Thapar Institute of Engg & Technology, Patiala

End-sem Exam; Chemical Reaction Engg-1(CH- 010) (5th Sem)

Time: 3 hr MM: 45 Date: 08/12/2006 Time: 14:00- 17:00 hrs

Attempt all questions.

1 Chemical X, a powdered solid, is slowly and continuously fed for half an hour into a well-stirred vat of water. The solid **very quickly** dissolves and hydrolyses to Y, which then **slowly** decomposes to Z as follows 6

$Y \rightarrow Z \quad -r_Y = KC_Y, \; k = 1.5\ hr^{-1}$.

The volume of liquid in the vat stays close to 3 m^3 throughout this operation and **if** no reaction of Y to Z occurred, the concentration of Y in the vat would be 100mol/m^3 at the end of the half hour addition of X.

(a) What is the maximum concentration of Y in the vat and at what time is this maximum reached?

(b) What is the concentration of product Z in the vat after 1 hour?

2 (a)Using autocatalytic reaction $A \rightarrow R$; $-r_A = 0.001\ C_A C_R$ mol/ (liter.s); we wish to process 1.5 liter/s of a C_{A0} = 10 mol/liter feed to the highest possible conversion in a reactor system consisting of four 100 liter MFRs connected as you wish and any feed arrangement. Sketch your recommended design and feed arrangement and determine the highest conversion possible. 4 + 4 + 2

(b) From the following data for the gas-phase decomposition of pure A, $A \rightarrow R + S$, in a mixed flow reactor.

Run Number:	1	2	3	4	5
X_A (C_{A0} =0.002 mol/liter):	0.22	0.63	0.75	0.88	0.96
Holding time (sec) :	0.43	5.10	13.5	44	192

Find a satisfactory rate equation.

(c) In a homogenous isothermal liquid reaction, $A \rightarrow R + S$; 20 % of the reactant A disappears in 34 min for initial A concentration of 0.04 and also for 0.8 mol/liter. What is the rate of disappearance of A

3. (a) For the first order series reactions $A \xrightarrow{k1} R \xrightarrow{k2} S$ being carried out in a mixed flow reactor show that the optimum residence time for producing maximum R is given by $\tau = 1/\sqrt{k_1 k_2}$

and max concentration of R is given as

$C_{R,max} / C_{A0} = 1/(\sqrt{k_2/k_1} + 1)^2$ 4 + 5

(b)At room temperature the second order irreversible liquid phase reaction proceeds as follows: $2A \rightarrow$ Products, $-r_A = [0.005\text{litre/(mole min)}]\ C_A^2$ C_{A0} =1 mol/liter. A batch reactor takes 18 minutes to fill and empty. What percent conversion and reaction time should we use so as to maximize the daily output of product R.?

4 (a) Applying heat balance over a mixed flow reactor operating under adiabatic conditions show that the temperature rise (for exothermic reaction) or temperature drop (for endothermic reaction) is directly proportional to the conversion X_A in the reactor. Assume that the variation of heat of reaction and specific heats of reactants and products with temperature is negligible.

(b) Michaelis and Mentene gave the following mechanism to explain the kinetics of enzyme-substrate reactions. 4 + 4

$A + E \overset{k1}{\rightarrow\leftarrow_{k2}} X$ with equilibrium constant K = [X]/[A][E]

$X \xrightarrow{k3} R + E$ and $[E_0] = [E] + [X]$

Where, $[E_0]$ = total enzyme conc; [E] =free unattached enzyme conc.

Find a kinetic expression for rate of consumption of substrate A in terms of [A], $[E_0]$,k1 ,k2, and k3

5 Under the action of mixed enzymes reactant A is converted to products as follows: $A \xrightarrow{k1,\ enzyme} R \xrightarrow{k2,\ enzyme} S$ $n_1 = n_2 = 1$; enzyme conc remains constant. The rate constants k1 and k2 depend on the pH of the system. When R is the desired product; $k1 = pH^2 - 8\ pH + 23$ with $2 < pH < 6$

$k2 = pH + 1$

(a)What pH level would you use for maximizing concentration of R from a mixed flow reactor for 60 % conversion of a given feed of pure A

(b)If it were possible to change pH level along the plug flow reactor, in what way (increase or decrease) you will change the pH for maximizing output concentration of R from the PFR (for a given feed). Justify your choice. 6

6 The liquid phase reaction of aniline with ethanol produces wanted monoethylaniline and unwanted diethyaniline: 6

$C_6H_5NH_2 + C_2H_5OH \xrightarrow{k1,\ H_2SO_4} C_6H_5NHC_2H_5 + H_2O$

$C_6H_5NHC_2H_5 + C_2H_5OH \xrightarrow{k2,\ H_2SO_4} C_6H_5N(C_2H_5)_2 + H_2O$ $k1 = 1.25\ k2$

(a) An equimolar feed is introduced into a batch reactor and reaction is allowed to proceed to completion. Find the concentration of reactants and products at the end of the run.

(b) Find the ratio of mono to diethyl aniline produced in a MFR for an alcohol to aniline feed ratio of 2 to 1 for 70 % conversion of alcohol.