KATHMANDU UNIVERSITY
End Semester Examination
February/March, 2025

Marks Scored:

Level : B.E.
Year : III

Course : CHEG 312
Semester : II

Exam Roll No. :

Time: 30 mins.

F. M. : 10

Registration No.:

Date : 03 MAR 2025

SECTION "A"
[20 Q. × 0.5 = 10 marks]

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

1. What is on the fourth level of the CRE pyramid?
   a. Mole balance b. Rate law c. Heat effects d. Stoichiometry

2. For a bioreaction following Michaelis- Menten kinetics, how would the rate of product formation change if the catalyst amount is halved?
   a. No change in rate b. The rate is halved
   c. The rate is doubled d. Insufficient information to calculate the rate

3. For an exothermic reaction,
   a. The equilibrium conversion remains unchanged with 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

4. The specific reaction rate for a certain reaction is 7.76 h^{-1} at 338.6 K. If the activation energy for the reaction is 65.7 kJ/mol, what is the specific reaction rate at 360 K?
   a. 31.1 h^{-1} b. 21.76 h^{-1} c. 14.76 h^{-1} d. 7.76 h^{-1}

5. The conversion for an isothermal irreversible reaction in an ideal PFR will _____ with decrease in space time
   a. Decrease b. Increase
   c. Remain unchanged d. Decrease exponentially

6. What is the solution for the second order catalyst decay?
   a. $a = 1\text{-}bt$ b. $a = e^{-bt}$ c. $a = 1/(1 + bt)$ d. $a = A_0t^{-b}$

7. The presence of a long tail in the residence time distribution curve of a packed bed reactor is an indication of
   a. Ideal plug flow b. Channeling c. Dead zone d. Bypass

8. In Langmuir treatment of adsorption
   a. Whole surface of the catalyst is essentially uniform and the adsorbed molecule has no effect on the rate of adsorption per site
   b. Whole surface of the catalyst does not have the same activity for adsorption and there is attraction between the adsorbed molecules
   c. All the adsorption does not take place by the same mechanism
   d. Extent of adsorption is more than one complete mono molecular layer on the surface

9. For multiple reactions, the flow pattern within the vessel affects the
   a. Size requirement
   b. Distribution of reaction products
   c. Conversion
   d. Both (a) and (b)

10. Which of the following will give maximum gas conversion?
   a. Fixed bed reactor
   b. Fluidized bed reactor
   c. Semi- fluidized bed reactor
   d. Plug flow catalytic reactor

11. If a solid-gas non-catalytic reaction occurs at very high temperature, the rate controlling step is the____________
   a. Ash layer
   b. Kinetics of the reaction
   c. Film diffusion
   d. Both diffusion and kinetics

12. Effectiveness factor of a catalyst pellet is a measure of the......... resistance.
   a. Pore diffusion
   b. Gas film
   c. Chemical reaction
   d. Surface area

13. For a gas phase elementary reaction $A + B \rightarrow C$, what is the effect on the reaction rate if we increase the pressure by 20% while maintaining constant temperature?
   a. Reaction rate increases by 0%
   b. Reaction rate increases by 20%
   c. Reaction rate increases by 80%
   d. Reaction rate increases by 100%

14. The first order gas phase reaction for $A \rightarrow 2B$ is carried out isothermally in batch mode. The rate of change of conversion with time is
   a. $dX_A/dt = k1*(1-X_A)$
   b. $dX_A/dt = k1*(1-X_A) / (1+X_A)$
   c. $dX_A/dt = k1*(1-X_A)* (1+0.5X_A)$
   d. $dX_A/dt = k1*(1-X_A)^2* (1+2X_A)$

15. Pick the 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

16. 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

17. 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.

18. If the equilibrium constant for a water gas shift reaction ($H_2O + CO \leftrightarrow CO_2 + H_2$) at 1000 K and 10 atm is 1.44, what is the equilibrium conversion? Assume an equimolar feed of water and carbon monoxide.
   a. 0.35
   b. 0.48
   c. 0.55
   d. 0.69

19. For the water gas shift reaction given in the previous question, what is the initial concentration of carbon monoxide in mol/dm^3?

a. 0.05 b. 0.06 c. 0.07 d. 0.08

20. For the water gas shift reaction given in the previous problem, what is the equilibrium concentration of carbon monoxide in mol/dm^3?

a. 0.0275 b. 0.0335 c. 0.0545 d. 0.0625

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SECTION "B"
[3 Q. × 5 = 15 marks]

*Attempt **ALL** questions.*

1. The reaction $H_2 + Br_2 \rightarrow 2HBr$ occurs by the formation of two intermediates as shown in the steps below.

   Initiation: $Br_2 \rightarrow 2Br^*$
   Propagation: $Br^* + H_2 \rightarrow HBr + H^*$
   $H^* + Br_2 \rightarrow HBr + Br^*$
   Inhibition: $H^* + HBr \rightarrow H_2 + Br^*$
   Termination: $2Br^* \rightarrow Br_2$

   The reaction rate constant for the five reactions are k_1, k_2, k_3, k_4 and k_5 respectively.
   Derive the rate law for the formation of HBr from the reactions above. [5]

