# CHEMICAL REACTION ENGINEERING-I (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 <u>any 5 (five)</u> from Group B to E, taking <u>at least one</u> 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 +  $\frac{1}{2}$  O<sub>2</sub> = NO<sub>2</sub> 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) Pick out the correct statement
  - (a) A chemical reaction occurs when the energy of the reacting molecule is less than the activation energy of the reaction
  - (b) Chemical equilibrium is a static state
  - (c) A photochemical reaction is catalysed by light
  - (d) Reactions with high activation energies are very temperature sensitive.
- (iii) A given reaction is much more temperature sensitive at
  - (a) low temperature

- (b) high temperature
- (c) all temperature levels (d) none of the above.
- (iv) 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.
- (v) 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 the above.

- The half life period of a first order reaction is given by (where, k = rate constant. (vi) (b) 0.693/k (a) 0.693k (d) 0.593/k. (c) 0.593k
- (vii) 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.
- (viii) The performance equations for constant density systems are identical for (b) P.F.R. and batch reactor (a) PFR and MFR
  - (c) MFR and batch

- (d) none of the above.
- (ix) 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 ,Conversion is cent per cent after three hours
  - (c) The time required to process one reactor volume of feed (measured at specified conditions) is 3 Hours
  - (d) none of the above.
- (x) Stimulus-response techniques are commonly used to characterize the extent of non-ideal flow in vessels. Tracer input signal is used as stimulus. Any material can be used
  - (a) as tracer if it can disturb the flow pattern in the vessel
  - (b) as tracer if it does not disturb the flow pattern in the vessel and it can be detected
  - (c) as tracer if it follows ideal flow patterns
  - (d) none of the above.

## Group – B

2. Show that the following scheme (a)

 $N_2O_5 \implies NO_2 + NO_3^*$  $NO_3^* \rightarrow NO^* + O_2$  $NO^* + NO_3^* \rightarrow 2 NO_2$ Is consistent with and can explain the observed first order decomposition of  $N_2O_5$ .

(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 collision theory.

6 + 6 = 12

An aqueous solution of ethyl acetate is to be saponified with sodium 3. (a) 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°C. The reaction is

essentially irreversible. Estimate the time required to saponify 95% of the ester at 40°C.

(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.

8 + 4 = 12

### Group – C

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

 $r_{NO_2} = 14000C_{No}^2 C_{O_2} \frac{kmol}{m^3 s}$ 

(b) 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.

7 + 5 = 12

- 5. (a) The elementary irreversible aqueous-phase reaction  $A + B \rightarrow R + S$  is carried out isothermally as follows. Equal volumetric flow rates of two liquid streams are introduced into a 4-liter mixing tank. One stream contains 0.020 mol A/liter, the other 1.400 mol B/liter. The mixed stream is then passed through a 16-liter plug flow reactor. We find that some R is formed in the mixing tank, its concentration being 0.002 mol/liter. Assuming that the mixing tank acts as a mixed flow reactor, find the concentration of R at the exit of the plug flow reactor as well as the fraction of initial A that has been converted in the system.
  - (b) Show that the performance equation of a recycle reactor changes to that of a mixed flow reactor if the recycle ratio (R) tend to infinity.

6 + 6 = 12

## Group – D

6. (a) Substance A in the liquid phase produces R and S by the following reactions R second order

 $A'_{\backslash}$ 

S first order

A feed ( $C_{A0} = 1$ ,  $C_{R0} = 0$ ,  $C_{S0}$ , = 0) enters two mixed flow reactors in series, ( $\tau = 2.5$  min,  $\tau$  = 10 min). Knowing the composition in the first reactor ( $C_{A1} = 0.4$ ,  $C_{R1} = 0.2$ ,  $C_{S1} = 0.7$ ), find the composition leaving the second reactor.

(b) A and B react with each other as follows:  $2A \rightarrow R$ ,  $r_R = k_1C_A^2$   $A + B \rightarrow S$ ,  $r_S = k_2C_AC_B$   $2B \rightarrow T$ ,  $r_T = k_3C_B^2$ 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?

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:

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

Let the molar cost ratio R/R = M (S is waste material of no value), and for convenience let  $k_1 = Nk_2C_{A0}$ . 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.
- (ii) Repeat part (i) with the hourly operating cost dependent on feed rate and given by  $\alpha + \beta F_{AO}$ .

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## Group – E

- 8. (a) Define mean residence time  $(\bar{t})$  and variance  $(\sigma^2)$  for non ideal reactor system and discuss in detail how these can be determined from tracer experiment.
  - (b) State the different types of models available for determination of non ideality of reactors and discuss them briefly.

## 6 + 6 = 12

9. The concentration reading in the following table represents a continuous response to a delta function input into a closed vessel which is used as a chemical reactor.

Time (t), min	0	5	10	15	20	25	30	35
Tracer concentration, gm/L fluid	0	3	5	5	4	2	1	0

The vessel is to be used to carry out a first order liquid phase reaction  $A \rightarrow R$  having rate constant (k) = 0.307 min<sup>-1</sup>. Find the fraction of reactant unconverted in this real reactor.

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