CHEMICAL REACTION ENGINEERING I
(CHE2204)

Time Allotted : 2½ hrs **Full Marks : 60**

Figures out of the right margin indicate full marks.

Candidates are required to answer Group A and ***any 4 (four) from Group B to E, taking one from each group.***

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

Group – A

1. Answer any twelve: **12 × 1 = 12**

Choose the correct alternative for the following

(i) The units of frequency factor in Arrhenius equation:
(a) is same as the rate constant (b) is different from the units of rate constant
(c) is unit less (d) None of the above

(ii) Molecularity of a chemical reaction
(a) Must be an integer (b) Can have a fractional value
(c) Can only apply to a non-elementary reaction (d) None of the above

(iii) The rate of a chemical reaction depends on the
(a) Time of reaction (b) Extent of reaction
(c) Concentration of reactants and temperature (d) Activation energy of the system

(iv) With increase in temperature, the equilibrium conversion of a reversible exothermic reaction
(a) Increases (b) Decreases
(c) Remains unaffected (d) None of the above

(v) The residence time of PFR and holding time for batch reactor are same for:
(a) Constant volume system (b) Variable volume system
(c) Either variable or constant volume system (d) None of the above

(vi) 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 or batch reactor (d) None of these

(vii) The ratio of volume of MFR to the volume of PFR (for identical flow rate, feed composition an conversion) for zero order reaction is
(a) 2 (b) 1.5
(c) 2.5 (d) 1

(viii) The reaction yield is defined as the ratio of ____
(a) Moles of reactant reacted to the moles of product formed
(b) Moles of product formed to the moles of reactant reacted
(c) Moles of desired product formed to the moles of undesired material formed
(d) Moles of product formed to the moles of reactant fed

(ix) The expression for residence time Distribution function E(t) for a pulse tracer input is given by
(a) $\dfrac{C(t)}{\int_0^\infty C(t)dt}$ (b) $\dfrac{C^2(t)}{\int_0^\infty C^2(t)dt}$
(c) $\dfrac{tC(t)}{\int_0^\infty tC(t)dt}$ (d) $\int_0^t C(t)dt$

(x) For a first order reaction, DamKohler number is expressed as
(a) kL/U (b) U/kL
(c) k/UL (d) kC_{A0}/UL

Fill in the blanks with the correct word

(xi) The equilibrium constant of chemical reaction ________ in the presence of catalyst.

(xii) For a _________ order chemical reaction, the half-life period is independent of the initial concentration of the reactant.

(xiii) Two MFR's of unequal size are connected in series to maximize production for a first order homogenous reaction, the sequence of connection should be___________.

(xiv) The expression for RTD of an ideal CSTR is ________________.

(xv) The expression for conversion for a first order reaction in a reactor using the tank in series model is ________________.

Group - B

2. (a) The aqueous reaction $A \rightarrow R + S$ proceeds as follows.

Time, min	C_A, mol/litre
0	0.1823
36	0.1433
65	0.1216
100	0.1025
160	0.0795
∞	0.0494

With C_{A0} = 0.1823 mol/liter, C_{R0} = 0, C_{S0} = 55 mol/liter. Find the rate equation for this reaction. *[(CO1)(Apply/HOCQ)]*

(b) Deduce the integrated form of first order reversible reaction. *[(CO1)(Remember/IOCQ)]*

8 + 4 = 12

3. (a) Find the volume expansion factor of the limiting reactant for the vapour phase reversible reaction if the initial vapour mixture contains 30 % C_2H_4, 60 % Br_2 and 10 % inert by volume.

$$C_2H_4 + Br_2 \leftrightarrow C_2H_4Br_2$$

[(CO1)(Analyse/IOCQ)]

(b) A zero order homogeneous gas reaction A = rR proceeds in a constant volume bomb, 20% inerts, and the pressure rises from 1 to 1.3 atm in 2 min. If the same reaction takes place in a constant pressure batch reactor, what is the fractional volume change in 4 min if the feed is at 3 atm and consists of 40% inerts. *[(CO1)(Apply/HOCQ)]*

5 + 7 = 12

Group - C

4. (a) A high molecular weight hydrocarbon gas A is fed continuously to a heated high temperature mixed flow reactor where it thermally cracks (homogeneous gas reaction) into lower molecular weight materials, collectively called R, by a stoichiometry approximated by $A \rightarrow 5R$. By changing the feed rate different extents of cracking are obtained as follows:

F_{A0}, millimol/hr	300	1000	3000	5000
$C_{Aout.}$ millimol / litre	16	30	50	60

The internal void volume of the reactor is V = 0.1 litre, and at the temperature of the reactor the feed concentration is C_{A0} = 100 millimol/litre. Find a rate equation to represent the cracking reaction. *[(CO2)(Apply/IOCQ)]*

