rxn}(T).\, F_{A0}X_A$$

2. The gas phase catalytic irreversible reaction A + B → C + D has the following rate law.

$$-r_A' = \frac{k' P_A P_B}{(1 + K_A P_A + K_B P_B + K_D P_D)^2}$$

   Suggest a mechanism and derive the rate law. [4]

SECTION "C"

[4Q. × 8 = 32 marks]

Attempt *ALL* questions.

3. The elementary gas phase reaction A + B ←→ 2C is carried out in a packed bed reactor. The entering molar flow rates are $F_{A0} = 5$ mol/s, $F_{B0} = 2F_{A0}$ and $F_I = 2F_{A0}$ with $C_{A0} = 0.2\ mol/dm^3$. The entering temperature is 325 K and a coolant fluid is available at 300 K. The following information is provided.

   $C_{pA} = C_{pB} = C_{pC} = 20$ cal/mol.K
   $k = 0.0002\ dm^6/kmol.s$ @ 300K
   $Ua = 320\ cal/s.m^3.K$
   $\rho_b = 1400\ kg/m^3$
   $K_C = 1000$ @ 305 K

   $C_{pI} = 18$ cal/mol.K
   $C_{pB} = 15$ cal/mol.K
   $E = 25$ kcal/mol
   $\Delta H^0_{rxn} = -20$ kcal/mol

   $\alpha = 0.00015\ kg^{-1}$
   $C_{pC} = 30$ cal/mol.K
   $m_C = 18$ mol/s
   $C_{p,coolant} = 18$ cal/mol

   a. Write the complete algorithm in order of the CRE pyramid for plotting conversion and temperature change along the length of the reactor. Please simplify the expressions to the extent possible with the values provided above for full points. [5]
   b. Derive an expression for equilibrium conversion. [3]

   The energy balance equation is given by

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

   For packed bed,

$$dW = \rho_b dV$$

4. Consider a culture of bacteria that secrete a product in a chemostat operated at steady state. The specific growth rate of bacteria is adequately described by the Monod equation, and the rate of product formation is described by Leudeking-Piret kinetics: $r_P = (\alpha\mu + \beta)^*C_C$, where $\mu = \mu_{max} C_S / (K_S+C_S)$. The liquid feed to the chemostat is sterile and the flow rates entering and exiting the chemostat are equal. The system is well characterized and the following constants are given:

$Y_{C/S} = 0.4$ g/g	$\alpha = 0.2$ g/g	$C_{S0} = 10$ g/L
$\mu_{max} = 0.7\ h^{-1}$	$\beta = 0.3$ g/g-h	$v_o = 15$ L/hr
$K_S = 0.2$ g/L	$Y_{P/S} = 0.8$ g/g	$V = 500$ L

a. Calculate the steady state concentration of the substrate. [3]
b. Calculate the steady state concentration of the cell. [3]
c. Calculate the flow rate at which washout occurs for a constant reactor volume. [2]

5. The elementary irreversible gas phase catalytic reaction A + B → C + D is to be carried out in a moving bed reactor at constant temperature. The reactor contains 2 kg of catalyst. The feed is stoichiometric in A and B. The entering concentration of A is 0.2 mol/dm^3. The catalyst decay law is zero order with $k_D = 0.2$ s. The reaction rate constant for the reaction is 1.0 dm^6 / (mol.kg cat.s) and volumetric flow into the reactor is 1 dm^3/s.
a. What conversion will be achieved for a catalyst feed rate of 0.5 kg/s? [5]
b. What is the maximum conversion that could be achieved for an infinite catalyst loading rate? [2]
c. At what catalyst loading rate will the catalyst activity be exactly zero? [1]

6. The third order liquid phase reaction A→ B was carried out in a reactor that has the following RTD

$E(t) = 0$ for t<1 min
$E(t) = 1.0$ for $1 \leq t \geq 2$ min
$E(t) = 0$ for t>2 min

The entering concentration of A is 2 mol/dm^3. For isothermal operation,
a. Calculate the mean residence time. [3]
b. Calculate the conversion predicted by a CSTR and a PFR. [2]
c. Calculate the conversion predicted by the segregation model. [3]

Additional information:
$k = 0.3$ dm^6/mol^2/min at 300 K
$\Delta H_{rxn} = -40{,}000$ cal/mol
$E/R = 20{,}000$
$C_{pA} = C_{pB} = 25$ cal/mol.K

Useful equations:

1. Simpson's 2 point rule
$$\int_{X_0}^{X_1} f(X)dX = \frac{h}{2}[f(X_0) + f(X_1)] \qquad h = X_1 - X_0$$
2. Simpson's 3 point rule
$$\int_{X_0}^{X_2} f(X)dX = \frac{h}{3}[f(X_0) + 4f(X_1) + f(X_2)] \qquad h = \frac{X_2 - X_0}{2}$$
3. Simpson's 4 point rule
$$\int_{X_0}^{X_3} f(X)dX = \frac{3}{8}h[f(X_0) + 3f(X_1) + 3f(X_2) + f(X_3)] \qquad h = \frac{X_3 - X_0}{3}$$
4. Simpson's 5 point rule
$$\int_{X_0}^{X_4} f(X)dX = \frac{h}{3}[f(X_0) + 4f(X_1) + 2f(X_2) + 4f(X_3) + f(X_4)] \qquad h = \frac{X_4 - X_0}{4}$$
5. Simpson's N + 1 points, where N is even
$$\int_{X_0}^{X_N} f(X)dX = \frac{h}{3}[f(X_0) + 4f(X_1) + 2f(X_2) + \cdots \ldots + f(X_N)] \qquad h = \frac{X_N - X_0}{N}$$