

III B.Tech II Semester Supplementary Examinations,  
November/December 2005  
CHEMICAL REACTION ENGINEERING-I  
(Chemical Engineering)

Time: 3 hours

Max Marks: 80

Answer any FIVE Questions  
All Questions carry equal marks

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1. (a) Define reaction rate constant. Develop an expression that facilitates calculation of units of rate constant for any order. [6]
- (b) Determine equilibrium conversion of A at 373<sup>0</sup>K for the following aqueous reaction.  

$$A \xrightleftharpoons[k_2]{k_1} R \quad \Delta G^0 = -3375 \text{ K cal/K mole}$$

$$\Delta H_r^0 = -18,000 \text{ K cal/K mole}$$
 Assume specific heats of all solutions are equal to that of water. [10]
2. (a) The decomposition of ammonia on a tungsten wire is carried out at 856<sup>0</sup>C and the following data are obtained.
 

Total Pressure, atm	0.300	0.330	0.359	0.418
Time, sec.	200	400	600	1000

 Check whether the reaction follows zero order kinetics. Find the reaction velocity constant.
- (b) For a second order reaction show that the half life period is  $t_{\frac{1}{2}} = 1 / K C_{A0}$   
 K- is the rate constant and  $C_{A0}$  - initial concentration of reactant. [8+8]
3. Experiment shows that the homogeneous decomposition of ozone proceed with a rate  $-r_{O_3} = K[O_3]^2[O_2]^{-1}$ . Suggest a two step mechanism to explain this rate and explain how would you further test this mechanism? [16]
4. The following reaction is carried out in mixed flow reactor at 400<sup>0</sup>C and 1 atm. Pressure. The reaction is second order irreversible,  $A \rightarrow B + C$ . Find the size of the reactor needed to obtain 95% conversion when the feed rate is 100 gm/sec. And the reaction velocity constant at 500<sup>0</sup>C is  $0.4 \text{ m}^3/\text{kg.mole.sec}$ . The molecular weight of A is 44. [16]
5. 100 litres/hour of radio active fluid having a half-life of 20 hr is to be treated by passing it through two ideal stirred tanks in series,  $V = 40,000$  litres each. In passing through this system, how much has the activity decayed? [16]
6. For a gaseous reaction  $A \rightleftharpoons R+S$  taking place on a porous catalyst, derive the rate expression if the adsorption of A controls the overall reaction. [16]
7. Derive the expression for effectiveness factor in a single cylindrical pore for a first order reaction. [16]

8. Write detailed notes on:

- (a) Integral and differential methods
- (b) Total volume and total pressure methods.

[8+8]

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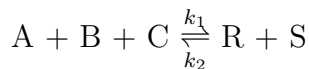
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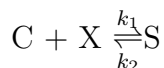
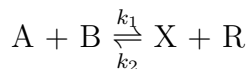
1. (a) For the reaction  $2A + \frac{1}{2} B \rightarrow C$  write the relation between the rate of formation and disappearance of the three components of the reaction. [6]
  - (b) A reaction has the stoichiometric equation  $2A \rightarrow R + S$  what is the order of the reaction. [2]
  - (c) The reaction with the following stoichiometric equation  $A + \frac{1}{2} B \rightarrow R$  has the rate expression  $r_A = kC_A C_B^{0.5}$ . What is the rate expression for the reaction written as  $2A + B \rightarrow 2R$  [2]
  - (d) A certain reaction has a rate given by  $r_A = 0.005C_A^2$ ,  $mol/cm^3 \cdot min$ . If the concentration is to be expressed in mol/lit and time in hours, what would be the value and units of the reaction rate constant? [6]
2. (a) The first order homogeneous decomposition,  $A \rightarrow 2.5 R$  is carried out in an isothermal batch reactor at 2 atm. With 20% inerts present, the volume increases by 60% in 20 min. In a constant volume reactor, find the time required for the pressure to reach 8 atm., if the initial pressure is 5 atm., 2 atm of which consists of inerts. [8]
  - (b) Explain how total volume and total pressure methods help in arriving at the kinetics of the given reaction. Derive relevant equations. [8]
3. Chemicals A, B and C combine to give R and S with steichiometry



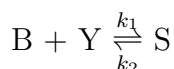
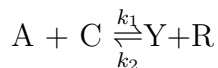
The observed rate is  $r_R = K \frac{C_A C_B C_C}{C_R}$ .

The following mechanisms have been proposed to explain the observed kinetics.

Mechanism I :



Mechanism II :



- (a) Are these mechanisms consistent with the kinetic expression?  
 (b) If neither is consistent, devise a scheme. [16]
4. From the following data find a satisfactory rate equation for gas phase decomposition of  $A \rightarrow R + S$ , taking place isothermally in a mixed reactor.
- |                    |       |      |      |      |       |
|--------------------|-------|------|------|------|-------|
| Space time in Sec: | 0.423 | 5.10 | 13.5 | 44.0 | 192.0 |
| Conversion :       | 0.22  | 0.63 | 0.75 | 0.88 | 0.96  |
- Initial concentration is 0.002 mole/lit. [16]
5. At present conversion is  $2/3$  for our elementary second-order liquid reaction  $2A \rightarrow 2R$  when operating in an isothermal plug flow reactor with a recycle ratio of unity. What will be the conversion if the recycle stream is shut off? [16]
6. (a) Define a catalyst and describe its properties.  
 (b) Compare physical adsorption and chemisorption.  
 (c) What is an adsorption isotherm? Define. [6+6+4]
7. Equimolar quantities of A, B and D are fed continuously to a mixed flow reactor where they combine by the elementary reactions
- $$\left. \begin{array}{l} A + D \xrightarrow{k_1} R \\ B + D \xrightarrow{k_2} S \end{array} \right\} \text{with } \frac{k_2}{k_1} = 0.2$$
- (a) If 50% of the incoming A is consumed find what fraction of the products formed is R.  
 (b) If 50% of the incoming D is consumed find what fraction of the products formed is R. [8+8]
8. Write brief notes on:
- (a) Optimum temperature progression.  
 (b) Product distribution in multiple reactions. [8+8]