2. A plant is removing a trace of Cl_2 from a waste gas stream by passing it over a solid granular adsorbent in a tubular packed bed. At present, 63.2% removal is being accomplished, but it is believed that greater removal could be achieved if the flow rate were increased by a factor of 4, the particle diameter was decreased by a factor of 3, and the packed tube length increased by 50%. What percentage of chlorine would be removed under the scheme proposed? [5]

3. A CSTR is being operated at steady state. The cell growth follows the Monod growth law without inhibition. The exiting substrate and cell concentrations are measured as a function of the volumetric flow rate (represented as the dilution rate), and the results are shown below. Of course, measurements are not taken until steady state is achieved after each change in the flow rate. Neglect substrate consumption for maintenance and the death rate, and assume that $Y_{p/c}$ is zero. For run 4, the entering substrate concentration was 50 g/dm^3 and the volumetric flow rate of the substrate was 2 dm^3/h.

   a. Determine the Monod growth parameters. [3]
   b. Estimate the stoichiometric coefficient $Y_{C/S}$. [2]

Run	C_s (g/dm^3)	D (day^{-1})	C_c (g/dm^3)
1	1	1	0.9
2	3	1.5	0.7
3	4	1.6	0.6
4	10	1.8	4

P.T.O.

SECTION "C"

[25 marks]

4. The first order reaction A → R is carried out in 3 PFRs in series. The reactant is fed into the first reactor (non-isothermal) at a flow rate of 100 mol/min at 25 °C. The reactor is heated by a thermal fluid until temperature reaches 100 °C. The second reactor operates adiabatically until a temperature of 650 °C is reached. After, reaching 650 °C, the reactor operates isothermally releasing heat. The final conversion achieved after the third reactor is 85%. Considering a system of three reactors, first is non-isothermal, second is adiabatic and third is isothermal,

   a. What is the conversion achieved after the first reactor? [2]
   b. What is the conversion achieved after the second reactor? [3]
   c. The volume of the isothermal reactor. [3]

The following information is provided.

$$k(min^{-1}) = 4 \times 10^3 \exp\left(-\frac{8000}{T}\right)$$

$$\Delta H_{rxn} = -150\ kJ/mol$$

$$C_{p,A} = C_{p,R} = 180\ J/(mol.K)$$

Heat exchange = 300 J/(m^2.s)

Heat exchange area = 1 m^2

5. The elementary isothermal gas-phase reaction A→ B + C is carried out in a moving bed reactor. The catalyst decays by sintering. The moving bed contains 100 kg of catalyst and the catalyst flow rate through the bed is adjusted so that the exiting catalytic activity is one fourth of the entering activity. The specific reaction rate for fresh catalyst is 10^{-4} dm3/g cat.s. Pure A enters at a concentration of 0.005 mol/dm^3 and a volumetric flow rate of 3.75 dm^3/s.

   a. Determine the general expression for catalyst activity as a function of time. [2]
   b. What is the conversion achieved with the given amount of catalyst? [4]
   c. What would be the conversion if there was no catalyst decay in the reactor? [2]

6. The second order liquid phase reaction 2A → B + C was carried out in a reactor that has the following RTD

$$E(t) = 0 \text{ for } 0 < t < 10 \text{ sec}$$

$$E(t) = 0.01*(t - 10) \text{ for } 10 < t < 20 \text{ sec}$$

$$E(t) = 0.01*(30 - t) \text{ for } 20 < t < 30 \text{ sec}$$

$$E(t) = 0 \text{ for } t > 30 \text{ sec}$$

The entering concentration of A is 2 mol/dm^3 and the specific reaction rate is 0.06 dm^3/mol.s.

   a. What is the conversion after 30 secs in a batch reactor? [2]
   b. What conversion would be achieved in a PFR? [3]
   c. What is the conversion predicted by the segregation model. [4]

Equations and Values

Energy balance equations

$$\frac{dT}{dt} = \frac{\dot{Q} - W_s - \sum F_{i0} C_{p,i}(T - \dot{T_{i0}}) + [-\Delta H_{rxn}][-r_A V]}{N_{A0}(\sum \theta_i C_{p.i} + \Delta C_p X)}$$

$$\frac{dE}{dt} = \dot{Q} + \dot{W} + \sum_{i=1}^{n} \Theta_i \, C_{p,i} F_{A0}(T_{i0} - T) - \Delta \mathrm{H}_{rxn}(T).X.F_{A0}$$

$$k_c \propto \frac{D_{AB}^{2/3}}{v^{1/6}} \frac{U^{1/2}}{d_p^{1/2}}$$

$$ln\frac{1}{1-X} = \frac{k_c a_c}{U} L$$

$$R = 8.314 \frac{J}{mol * K} = 82.058\ cm^3.\frac{atm}{K.mole} = 8.2 \times 10^{-5} m^3.\frac{atm}{K.mole} = 1.987 \frac{cal}{mol.K}$$

Simpson's 2 point rule

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

1. Simpson's 3 point rule

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

2. Simpson's 4 point rule

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

3. Simpson's 5 point rule

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

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

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