

III B.Tech II Semester Regular Examinations, Apr/May 2006
CHEMICAL REACTION ENGINEERING-I
 (Chemical Engineering)

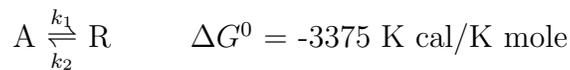
Time: 3 hours

Max Marks: 80

Answer any FIVE Questions
 All Questions carry equal marks

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 373⁰K for the following aqueous reaction.

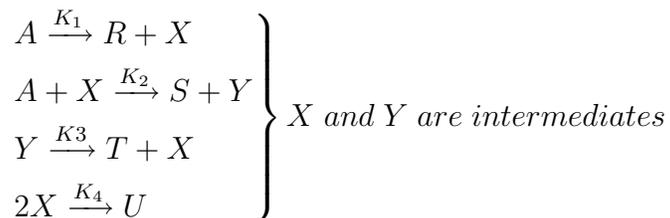


$$\Delta H_r^0 = -18,000 \text{ K cal/K mole}$$

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

2. A zero order homogeneous gas reaction $A \rightarrow rR$ proceeds in a constant volume bomb. With 20 % inerts, and the pressure rises from 1 to 1.3 atm. in 2 minutes. If the same reaction takes place in a constant pressure batch reactor, what is the fractional change in 4 minutes if the feed is at 3 atm. and consist of 40% inerts. [16]

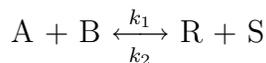
3. The reaction $3A \rightarrow 2R + S + T + U$ has the following mechanism.



Show that $-r_A$ can be represented as $-r_A = KC_A^{3/2}$

Specify all the assumptions that are made. [16]

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. Substance A reacts according to second order kinetics and conversion is 95% from a single flow reactor. We buy a second unit identical to the first. For the same conversion, by how much is the capacity increased if we operate these two units in parallel or in series?
- (a) The reactors are both plug flow.
(b) The reactors are both mixed flow. [8+8]
6. For the solid catalyzed reaction $A \rightleftharpoons R$ derive the expression for the rate of reaction if desorption of R is rate controlling. [16]
7. At 1000⁰K and 1 atm substance A is 2 mole % dissociated according to the following reaction $2A = 2B + C$.
- (a) Calculate the mole % dissociated at 200⁰ K and 1 atm.
(b) Calculate the mole % dissociated at 200⁰ K and 0.1atm.
- i. Average C_p of A = 8 cal/mol.⁰ K
ii. Average C_p of B = 8 cal/mol.⁰ K
iii. Average C_p of C = 8 cal/mol.⁰ K
- At 25⁰C and 1 atm 2000 cal are released when 1 mole A is formed from the reactants B and C. [8+8]
8. Write short notes on:
- (a) Order and molecular
(b) Empirical rate equations. [8+8]

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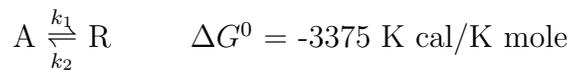
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1. (a) Define reaction rate constant. Develop an expression that facilitates calculation of units of rate constant for any order. [6]

- (b) Determine equilibrium conversion of A at 373⁰K for the following aqueous reaction.



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

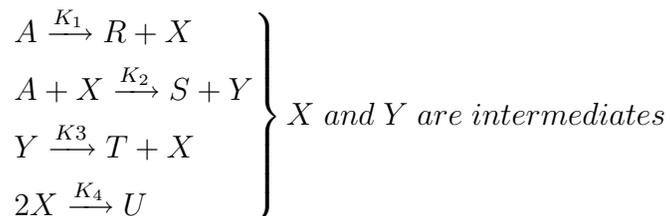
Assume specific heats of all solutions are equal to that of water. [10]

2. Pure gaseous A decomposes to completion according to the reaction $A \rightarrow R + S$ in a then walled capillary tube which acts as a batch reactor. The required temperature is maintained in the tube by placing it into a bath of boiling water. The following data are obtained.

Time (min.)	0.5	1	1.5	2	3	4	6	10
Length of Capillary occupied by reactions mixture(mm),	6.1	6.8	7.2	7.5	7.85	8.1	8.4	8.7 9.4

Find a rate equation in units of moles, liters and minutes for the decomposition. Pressure in the capillary measures 1000mm Hg guage. [16]

3. The reaction $3A \rightarrow 2R + S + T + U$ has the following mechanism.



Show that $-r_A$ can be represented as $-r_A = KC_A^{3/2}$

Specify all the assumptions that are made. [16]

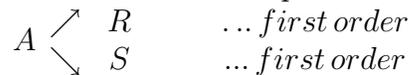
4. A high molecular weight hydrocarbon stream A is fed continuously to a high temperature mixed reactor where it thermally cracks (homogeneous gas reaction) into lower molecular weight materials, R by the reaction, $A \rightarrow 5 R$ By changing the feed rate different extents of cracking are obtained as follows:

F_A , millimol/hr	300	1000	3000	5000
C_A , millimol/hr	16	30	50	60

The internal void volume of the reactor is 0.1 litre and the feed concentration is 100 millimol/liter. Find rate equation to represent the cracking reaction. [16]

