Ref. No. Ex./Ch.E/T/312/2017

B. Chemical Engineering 3rd Year 1ST Semester Examination, 2017

Chemical Reaction Engineering I

Time: Three Hours　　　　　　　　　　　　　　　　　　Full Marks: 100

(50 marks for each part)
Use a separate Answer-Script for each part

Part I
Answer any three questions
All questions *do not* carry equal marks
Assume missing data, if any

1 .(i) Consider a reversible reaction $A + B \Leftrightarrow C + D$ being conducted in an isothermal semibatch reactor where B is continuously being fed at a constant rate to a batch of another reactant A. Derive an expression relating conversion of A, X with time. **[6]**

1. (ii) In the context of dispersion model for non-ideal reactor, define 'DamkÖhler Number' and 'Peclet Number' stating their significance. **[4]**

1.(iii) A vapor phase decomposition reaction A → R+S is carried out in a CSTR. Initial concentration of pure A is 0.0050 kmol/m^3. The following data is obtained in different runs:

Run No.	1	2	3	4	5
τ, s	0.4	5.0	14	45	195
X_A	0.2	0.6	0.76	0.9	0.97

Determine a suitable rate equation for this vapor phase decomposition reaction.

[6]

2. (i) At 1 atm, 298K a small constant volume reactor was filled with pure reactant A. The temperature is then rapidly raised to 373K and the readings in the following table are obtained. The stoichiometry of the reaction is 2A → B, and after leaving the reactor for long duration the contents are analyzed and no A can be found. Find a rate equation in units of moles, L and minutes which will satisfactorily fit the data.

Time, min	0	1	2	3	4	5	6	7	8	9	10	15	20
P (atm)	1.252	1.10	1.00	0.980	0.940	0.90	0.860	0.840	0.82	0.805	0.800	0.754	0.728

[8]

2.(ii) The second order reversible liquid phase reaction $P + Q \Leftrightarrow R + S$ (forward rate constant= 8.5 L/mol.min and backward rate constant= 6.5 L/mol.min)is to be carried out in a CSTR of volume 150 L. The concentrations of the reactants P and Q at the storage tanks are 2.6 mol/L and 2.0 mol/L respectively. The reactants are introduced at equal volumetric flow rates in the reactor. It is desired to attain 50% conversion of the limiting reactant. Calculate the necessary flow rate of each reactant stream. **[8]**

4. (i) Propylene oxide (PO) is reacted with excess water in presence of inert methanol (M) using an adiabatic CSTR which is fed with PO at a rate of 19.56 kmol/h for production of Propylene glycol (PG). The feed stream consists of (a) an equivalent mixture of propylene oxide and methanol containing 1.32 m^3/h each and (b) water containing 0.1% H_2SO_4. Volumetric flow rate of water is 6.6 m^3/h. The corresponding molar feed rates of water and methanol are 364.9 kmol/h and 32.66 kmol/h respectively. The temperature of both feed streams is 15 $^\circ$C prior to mixing. There is an immediate rise of temperature by 8 $^\circ$C on mixing. Volume of the reactor available in the laboratory is 1.2 m^3. The reaction is of first order with respect to PO and zero order with respect to water and the rate constant is $k=16.96\times10^{12}\exp(-18000/1.987\,T)\ h^{-1}$. What will be the steady state conversion and temperature? The temperature should not exceed 75°C to avoid vaporization of PO.

(a) Check the suitability of this reactor for this purpose. **[12]**

Data: $C_{pm}(PO)$= 35 Cal/mol. K; $C_{pm}(H_2O)$= 18 Cal/mol. K; $C_{pm}(PG)$= 46 Cal/mol. K; $C_{pm}(M)$=19.6Cal/mol.K.; $\Delta H_{r(20^\circ C)}$ = -20222Cal/mole PO.

(ii) Write the general expression to evaluate the conversion in a nonideal reactor as per Segregation model. **[4]**

4. (i)Starting with pulse tracer unsteady mole balance equation in presence of dispersion, explain the procedure to compute the dispersion coefficient/reactor Peclet number(Pe_R) using RTD data considering Danckwerts *closed-closed* boundary conditions. **[6]**

(ii) Stating the pertinent equations, explain the procedure to determine reactor dead volume using RTD data through applications of open-open boundary conditions (long tubes, Pe_R>100) as per dispersion model for nonideal reactor.

