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

(iii) In a tubular plug flow reactor,
(a) Radial mixing is complete, axial mixing is negligible
(b) Axial mixing is complete, radial mixing is negligible
(c) Axial mixing is complete, radial mixing is complete
(d) Both radial and axial mixing are negligible.

(iv) 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.

(v) 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%, and under these conditions the residence time is
(a) 1 sec (b) 2 sec (c) ½ sec (d) None of the above.

(vi) 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.

(vii) A batch reactor is characterised by
(a) Variation in extent of reaction with time
(b) Variation of composition at different position of the reactor
(c) non variation in extent of reaction with time
(d) none of the above.

(viii) A liquid phase reaction is 50% complete in one hour and 75% complete in two hours The reaction is
(a) Zero order (b) First order (c) Second order (d) None of the forgoing.

(ix) The performance equations for constant density systems are identical for
(a) PFR and MFR (b) P.F.R. and batch reactor
(c) MFR and batch (d) none of the above.

(x) For an ideal plug flow reactor, the value of Peclet number is
(a) 0 (b) 1 (c) 2 (d) infinity.

## Group- B

2 . (a) For a gas phase reversible reaction, A ⇄ mB, equilibrium constants based on partial pressures and concentrations are, respectively, $K_p$ and $K_c$. Find the relationship between the constants. [(CO1)(Remember(LOCQ))]

(b) Consider a reaction A → B + C. When conducted in a constant volume batch reactor at a constant temperature, the following data were obtained.

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| Time (min) | 0 | 5 | 9 | 15 | 22 | 30 | 40 | 60 |
| Concentration of A (mol/dm³) | 2 | 1.6 | 1.35 | 1.1 | 0.87 | 0.70 | 0.53 | 0.35 |

Use the integral method of rate analysis to determine order and rate constant of the reaction. [(CO1)(Analyze(IOCQ))], [(CO1)(Evaluate(HOCQ))]

**4 + (4 + 4) = 12**

3 . (a) Design of industrial reactors necessitates knowledge of chemical kinetics. Justify the statement by writing mass balance equation of a batch reactor.

[(CO1)Apply(LOCQ)]

(b) Consider a liquid-phase reaction A → B + C. For studying kinetics of this reaction, experiments have been conducted in a continuously-operated ideally-stirred flow reactor with varying flow rates and following data at steady-state have been obtained.

Feed: Pure A having concentration of 2 mol/ dm³

| | | | | | |
|---|---|---|---|---|---|
| Experiment no. | 1 | 2 | 3 | 4 | 5 |
| Time (min) | 15 | 38 | 100 | 300 | 1200 |
| Exit conc (mol/ dm³ ) | 1.5 | 1.25 | 1.0 | 0.75 | 0.5 |

Determine the reaction order and rate constant. [(CO1)(Analyze/IOCQ)]

(c) In part (b), for studying the kinetics, if experiments are conducted at somewhat higher temperature, what kind of experimental results will you expect? What theoretical framework do you have in mind behind your expectations?

[(CO1)Create(HOCQ]

**3 + 6 + 3 = 12**

## Group - C

4. (a) A daily production of 50 tonnes of ethyl acetate from alcohol and acetic acid is 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 $100^0$C is

$$(-r_A) = k\,(C_AC_B - C_PC_Q / K),\ \text{where, } k = 7.93 \times 10^{-6}\ m^3/\ \text{kmol.s and } K = 2.93$$

The feed solution contains 23 wt% of acid, 46 wt% of alcohol and no ester. The required conversion of acid is 35%. The density may be assumed to have a constant value 1020 kg/$m^3$. The plant must be operated day and night and times for filling, emptying and cleaning operation of a reactor is 1 hour. What would be the required reactor volume if one batch reactor vessel is used? [(CO2)Apply(HOCQ]

(b) At 650°C phosphine vapor decomposes as follows:

$$4PH_3 \rightarrow P_4 + 6H_2,\quad -r_{phos} = (10hr^{-1})\ C_{phos}$$

What size of plug flow reactor operating at 649°C and 11.4 atm is needed for 75% conversion of 10 mol /hr of phosphine in a 2/3 phosphine-1/3 inert feed?

[(CO2)(Analyze/IOCQ)]

**6 + 6 = 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 $85^0$C 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 to achieve 85% conversion of A if the reactor employed is:

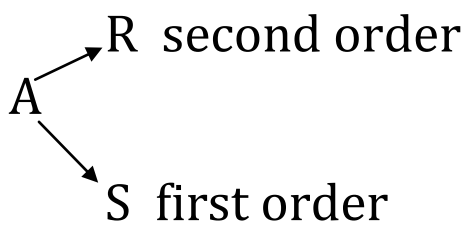
(i) One mixed flow reactor

(ii) One plug flow reactor. (CO2)(Analyze/IOCQ)]

**(6 + 6) = 12**

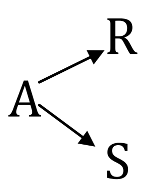
## Group - D

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




A feed ($C_{A0}$ = 1, $C_{R0}$ = 0, $C_{S0}$, = 0.3) enters two mixed flow reactors in series, ($\tau_1$ = 2.5 min, $\tau_2$, = 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. [(CO3)(Analyze/HOCQ)]

(b) The stoichiometry of 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 a feed $C_{A0}$ = 100 and exit concentration CAf = 20, find $C_R$ at the exit from a plug flow reactor. [(CO3)(Remember/LOCQ)]

**6 + 6 = 12**

7. A 20 liter MFR is to treat a reactant which decomposes as follows

$$A \longrightarrow R, \quad r_R = 4hr^{-1}C_A$$
$$A \longrightarrow S, \quad r_S = 1hr^{-1}C_A$$

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/lit, 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)(Analyze/IOCQ)]

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## Group - E

8. (a) Discuss in details how RTD function E (t) can be determined from the tracer concentration C (t). [(CO4)(Remember/LOCQ)]
(b) Discuss in details the Tank in Series model. [(CO5)(Understand/LOCQ)]

**6 + 6 = 12**

9. The first order reaction A $\longrightarrow$ B is carried out in a 10 cm diameter tubular reactor 6.36 m in height. The rate constant is 0.25 $min^{-1}$. The result of tracer test carried out on this reactor is shown in Table A:

Table A: Effluent Tracer Concentration as a Function of Time

| t (min) | 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 |

Calculate conversion using the closed vessel dispersion model. Given Variance = 6.10 min. [(CO5)(Analyze/IOCQ)]

**12**

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| Cognition Level | LOCQ | IOCQ | HOCQ |
|---|---|---|---|
| Percentage distribution | 26.05 | 54.16 | 19.79 |

**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.