CHEMICAL REACTION ENGINEERING I
(CHEN 2204)

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) Fractional conversion is independent of initial concentration for a
(a) Zero order reaction (b) First order reaction
(c) Second order reaction (d) Half order reaction

(ii) In homogeneous system, rate of a chemical reaction depends on
(a) Temperature (b) Pressure (c) Composition (d) All of these

(iii) For a first order reaction having rate constant of 1 min^{-1}, half life period is
(a) 0.6 (b) 0.5 (c) 1 (d) none of the above.

(iv) Order of a chemical reaction
(a) can have fractional value (b) must be an integer
(c) can only apply to a nonelementary reaction (d) none of the above.

(v) The rate constant of a reaction depends on the
(a) time of reaction (b) extent of reaction
(c) initial concentration of reactants (d) temperature of the system.

(vi) In a chemical reaction, the time required to reduce the concentration of reactant from 100 mol/lit to 50 mol/lit is same as that required to reduce it from 2 mol/lit to 1 mol/lit in the same volume. Then the order of this reaction is
(a) Zero (b) 2 (c) 1 (d) none of the above.

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

(viii) 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) 0 (b) 1 (c) 2 (d) 1.5.

(ix) The vessel dispersion number is
(a) D_a/UL (b) UL/D_a (c) D_a/U (d) D_a*UL.

(x) The ratio of rate of consumption of a reactant by reaction to rate of transport by convection is

(a) Reynolds number (b) Peclet number
(c) Schmidt number (d) Damkohler number.

Fill in the blanks with the correct word

(xi) A space velocity 5 hr^{-1} means_________.

(xii) In a continuous flow stirred tank reactor, the composition of the exitstream is same as that _________.

(xiii) The Dankwerts boundary conditions for a closed-closed vessel in dimensionless form are _________.

(xiv) Reactions with high activation energies are very temperature_________.

(xv) There is no correspondence between stoichiometry and the rate equation in case of a / an _________ reaction.

Group - B

2. (a) Show that the following scheme

$$N_2O_5 \rightleftharpoons NO_2 + NO_3^*$$
$$NO_3^* \rightarrow NO^* + O_2$$
$$NO^* + NO_3^* \rightarrow 2\,NO_2$$

is consistent with and can explain the observed first order decomposition of N_2O_5. *[(CO1)(Remember/LOCQ)]*

(b) Milk is pasteurized if it is heated to 63°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. *[(CO1)(Analyse/LOCQ)]*

(c) After 8 minutes in a batch reactor, reactant (C_{A0} = 1 mol/litre) is 80% converted; after 18 minutes, conversion is 90%. Find a rate equation to represent this reaction. *[(CO1)(Evaluate/IOCQ)]*

4 + 4 + 4 = 12

3. (a) A 10-minute experimental run shows that 75% of liquid reactant is converted to product by a half-order rate. What would be the fraction converted in a half-hour run? *[(CO1)(Apply/LOCQ)]*

(b) A zeroorder homogeneous gas reaction A ->rR proceeds in a constant volume bomb, 20% inertsand 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)(Evaluate/IOCQ)]*

6 + 6 = 12

Group - C

4. (a) Deduce the performance equation of a batch reactor. *[(CO2)(Apply/LOCQ)]*

(b) A daily production of 50 tons of ethyl acetate from alcohol and acetic acid his required. The reaction proceeds according to

$$C_2H_5OH\ (A) + CH_3COOH\ (B) \rightleftharpoons CH_3COOC_2H_5\ (P) + H_2O\ (Q)$$

The reaction rate in the liquid phase at 100^0C is $(-r_A) = k\,(C_AC_B - C_PC_Q / K)$,where, $k = 7.93 \times 10^{-6}\ m^3/\ kmol.s$ and $K = 2.93$. The feed solution contains 23wt% of acid, 46 wt% of alcohol and no ester. The required conversion of acid is35%. The density may be assumed to have a constant value 1020 kg / m^3. Theplant must be operated day and night and times for filling, emptying andcleaning operation of a reactor is1hour. What would be the required reactorvolume if one batch reactor vessel is used? *[(CO2)(Apply/HOCQ)]*