[8]

(iii) Explain graphically the optimum temperature progression of a reversible exothermic reaction. **[4]**

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BACHELOR OF CHEMICAL ENGINEERING EXAMINATION, 2017

(3rd Year, 1st Semester)

Chemical Reaction Engineering - I

Answer any ***TWO***

Assume any **missing** data

PART: II

1.a. An exothermic reversible reaction $A \Leftrightarrow B$ with rate equation has the following kinetic parameters:

$$-r_A = k_1 C_{A0}(1 - x_A) - k_2 C_{A0} x_A$$

$$k_1 = k_{10} e^{-\Delta E_1/RT} ; k_{10} = 21\ s^{-1}; \Delta E_1 = 32{,}200\ KJ/Kmol$$

$$k_2 = k_{20} e^{-\Delta E_2/RT} ; k_{20} = 4200\ s^{-1}; \Delta E_2 = 64{,}400\ KJ/Kmol$$

The reaction is to be carried out in a continuous flow reactor in which optimum temperature policy is maintained. Calculate the space time required for 80% conversion of A. the feed concentration of A is 0.8 kmol/m^3 and reaction temperature is to be restricted to remain below 900 K. Show that space time for CSTR is 6.4 times larger than PFR.

b. An elementary liquid phase reaction A + B $\Leftrightarrow$ C takes place in a continuous flow reactor using a equimolar quantities of A & B. Calculate the volume necessary to achieve 98% of the equilibrium conversion for CSTR and PFR.

k_1 = 0.01 lt/mol-min

K_e = 2 lt/min

F_{A0} = 10 mol/min

$C_{A0} = C_{B0}$ = 2 mol/lt

c. After the start up of a CSTR, show that for a first order reaction, time required to reach concentration 99% of the steady state concentration, $t_s = 4.6 \frac{\tau}{1+k\tau}$; where symbols carry their usual meaning.

15+6+4

2.a. Recycle plug flow reactor (PFR) is mainly used for autocatalytic reactions. Explain why with elaboration of characteristics of autocatalytic reactions.

b. What are the merits and demerits of step experiments over pulse for RTD determination by tracer injection technique?

c. $A \xrightarrow{k_1} B \xrightarrow{k_2} C$ type of series reactions (considering all the steps are first order), show that maximum concentration of B, C_{Bmax} will be

$$\frac{C_{Bmax}}{C_{A0}} = \left(\frac{k_1}{k_2}\right)^{\frac{k_2}{k_2-k_1}}; \qquad when\ k_1 \neq k_2$$

$$\frac{C_{Bmax}}{C_{A0}} = \frac{1}{e}; \qquad when\ k_1 = k_2$$

d. Acetic anhydride is hydrolyzed in three stirred tank reactor operated in series. The feed flows to the first reactor (V= 1lt) at a rate of 400 cc/min. The second and third reactors have volume of 2lt and 1.5 lt, respectively. The first order irreversible rate constant is 0.158 min^{-1} at 25°C. Calculate the fraction hydrolyzed in effluent from the third reactor. The rate equation is: r = $0.158C_1$.

6+5+6+8

3.a. A + B → R (desired)
→ S (undesired)

$$\frac{dC_R}{dt} = C_A C_B^{0.3} mol/lt - min$$

$$\frac{dC_S}{dt} = C_A^{0.5}\ C_B^{1.8} mol/lt - min$$

Feed is a mixture of pure A and pure B (each has concentration of 20 mol/lt). Find the fraction of impurity in product for feed of 90% conversion of A in case of plug flow reactor and CSTR.

b. Show that $x_A = \frac{D_a}{1+D_a}$ for first order liquid phase (at constant pressure) reaction kinetics where x_A is the conversion of reactant and D_a is the Damkohler number.

c. Why and when either "Inter-stage cooling" or "Cold-shot cooling" are done in case of stage reactions?

d. The first order homogeneous gaseous decomposition A → 2.5 R is carried out in an isothermal batch reactor at 2 atm with 20% inert and the volume increases by 60% in 20 mins. In a constant volume reactor, find out the time required for the pressure to reach 8 atm if the initial pressure is 5 atm, 2atm of which consist of inerts.

8+4+6+7