CHEMICAL REACTION ENGINEERING
(CHEN 3102)

Time Allotted : 3 hrs **Full Marks : 70**

Figures out of the right margin indicate full marks.

Candidates are required to answer Group A and any 5 (five) from Group B to E, taking at least one from each group.

Candidates are required to give answer in their own words as far as practicable.

Group – A
(Multiple Choice Type Questions)

1. Choose the correct alternative for the following: **10 × 1 = 10**

(i) For the reaction NO + ½ O_2 = NO_2 carried out in presence of Pt-Rh catalyst, the reaction:
(a) is considered as homogeneous
(b) is considered as heterogeneous
(c) may be either homogeneous or heterogeneous
(d) none of the above.

(ii) The units of frequency factor in Arrhenius equation
(a) is same as that of the rate constant
(b) is different from the units of the rate constant
(c) is unitless
(d) none of the above.

(iii) From the Arrhenius law the frequency factor
(a) does affect the temperature sensitivity of a reaction
(b) does not affect the temperature sensitivity of a reaction
(c) is dimensionless
(d) is a measure of activation energy.

(iv) For a reaction having order (n) greater than unity, the best combination of reactors will be
(a) PFR, small mixed, large mixed
(b) large mixed, small mixed, PFR
(c) small mixed, large mixed, PFR
(d) small mixed, PFR, large mixed.

(v) The order of a Chemical Reaction corresponds to Molecularity for
(a) non elementary reaction (b) elementary reaction
(c) enzyme catalyzed reaction (d) isothermal reactions.

(vi) 1 liter/sec of gaseous reactant A is introduced into a mixed flow reactor having volume 4 liters. The stoichiometry is A → 3R. The conversion is 50%. Under these conditions the residence time is
(a) 1 sec (b) 2 sec (c) ½ sec (d) none of the above.

(vii) If the desired product is in the sequence of a series reaction the best product distribution is obtained in
(a) mixed flow reactor (b) plug flow reactor
(c) either plug flow reactor or batch reactor (d) none of the above.

(viii) Maximum Mixedness model is a
(a) zero parameter model (b) one parameter model
(c) two parameter model (d) multi parameter model.

(ix) The fractional volume change of the system between no conversion and complete conversion for the isothermal gas phase reaction, $A \rightarrow 3B$ with 50% A and 50%, inert initially present is
(a) 2 (b) 1 (c) 0.5 (d) 0.

(x) For reaction under pore diffusion regime, the reaction rate
(a) varies directly with catalyst particle size
(b) varies inversely with catalyst particle size
(c) is independent of catalyst particle size
(d) none of the above.

Group – B

2. Under the influence of oxidizing agents hypophosphorous acid is transferred into phosphorous acid: $H_3PO_2 \rightarrow H_3PO_3$
The kinetics of this transformation present the following features. At low concentration of oxidizing agent $r_{H_3PO_3}$ = k[oxidizing agent] [H_3PO_2]
At high concentration of oxidizing agent $r_{H_3PO_3}$ = k/[H^+] [H_3PO_2]
To explain the observed kinetics, it has been postulated that with hydrogen ion as catalyst normal unreactive H_3PO_2 is transferred into an active form, the nature of which is unknown. This intermediate then reacts with the oxidizing agent to give H_3PO_3. Show that this scheme does explain the observed kinetics. **12**

3. (a) Milk is pasteurized if it is heated to 63^{0}C for 30 min, but if it is heated to 74°C it only needs 15 s for the same result. Find the activation energy of this sterilization process.

(b) Prove that for a 2nd order irreversible bimolecular reaction, A + 2B → Products
$\ln \frac{M-2X_A}{M(1-X_A)} = C_{A0}(M-2)kt$ where, $M = C_{B0}/C_{A0}$ & M # 2
(Symbols stand for usual notations)

6 + 6 = 12

Group – C

4. (a) For the Diels – Alder reactions of benzoquinone (B) and cyclopentane (C) at 25^{0}C B + C = adduct, $(-r_C) = k\, C_B\, C_C$, volume changes on reaction may be neglected. At 25^{0}C , the reaction rate constant is equal to 9.92 × 10^{-3} m^3/kmol.s. If one employs a well stirred isothermal batch reactor to carry out this reaction, determinethe holding time necessary to achieve 95% conversion of the limiting regeant using initial concentration of 0.1 and 0.08 kmol/m^3 for B and C respectively.