5 + 7 = 12

5. Cumene hydroperoxide is converted to phenol and acetone in presence of small amount of acid as follows:

$$(C_6H_5)\ C\ (CH_3)_2\ OOH\ (A) \rightarrow (C_6H_5)\ OH\ (P) + (CH_3)_2CO\ (Q)$$

The reaction takes place in liquid phase and the rate equation at 85^0C is given by $(-r_A) = 4.12\ hr^{-1}C_A$. The flow rate into the reactor is 26.9 m^3/hr. Find the reactor volume after deducing the relevant formula to achieve 85% conversion of A ifthe reactor employed is

(i) One mixed flow reactor

(ii) One plug flow reactor. *[(CO2)(Evaluate/HOCQ)]*

6 + 6 = 12

Group - D

6. (a) A 20 litre MFR is used to treat a reactant which decomposes as follows

$$A \rightarrow R \qquad r_R = 4hr^{-1}C_A$$
$$A \rightarrow S \qquad r_S = 1hr^{-1}C_A$$

Find the feed rate and conversion of reactant so as to maximize profits. What are these on an hourly basis?

Data: Feed material A costs \$1/mol at C_{A0} = 1 mol/litre, product R sells for \$5/mol and S has no value. The total operating cost of reactant and product separation equipment is \$25/hr + \$1.25/mol A feed to the reactor. Unconverted A is not recycled. *[(CO3)(Evaluate/HOCQ)]*

(b) For the elementary reactions

$$A \xrightarrow{k_1} R \xrightarrow{k_2} S \qquad k_2 = k_1 + k_3$$
$$A \xrightarrow{k_3} T$$

Find C_{Rmax} / C_{A0} and τ_{opt} in a plug flow reactor. *[(CO3)(Evaluate/HOCQ)]*

6 + 6 = 12

7. (a) Substance A in a liquid reacts to produce R and S as follows:

A ->R, first order,

A -> S, first order

A feed (C_{A0}= 1, C_{R0}= 0, $C_{S0,}$ = 0) enters two mixed flow reactors in series, (τ =*2.5*min,τ, = *5* min). Knowing the composition in the first reactor (C_{A1}= 0.4, C_{R1}= 0.4, C_{S1}= 0.2), find the composition leaving the second reactor.

[(CO3)(Evaluate/HOCQ)]

(b) For the elementary reaction A-> R-> S carried out in a PFR, find the value of C_{Rmax}. *[(CO3)(Evaluate/HOCQ)]*

6 + 6 = 12

Group - E

8. (a) Derive the expressions for residence time distribution and mean residence time in a laminar flow reactor. *[(CO4)(Analyse/IOCQ)]*

(b) A first order reaction is carried out in a 10 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.

Table Tracer concentration versus time (mm graph required)

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

[(CO5)(Evaluate/HOCQ)]

4 + (4 + 4) = 12

9. (a) For a closed vessel represented by the dispersion model whose tracer response data are given below,

(i) Calculate the vessel dispersion number and mean residence time.

(ii) Calculate the fractional conversion obtained from the reactor when a first order reaction with rate constant 0.3 min^{-1} is carried out in the reactor.

t, min	0	5	10	15	20	25	30	35
C_{pulse}, g/l	0	3	5	5	4	2	1	0

[(CO4,CO5)(Evaluate/IOCQ)]

(b) Write the equation for variation of tracer concentration with time and axial distance in a packed bed reactor in dimensionless form. Explain the difference between closed-closed and open-open vessel by stating the appropriate boundary conditions. Sketch the variation of dispersion of fluid in packed bed with Reynolds number. *[(CO4)(Remember/LOCQ)]*

(3 + 3) + (1 + 3 + 2) = 12

Cognition Level	LOCQ	IOCQ	HOCQ
Percentage distribution	26.04	20.83	53.13

Course Outcome (CO):

After the completion of the course students will be able to

1. Determine rate equation of a chemical reaction from its kinetic experimental data.
2. Design a suitable reactor for a given chemical reaction.
3. Optimize the size and combination of chemical reactors in view to maximize yield and productivity of a material.
4. Compare the performance of ideal and non-ideal reactors using E(t) and F(t) curves.
5. Analyse a non-ideal reactor and predict conversion of a given chemical reaction.

**LOCQ: Lower Order Cognitive Question; IOCQ: Intermediate Order Cognitive Question; HOCQ: Higher Order Cognitive Question.*