5. (a) Define recycle ratio. What is the effect of varying the recycle ratio from zero to infinity on the performance of the recycle reactor?
 (b) Develop the performance equation for a recycle reactor. Write the performance equation for the two extremes of the recycle ratio. [4+12]
6. For the solid catalyzed reaction $A \rightleftharpoons R$ derive the expression for the rate of reaction if desorption of R is rate controlling. [16]

7. Substance A in a liquid reacts to produce R and S as follows:



A feed ($C_{A0} = 1$, $C_{R0} = 0$, $C_{S0} = 0$) enters two mixed reactors in series ($\tau_1 = 2.5$ min, $\tau_2 = 5$ min). Knowing the composition in the first reactor ($C_{A1} = 0.4$, $C_{R1} = 0.4$, $C_{S1} = 0.2$), find the composition leaving the second reactor. [16]

8. Write short notes on:

- (a) Batch and flow reactors
 (b) Law of mass action. [8+8]

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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]

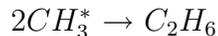
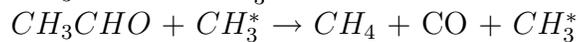
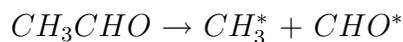
2. (a) A tri molecular elementary reaction $A + 2B \rightarrow R$ takes place in a constant volume batch reactor. Starting with $C_{A0} = 0.2$ mole/lit. and $C_{B0} = 0.4$ mole/lit. the following data are obtained

t, min.	10	20	30	40	50	60
C_A mole/lit	0.174	0.156	0.143	0.132	0.124	0.117

 Find a suitable rate equation

- (b) Derive the equation used to solve the above problem. [8+8]

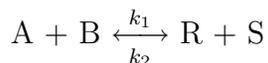
3. (a) What is a chain reaction? Define chain length.
- (b) Thermal decomposition of acetaldehyde is postulated to proceed by the chain mechanism



observing the rate of first reaction is small in comparison with the second when chains are long, show that

$$\frac{-d[CH_3CHO]}{dt} = K[CH_3CHO]^{1.5} \quad [4+12]$$

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. (a) What are autocatalytic reactions? Explain with a typical rate-concentration curve. Give some important examples of autocatalytic reactions.
(b) Which reactor is more efficient for carrying out autocatalytic reactions at various conversion levels? Explain with the help of $1/(-r_A)$ versus X_A graph. [8+8]
6. For the solid catalyzed reaction $A \rightleftharpoons R+S$ derive the expression for the rate of reaction if desorption of R is rate determining step. [16]
7. At 1000^0K and 1 atm substance A is 2 mole % dissociated according to the following reaction $2A = 2B + C$.
(a) Calculate the mole % dissociated at 200^0K and 1 atm.
(b) Calculate the mole % dissociated at 200^0K and 0.1atm.
i. Average C_p of A = 8 cal/mol. ^0K
ii. Average C_p of B = 8 cal/mol. ^0K
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- At 25^0C and 1 atm 2000 cal are released when 1 mole A is formed from the reactants B and C. [8+8]
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1. (a) What are the variables affecting the reaction rate. List out the different forms of definition of reaction rate. [8]
- (b) The following rate equation is reported for vapor- phase reaction $-dP_A/dt = 3.66P_{A_2,atm}/hr$
 - i. What are the units of the rate constant?
 - ii. What is the value of the rate constant if the rate equation is written in terms of molar concentration of A? [8]
2. The gas reaction $2A \rightarrow R + 2S$ is approximately second order with respect to A. When pure A is introduced at 1 atm. into a constant volume batch reactor, the pressure rises 40% in 3 minutes. For a constant pressure batch reactor find
 - (a) the time required for the same conversion [8]
 - (b) the fractional increase in volume at that time. [8]
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 vapor phase decomposition of acetaldehyde at 520^0C and 1 atm. Pressure is carried out in a plug flow reactor. The decomposition occurs according to the reaction,

$$CH_3CHO \xrightarrow{k} CH_4 + CO$$
 , $k = 0.43m^3 / Kg.molesec$.The reaction is second order and irreversible. Calculate the volume of reactor required to produce 80% conversion when rate of flow of aldehyde is $0.1 kg/sec$. [16]
5. An aqueous reactant stream (4 mol A/liter) passes through a mixed flow reactor followed by a plug flow reactor. Find the concentration at the exit of the plug flow reactor if in the mixed flow reactor $C_A = 1$ mol/liter. The reaction is second-order with respect to A, and the volume of the plug flow unit is three times that of the mixed flow unit. [16]

6. The irreversible reaction $A \rightarrow R + S$ is catalyzed by a solid catalyst. Mechanism of reaction may be taken as: Adsorption of A followed by surface reaction forming adsorbed R and unadsorbed S. If surface reaction is the controlling step, derive an overall rate equation. [16]
7. Derive the energy balance equation for an adiabatically operated CSTR. [16]
8. Write short notes on:
- (a) Order and molecular
 - (b) Empirical rate equations. [8+8]