(b) The elementary liquid-phase reaction $A + 2B \leftrightarrow R$ with rate equation $-r_A = -\frac{1}{2}r_B = (12.5\ \text{litre}^2/\text{mol}^2\text{min})C_A C_B^2 - (1.5\ \text{min}^{-1})C_R$, mol/litre.minis to take place in a 6-liter steady-state mixed flow reactor. Two feed streams, one containing 2.8 mol A /litre and the other containing 1.6 mol B / litre, 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. *[(CO2)(Analyse/HOCQ)]*

6 + 6 = 12

5. (a) At present the elementary liquid-phase reaction $A + B \rightarrow R + S$ takes place in a plug flow reactor using equimolar quantities of A and B. Conversion is 96%, $C_{A0} = C_{B0}$ = 1 mol/litre. If a mixed flow reactor ten times as large as the plug flow reactor were hooked up in series with the existing unit, which unit should come first and by what fraction could production be increased for that setup?
Note: Conversion is to remain unchanged. *[(CO3)(Apply/HOCQ)]*

(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/litre and mean residence time of 96 sec in the first reactor, the concentration in the first reactor is 0.5 mol A/litre and in the second is 0.25 mol A/litre. Find the kinetic equation for the decomposition. *[(CO3)(Apply/IOCQ)]*

7 + 5 = 12

Group - D

6. (a) A and B react with each other as follows.

$$2A \rightarrow R \qquad r_R = k_1 C_A^2$$
$$A + B \rightarrow S \qquad r_S = k_2 C_A C_B$$
$$2B \rightarrow T \qquad r_T = k_3 C_B^2$$

What ratio of A and B should be maintained in a mixed flow reactor so as to maximize the fractional yield of desired product S? *[(CO4)(Apply/HOCQ)]*

(b) We have a mixture consisting of 90 mol% A (45 mol/litre) and 10 mol% impurity B (5 mol/litre). To be of satisfactory quality the mol ratio of A to B in the mixture must be 100 to 1 or higher. D reacts with both A and B as follows:

$$A + D \rightarrow R \qquad (-r_A) = 21 C_A C_D$$

$$B + D \rightarrow S \quad (-r_B) = 147 C_B C_D$$

Assuming that the reactions go to completion, how much D need be added to a batch of mixture to bring about the desired quality?

[(CO4)(Apply/HOCQ)]

6 + 6 = 12

7. For the following series reaction

$$A \xrightarrow{k_1} R \xrightarrow{k_2} S$$

find the maximum concentration of R if the reaction is carried out in a

(i) Plug Flow reactor

(ii) Mixed Flow Reactor

Note that initially only A was present (C_{A0}) and $k_1 \neq k_2$.

[(CO4)(Analyse/HOCQ)]

(6 + 6) = 12

Group - E

8. (a) Derive the expression of residence time distribution function in a reactor when a tracer is injected in the form of

(i) A pulse input

(ii) A step input.

[(CO5)(Analyse/IOCQ)]

(b) A sample of tracer is injected as a pulse to a reactor and the effluent concentration measured as a function of time resulting in the data given below.

(i) Construct figures showing the variation of residence time distribution as function of time (graph required)

(ii) Determine the fraction of material leaving the reactor that has spent between 3 and 6 min in the reactor.

(iii) Determine the fraction of material that has spent 3 min or less in the reactor.

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

[(CO5)(Analyse/HOCQ)]

(c) Assuming that a closed vessel is well represented by a dispersion model, calculate the vessel dispersion number and mean residence time with the following tracer response data.

t, min	C_{pulse}, g/litre
0	0
5	2
10	5
15	5
20	4
25	1.5
30	1
35	0

[(CO5)(Apply/IOCQ)]

3 + 6 + 3 = 12

9. (a) Compute the conversion of a first order reaction in a tubular reactor assuming that the dispersion model represents the flow pattern in the reactor. Given: The rate constant of the reaction is 0.307 min^{-1}, mean residence time 15 min and the vessel dispersion number is 0.14. *[(CO6)(Analyse/IOCQ)]*

(b) A first order reaction is carried out in a 12 cm diameter tubular reactor 6.4 m in length. The specific reaction rate is 0.2 min^{-1}. The results of the tracer test are given below. Calculate the conversion using the (i) closed vessel dispersion model (ii) tank-in-series model

t, s	0	1	2	3	4	5	6	7	8	9	10	12	14
C mg/l	0	1	5	8	10	8	6	4	3	2.2	1.5	0.6	0

(mm graph required)

[(CO6)(Analyse/HOCQ)]

4 + (4 + 4) = 12

Cognition Level	LOCQ	IOCQ	HOCQ
Percentage distribution	0	31.25	68.75