

III B.Tech Supplementary Examinations, Aug/Sep 2008  
 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) A first order gaseous reaction  $A \rightarrow 2R + S$  takes place isothermally in a constant pressure experimental reactor. Starting with a mixture of 75% A and 25% inerts the volume doubles in 8 minutes. What is the conversion achieved? [8]
- (b) Write a note on excess reactant and stoichiometric proportion methods. [8]
3. For the non elementary reaction  $A + 2B \rightarrow R + S$  if the mechanism suggested is
 
$$A + B \xrightleftharpoons[k_2]{k_1} R + X$$

$$B + X \xrightarrow{K_3} S$$
 where X is the unstable intermediate compound,
  - (a) Derive an expression for rate of disappearance of A
  - (b) Explain how the rate constants can be evaluated using the rate law. [8+8]
4. Sulfuryl chloride ( $SO_2Cl_2$ ) is to be dissociated in a plug flow reactor to sulfur dioxide and chlorine at 330<sup>0</sup>C with rate constant of  $1.32 \times 10^{-3}$  per min. for a feed rate of 25 kg/hr of pure  $SO_2Cl_2$ . And 90% conversion. Determine (i) volume of reactor (ii) Space velocity (iii) Actual residence time. [16]
5. At present we have 90% conversion of a liquid feed ( $n = 1$ ,  $C_{AO} = 10$  mol/liter) to our plug flow reactor with recycle of product ( $R = 2$ ). If we shut off the recycle stream, by how much will this lower the processing rate of our feed to the same 90% conversion? [16]
6. Determine the order of reaction and the weight of catalyst needed for 35% conversion of A to R for a feed of 2000 mol/hr of pure A at 117<sup>0</sup>C and 3.2 atm. For this reaction the stoichiometry is  $A \rightarrow R$  and the kinetic data are given as follows:

Code No: RR320802

**Set No. 1**

Run	1	2	3	4
$C_{A,in}$ , mol/liter	0.100	0.080	0.060	0.040
$C_{A,out}$ , mol/liter	0.084	0.070	0.055	0.038

Assume plug flow in the packed bed reactor. [16]

7. Derive the energy balance equation for adiabatic operation of PFR. [16]

8. Write detailed note on:

(a) Design procedure for flow reactor

(b) Shifting order reactions. [8+8]

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1. For the general reaction scheme  $aA + bB \rightarrow rR + sS$  explain and derive expressions for the following. [4×4=16]
- General mole relation (Stoichiometric equation)
  - Fractional conversion
  - Rate of reaction
  - Law of mass action

Show what form they take when the reaction under consideration is a constant volume reaction.

2. A tri molecular elementary reaction  $A + 2B \rightarrow \text{Products}$ , takes place in a batch reactor. Using the following data find a suitable rate equation.
- |                                 |       |       |       |       |       |       |
|---------------------------------|-------|-------|-------|-------|-------|-------|
| Time, min                       | 0.0   | 1.0   | 2.0   | 3.0   | 4.0   | 5.0   |
| Concentration of A,<br>mole/lit | 0.500 | 0.250 | 0.189 | 0.158 | 0.138 | 0.125 |

The component B is introduced at 1 mole/lit. along with component A. Derive the equation used. [16]

3. A reaction  $2A + B \rightarrow A_2B$  is non-elementary and has the rate equation as  $r_{A_2B} = K[A][B]$ . Suggest and verify a suitable mechanism which is consistent with observed rate law. [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,  $A \rightarrow 5R$  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) Derive an expression for the concentration of reactant in the effluent from a series of mixed reactors of different sizes. Let the reaction follow first order kinetics and let the holding time in the  $i^{th}$  reactor be  $t_i$ .
- (b) Show that this expression reduces to the appropriate equation when the reactors are all the same size. [8+8]

6. For the solid catalyzed reaction  $A+B \rightleftharpoons R$  derive the expression for the rate of reaction if adsorption of B 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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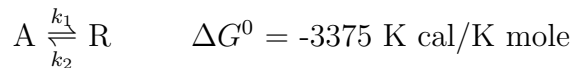
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1. (a) Define reaction rate constant. Develop an expression that facilitates calculation of units of rate constant for any order. [6]

- (b) Determine equilibrium conversion of A at 373<sup>0</sup>K for the following aqueous reaction.



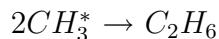
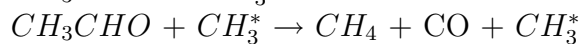
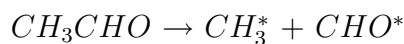
$$\Delta H_r^0 = -18,000 \text{ K cal/K mole}$$

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. (a) What is a chain reaction? Define chain length.

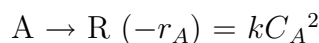
- (b) Thermal decomposition of acetaldehyde is postulated to proceed by the chain mechanism



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 decomposition of gaseous A proceeds as follows



A tubular reactor of 2 liters volume is fed at 2  $m^3/hr$  of pure A at 300<sup>0</sup>C and 20 atm. Conversion of reactant is 65%. In a commercial plant, it is desired to treat 100 $m^3/hr$  of feed gases at 40 atm and 300<sup>0</sup>C containing 60%A and 40% diluents to obtain 85% conversion of A. Find the volume of reactor required. [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. (a) Describe the different types of catalysts with examples.  
(b) Explain the three mechanisms by which a reactant absorbed onto the catalyst surface is capable of reacting to form the product. [10+6]
7. Obtain the expression for steady state energy balance for a CSTR under non-isothermal conditions. [16]
8. Write detailed notes on:
  - (a) Integral and differential methods
  - (b) Total volume and total pressure methods. [8+8]

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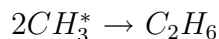
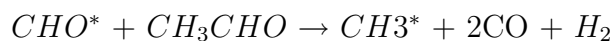
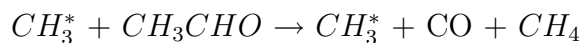
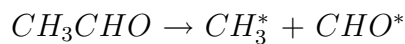
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1. (a) The hydrogenation of acetylene over a catalyst is represented by the reaction  $C_2H_2 + H_2 \rightleftharpoons C_2H_4$ . Compute the standard heat of reaction. The following data is available. [10]

Temperature $^{\circ}K$	298	600	1000
Equilibrium constant, $atm^{-1}$	5.1931024	1.194109	501.4

- (b) How do you compute the equilibrium composition in case of multiple reactions? Discuss. [6]
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. The pyrolysis of acetaldehyde is to take place according to the mechanism.



Derive the rate expression for the decomposition of acetaldehyde. Under what conditions the rate law reduces to  $-r_{CH_3CHO} = K[CH_3CHO]^{3/2}$  [16]

4. A homogeneous liquid phase reaction  $A \rightarrow R$ ,  $(-r_A) = kC_A^2$  takes place with 50% conversion in a mixed reactor. What will be the conversion, if this reactor is replaced by one 6 times as large, all else remaining unchanged. What will be the conversion if the original reactor is replaced by a plug flow reactor of equal size, all else remaining same. [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 adsorption of A is rate controlling. [16]
7. For the first order reactions  $A \xrightarrow{k_1} R \xrightarrow{k_2} S$  occurring in a mixed reactor develop the expression for  $C_{R,max}$  and  $\tau_{m,opt}$ . [16]
8. Write detailed note on:
- (a) Enzyme - substrate reactions
  - (b) Methods of analysis of kinetic data. [8+8]

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