B.TECH/CHE/5TH SEM/CHEN 3102/2016

CHEMICAL REACTION ENGINEERING
(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) Reactor design
(a) invariably relies on experimentally determined rates
(b) invariably relies on theoretically predicted rates
(c) does not rely on theoretically predicted rates
(d) both (a) and (c).

(ii) The frequency factor in Arrhenius law
(a) does affect the temperature sensitivity of a reaction
(b) does not affect the temperature sensitivity of a reaction
(c) is dimensionless
(d) is a measure of activation energy

(iii) For a reaction having order (n) greater than unity, the best combination of reactors will be
(a) PFR, small mixed, large mixed.
(b) Large mixed, small mixed, PFR.
(c) Small mixed, large mixed, PFR.
(d) Small mixed, PFR, large mixed.

(iv) The molecularity of a chemical reaction can be
(a) zero (b) fractional
(c) negative (d) always an integer.

(v) Half-life period for a first order reaction is ..... the initial concentration of the reactant.
(a) directly proportional to (b) inversely proportional to
(c) independent of (d) none of these.

(vi) 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.

(vii) 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 reactor or batch reactor
(d) none of the above.

(viii) For reaction under pore diffusion regime, the reaction rate
(a) varies directly with catalyst particle size
(b) varies inversely with catalyst particle size
(c) is independent of catalyst particle size
(d) none of the above.

(ix) For RTD in Open-open system, when the extent of dispersion becomes same as mean residence time, the value of Peclet number would be close order of
(a) zero (b) infinity (c) unity (d) two.

(x) For an ideal plug flow reactor, the value of Peclet number is
(a) 0 (b) ∞ (c) 1 (d) 10.

Group – B

2. (a) (i) The decomposition of A at 400^0 C for pressures between 1 and 10 atm follows a first order rate law. Show that the following mechanism.
$A + A \rightleftharpoons A^* + A$
$A^* \rightarrow R + S$
is consistent with the observed kinetics.

(ii) Different mechanisms can be proposed to explain first order kinetics. To claim that this mechanism is correct in the face of other alternatives requires additional evidence. For this purpose what further experiments would you suggest we run and what results would you expect to find?

(b) In a certain Chemical Reaction the half-life becomes doubled when the concentration is doubled. Find the order of the reaction.

(3 + 3) + 6 = 12

3. (a) For a certain chemical reaction $A \rightarrow$ Error! Bookmark not defined. R, the following data were obtained:

Temperature, ^0C	100	110	120	130	140	150
Rate constant, s^{-1}	1.055×10^{-16}	1.070×10^{-15}	9.25×10^{-15}	6.94×10^{-14}	4.58×10^{-13}	$3.19\ 10^{-12}$

Find the activation energy and frequency factor for this reaction.

(b) For the reactions in series, $A \xrightarrow{k_1} R \xrightarrow{k_2} S$, $k_1 = k_2$
Find the maximum concentration of R and the time when it is reached.

6 + 6 = 12

Group – C

4. (a) A daily production of 50 tons 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 100^0C 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 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 is1 hour. What would be the required reactor volume if one batch reactor vessel is used?

(b) It has been reported that the reaction
$C_2H_4OHCl + NaHCO_3 \rightarrow C_2H_4(OH)_2 + NaCl + CO_2$
is elementary with rate constant k = 5.2 liter/mol.hr at 82^0C. On the basis of this information we wish to construct a pilot plant to determine the economic feasibility of producing ethylene glycol from two available feeds, a 15 wt% aqueous solution of $NaHCO_3$ and a 30 wt% aqueous solution of C_2H_4OHCl. What volume of tubular (plug flow) reactor will produce 20 kg/hr ethylene glycol at 95% conversion of an equimolar feed produced by intimately mixing appropriate quantities of the two feed streams. Assume all operations at 82^0C, at which temperature the specific gravity of mixed reacting fluid is 1.02.

7 + 5 = 12

5. (a) The elementary irreversible aqueous-phase reaction A + B → 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) A first order reaction is to be treated in a series of two mixed flow reactors. Show that the total volume of the two reactors is the minimum when the reactors are equal in size.

6 + 6 = 12

Group – D

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

(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.

6 + 6 = 12

7. (a) The catalytic reaction $A \rightarrow 4R$
is run at 3.2 atm and 117°C in a plug flow reactor which contains 0.01 kg of catalyst and uses a feed consisting of the partially converted product of 20 liters/hr of pure unreacted A. The results are as follows:

Run	1	2	3	4
C_{Ain}, mol/liter	0.100	0.080	0.060	0.040
C_{Aout}, mol/liter	0.084	0.070	0.055	0.038

Find a rate equation to represent this reaction.

(b) Discuss in details the different methods used for preparation of catalyst.

7 + 5 = 12

Group – E

8. (a) Show that the complete RTD function for a Laminar Flow is:

$$E(t) = 0 \text{ for } t < \frac{\tau}{2} \text{ and } \frac{\tau^2}{2t^3} \text{ for } t \geq \frac{\tau}{2}$$

(b) Determine mean conversion in a PFR following Segregation model.

7 + 5 = 12

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

t (min)	0	1	2	3	4	5	6	7	8	9	10	12	14
C (g/m^3)	0	1	5	8	10	8	6	4	3.0	2.2	1.5	0.6	0

The measurements represent the exact concentrations at the times listed and not average values between the various sampling tests. Construct figures showing C(*t)* and E (*t*) as functions of time.

(b) What do you mean by dead zone of a reactor? What is the significance of Damkohler no.

9 + 3 = 12