CHEMICAL REACTION ENGINEERING - I
(CHEN 3102)

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

Figures out of the right margin indicate full marks.

Candidates are required to answer Group A and <u>any 4 (four)</u> from Group B to E, taking <u>one</u> 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) For the reaction $SO_2 + ½ O_2 = SO_3$ 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) Reactions with high activation energy are
(a) very temperature sensitive (b) temperature insensitive
(c) always irreversible (d) always reversible.

(iii) Higher free energy of activation of a chemical reaction (at a given temperature) implies
(a) higher rate of reaction (b) higher equilibrium conversion
(c) slower rate of reaction (d) none of (a), (b) & (c).

(iv) With increase in temperature, the equilibrium conversion of a reversible exothermic reaction
(a) increases (b) decreases
(c) remains unaffected (d) none of (a), (b) & (c).

(v) There is no correspondence between stoichiometry and the rate equation in case of a / an _______________ reaction.
(a) non elementary (b) elementary
(c) series (d) parallel

(vi) Rate constant 'k' and absolute temperature T are related by Collision theory (for bimolecular reaction) as
(a) $k \infty T^{1.5}$ (b) $k \infty T^{0.5}$
(c) $k \infty T$ (d) $k \infty \exp(-E/RT)$

(vii) For a _________ order chemical reaction, the half- life period is independent of the initial concentration of the reactant A.
(a) first (b) third (c) second (d) zero

(viii) A space time of 3 hours for a flow reactor means that
(a) it takes three hours to dump the entire volume of the reactor with feed,
(b) three reactor volumes of feed can be processed every hour
(c) the time required to process one reactor volume of feed (measured at specified conditions) is 3 Hours
(d) none of the above.

(ix) The vessel dispersion number for Plug Flow is
(a) 0 (b) 500 (c) 750 (d) infinity.

(x) The single parameter model proposed for describing non ideal flow is
(a) maximum mixedness model (b) segregation model
(c) dispersion model (d) bypassing/dead space model.

Fill in the blanks with the correct word

(xi) In an autocatalytic reaction one of the_______acts as a catalyst. (Fill in the blank)

(xii) The use of space time is preferred over the mean residence time in the design of _________ reactor.

(xiii) All liquid phase reactions are considered as _________ volume reaction.

(xiv) In RTD the two most used methods of injection of tracers are Pulse Input and _______ input.

(xv) In RTD the third moment is also taken about the mean and is related to the _________.

Group - B

2. (a) Consider the reaction A +B→ Products, show that, $\ln\dfrac{M-X_A}{M(1-X_A)} = C_{A0}(M-1)kt$ for M not equal to 1, symbols stand for usual notation. *[(CO1)(Analyze/IOCQ)]*
(b) At 500 K the rate of a bimolecular reaction is ten times the rate at 400 K. Find the activation energy of this reaction from the Collision theory. *[(CO1)(Evaluate/HOCQ)]*

6 + 6 = 12

3. (a) An aqueous solution of ethyl acetate is to be saponified with sodium hydroxide. The initial concentration of ethyl acetate is 5.0 g/liter and that of caustic soda is 0.10 normal. Values of the second-order rate constant, in liters/(g mole)(min), are k = 23.5 at 0°C and 92.4 at 20^{0}C. The reaction is essentially irreversible. Estimate the time required to saponify 95% of the ester at 40°C. *[(CO1)(Apply(LOCQ))]*
(b) Find the first order rate constant for the disappearance of A in the gas reaction 2A = R if on holding the pressure constant the volume of the reaction mixture, starting with 80% A decreases by 20% in 3 min. *[(CO1)(Analyze(IOCQ))]*
(c) Deduce the integrated form of a half order reaction. *[(CO1)(Evaluate(HOCQ))*

5 + 5 + 2 = 12

Group - C

4. (a) Deduce the performance equation of an ideal plug flow reactor. *[(CO2)(Apply/IOCQ)]*