(b) The elementary liquid-phase reaction
$A + 2B \rightleftharpoons R$
with rate equation $-r_A = -\frac{1}{2} r_B = (12.5\ liter^2/mol^2\ min)C_A C_B^2 - (1.5\ min^{-1})\, C_R$, mol/lit.min is to take place in a 6-liter steady-state mixed flow reactor. Two feed streams, one containing 2.8 mol A/liter and the other containing 1.6 mol B/liter, are to be introduced at equal volumetric flow rates into the reactor, and 75% conversion of limiting component is desired. What should be the flow rate of each stream? Assume a constant density throughout.

6 + 6 = 12

5. (a) The data in table below have been obtained on the decomposition of gaseous reactant A in a constant volume batch reactor at 100°C. The stoichiometry of the reaction is 2A → R + S. What size plug flow reactor (in liters) operating at 100°C and 1 atm can treat 100 mol A/hr in a feed consisting of 20% inerts to obtain 95% conversion of A?

t,sec	**0**	**20**	**40**	**60**	**80**	**100**	**140**	**200**	**260**	**330**	**420**
p_A, atm	1.00	0.80	0.68	0.56	0.45	0.37	0.25	0.14	0.08	0.04	0.02

(b) The kinetics of the aqueous-phase decomposition of A is investigated in two mixed flow reactors in series, the second having twice the volume of the first reactor. At steady state with a feed concentration of 1 mol A/liter and mean residence time of 96 sec in the first reactor, the concentration in the first reactor is 0.5 rnol A/liter and in the second is 0.25 rnol A/liter. Find the kinetic equation for the decomposition.

6 + 6 = 12

Group – D

6. (a) Kinetic experiments on the solid catalyzed reaction A → 3R are conducted at 8 atm and 700°C in a basket type mixed reactor 960 cm^3 in volume and containing 1 gm of catalyst of diameter d, = 3 mm. Feed consisting of pure A is introduced at various rates into the reactor and

the partial pressure of A in the exit stream is measured for each feed rate. The results are as follows:

Feed rate, liter/hr	100	22	4	1	0.6
p_{Aout}/p_{ain}	0.8	0.5	0.2	0.1	0.05

Find a rate equation to represent the rate of reaction on catalyst of this size.

(b) Prove that an nth order chemical reaction will behave as $\frac{n+1}{2}th$ order reaction under strong pore diffusion control regime.

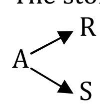
(c) The following kinetic data on the reaction A → R are obtained in an experimental packed bed reactor using various amounts of catalyst and a fixed feed rate F_{A0} = 10 kmol / hr.

W, kg cat	1	2	3	4	5	6	7
X_A	0.12	0.20	0.27	0.33	0.37	0.41	0.44

How much catalyst would be needed if the reactor employed is a mixed flow reactor for 40% conversion and a feed rate of 400 kmol/hr?

5 + 3 + 4 =12

7. (a) The stoichiometry of a liquid-phase decomposition is known to be

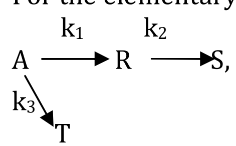


In a series of steady-state flow experiments (C_{A0} = 100, C_{R0} = C_{S0} = 0) in a laboratory mixed flow reactor the following results are obtained:

C_A	90	80	70	60	50	40	30	20	10	0
C_R	7	13	18	22	25	27	28	28	27	25

Further experiments indicate that the level of C_R and C_S have no effect on the progress of the reaction. With C_{A0} = 200 and C_{Af} = 20 find C_R at the exit from a plug flow reactor.

(b) For the elementary reactions



$k_2 = k_1 + k_3$

Find C_{Rmax} / C_{A0} and τ_{opt} in a mixed flow reactor.

7 + 5 = 12

Group – E

8. (a) Determine mean conversion in a PFR following Segregation model.

(b) Show for a One parameter Tank-in Series (RTD) model, the variance decreases as the number of tanks increases.

6 + 6 = 12

9. The first-order reaction A → B is carried out in a 10 cm diameter tubular reactor 6.36 m in length. The specific reaction rate is 0.25 min^{-1}. The results of a tracer test carried out on this reactor are shown below:

t (min)	0	1	2	3	4	5	6	7	8	9	10	12	14
C (g/m^3)	0	1	5	8	10	8	6	4	3.0	2.2	1.5	0.6	0

Calculate conversion using the tanks-in-series model.

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