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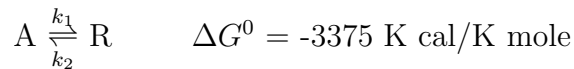
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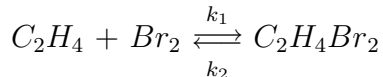
1. (a) Define reaction rate constant. Develop an expression that facilitates calculation of units of rate constant for any order. [6]
- (b) Determine equilibrium conversion of A at 373<sup>0</sup>K for the following aqueous reaction.



$$\Delta H_r^0 = -18,000 \text{ K cal/K mole}$$

Assume specific heats of all solutions are equal to that of water. [10]

2. For the reaction in series  $A \rightarrow R \rightarrow S$  with  $k_1 \neq k_2$ , find the maximum concentration of R and when it is reached in a batch reactor?  $k_1$  and  $k_2$  are the rate constants for the first and second reactions. Show what happens if  $K_1 = K_2$ . [16]
3. Experiment shows that the homogeneous decomposition of ozone proceed with a rate  $-r_{O_3} = K[O_3]^2[O_2]^{-1}$ . Suggest a two step mechanism to explain this rate and explain how would you further test this mechanism? [16]
4. At 600<sup>0</sup>K the gas phase reaction,



has rate constants  $k_1 = 500 \text{ m}^3 / (\text{K mole.hr})$  and  $k_2 = 0.032 \text{ hr}^{-1}$ . If a plug flow reactor is to be fed 600  $\text{m}^3/\text{hr}$  of gas containing 60%  $Br_2$ , 30%  $C_2H_4$  inerts by volume at 600<sup>0</sup>K and 1.5 atm., calculate the volume of reaction vessel required to obtain 60% conversion of ethylene. [16]

5. From steady-state kinetics runs in a mixed flow reactor, we obtain the following data on the reaction  $A \rightarrow R$ .

t, sec	$C_{AO}$ , mmol/liter	$C_A$ , mmol/liter
60	50	20
35	100	40
11	100	60
20	200	80
11	200	100

Find the space time needed to treat a feed of  $C_{AO} = 100 \text{ mmol/litre}$  to 80% conversion.

- (a) In a plug flow reactor  
(b) In a mixed flow reactor. [8+8]
6. For the following gas phase solid catalyzed reaction:  
 $A+B \rightleftharpoons R+S$ . Obtain the expression for the rate of reaction if adsorption of A is the controlling step. [16]
7. For the first order reactions  $A \xrightarrow{k_1} R \xrightarrow{k_2} S$  taking place in a plug flow reactor derive the expression for  $C_{R,max}$  and  $\tau_{p,opt}$ . [16]
8. Write short notes on:
- (a) Bio chemical reactions  
(b) Catalytic reactions [8+8]

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1. (a) i. For the reaction  $\frac{1}{2} O_2 + 2NO_2 \rightarrow N_2O_5$  Write the relation between the rates of formation and disappearance of all the components involved in the reaction. [4]
- ii. Write the units of specific reaction rate constant in the eqn:  $-r_A = 0.08C_A^{0.5}$  [2]
- iii. Define the molecularity of a reaction with an example [2]
- iv. Define elementary reaction with example [2]
- v. Define multiple reactions with example [2]
- (b) Sketch the energies involved in the transformation of reactants to products for exothermic and endothermic reaction. [4]

2. (a) Explain how total pressure data help in finding the rate equation. [6]
- (b) The reaction  $2A \rightarrow R$  is studied isothermal at  $36^\circ C$  in a constant volume batch reactor. Using the following data obtain the rate equation in units of moles, liters and minutes. [10]

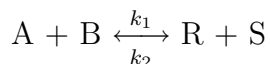
Time, min	3	7	14	23	34	48	68	95
Total Pressure, mm Hg	620	600	575	550	525	500	474	450

3. (a) Distinguish between elementary and non elementary reactions.
- (b) Show that the following scheme
 
$$N_2O_5 \rightleftharpoons NO_2 + NO_3^*$$

$$NO_2 + NO_3^* \rightarrow NO^* + O_2 + NO_2$$

$$NO^* + NO_3^* \rightarrow 2NO_2$$
 is consistent with and can explain the observed first order decomposition of  $N_2O_5$ . [4+12]

4. The liquid phase reaction,



$$k_1 = 8 \text{ liter/mole. Min.}$$

$$k_2 = 4 \text{ liter/ mole. Min.}$$

is to take place in a 200 liter steady state mixed reactor. Two feed streams, one containing 3.0 mole A/liter, and the other containing 2.0 moles/liter are to be introduced in equal volumes into the reactor and 60 % conversion of limiting component

- is desired. What should be flow rate of each stream? Assume a constant density throughout. [16]
5. 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. [16]
6. For the solid catalyzed reaction  $A+B \rightleftharpoons R+S$  derive the expression for the rate of reaction if desorption of R is rate controlling. [16]
7. Derive the energy balance equation for adiabatic operation of PFR. [16]
8. Write short notes on:
- (a) Law of mass action
  - (b) Single and multiple reactions. [8+8]

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