(b) The gas leaving an ammonia oxidation plant consists of 10% NO, 1% NO_2, 8% O_2 and rest inert. The gas is allowed to oxidize NO (A) + 1/2O_2 (B) = NO_2 (R) until NO_2: NO ratio reaches 8:1 and the oxidized gas is then absorbed in water to produce nitrisc acid. Calculate the size of the tubular reactor (assuming plug flow) operating at 20^0C and I atm needed to NO to NO_2 oxidation for a gas feed rate of 1000 m^3/hr (measured at 0^0C and 1 atm). The reaction rate equation is

$r_{NO_2} = 14000 C_{No}^2 C_{O_2} \frac{kmol}{m^3 s}$ *[(CO2)(Apply/HOCQ)]*

(c) An aqueous reactant stream (4mol A/lit) passes through a mixed flow reactor followed by a plug flow reactor. Find the concentration at the exit of the plug flow reactor if in the mixed flow reactor $C_{A\,=}$ 1 mol/lit. The reaction is first order with respect to A and the reactor volumes are equal. *[(CO2)(Apply(IOCQ))]*

3 + 5 + 4 = 12

5. (a) Deduce the performance equation of a MFR. *[(CO2)(Apply(LOCQ))]*

(b) We are planning to operate a batch reactor to convert A into R. This is a liquid reaction, the stoichiometry is A → R, and the rate of reaction is given in the following table. How long must we react each batch for the concentration to drop from C_A = 1.3 mol /liter to C_{Af} = 0.3 mol / liter?

Data:

C_A mol /liter	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	1.0	1.3
- r_A, mol / liter. min	0.1	0.3	0.5	0.6	0.5	0.25	0.10	0.06	0.05	0.045

[(CO2)(Evaluate(HOCQ))]

5 + 7 = 12

Group - D

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

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

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? *[(CO3)(Evaluate(HOCQ))]*

(b) For the elementary reactions $A \overset{k_1}{\rightarrow} R \overset{k_2}{\rightarrow} S$ Carried out in a MFR, find the value of $C_{R\,max}$.

[(CO3)(Evaluate/HOCQ)]

6 + 6 = 12

7. Chemical R is to be produced by the decomposition of A in a given mixed reactor. The reaction proceeds as follows:

$$A \rightarrow R, \quad r_R = k_1 C_A$$
$$2A \rightarrow S, \quad r_S = k_2 C_A^2$$

Let the molar cost ratio $\$_R/\$_A$ = M (S is waste material of no value), and for convenience let $k_1 = N k_2 C_{A0}$. In the feed C_{A0} is fixed.

(i) Ignoring operating costs, find what conversion of A should be maintained in the reactor to maximize the gross earnings and therefore the profits. *[(CO3)(Analyze(IOCQ))]*

(ii) Repeat part (i) with the hourly operating cost dependent on feed rate and given by $\alpha + \beta F_{A0}$. *[(CO3)(Evaluate(IOCQ))]*

(iii) Taking an example of a parallel reaction, define the term instantaneous yield. *[(CO3)(Evaluate/IOCQ)]*

(5 + 5 + 2) = 12

Group - E

8. (a) A sample of the tracer hytane at 320K was injected as a pulse to a reactor, and the effluent concentration was measured as a function of time, as per the data shown in the following table.

t (min)	0	1	2	3	4	5	6	7	8	9	10	12	14	17	20	23
C (g/m³)	0	1	5	8	10	12	11	9	8	6.5	5	3.0	2.2	1.5	0.6	0

Construct figure showing C(t) as functions of time. *[(CO4)(Evaluate(HOCQ))]*

(b) Construct a figure showing E(t) as functions of time. *[(CO4)(Evaluate(HOCQ))]*

(c) Determine the fraction of material leaving the reactor that has between 7 and 17 minutes. *[(CO4)(Evaluate(HOCQ))]*

4 + 4 + 4 = 12

9. (a) Determine the following RTD function for a laminar flow reactor:

$$E(t) = \begin{cases} 0 & t < \dfrac{\tau}{2} \\ \dfrac{\tau^2}{2t^3} & t \geq \dfrac{\tau}{2} \end{cases}$$

[(CO4)(Evaluate/HOCQ)]

(b) Determine mean conversion in a PFR following Segregation model. *[(CO5) (Analyze/IOCQ)]*

6 + 6 = 12

Cognition Level	LOCQ	IOCQ	HOCQ
Percentage distribution	10.42	37.5	52.08

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.*