III-B.Tech II-Semester Regular Examinations-April/May-2005 CHEMICAL REACTION ENGINEERING-I (Chemical Engineering)

Time: 3 hours

Max. Marks: 80

Answer and FIVE questions All questions carry equal marks

- 1. Compute the decomposition pressure of limestone at 1000° K. The following data is available. H_{f^0} (298° K) =43.57 kcal/gmole ; S_{f^0} (298° K) =38.40 kcal/gmole C_P (CaCO₃) =19.68 +11.89×10⁻³ T ; C_P (CaO) =10 +4.84×10⁻³ T; C_P (CO₂) =6.85 +8.53×10⁻³ T Where T is in ° K and C_P is in cal/gmole.°K.
- 2. For the reaction in series $A \rightarrow R \rightarrow S$ with $k1 \neq k2$, find the maximum concentration of R and when it is reached in a batch reactor? k1 and k2 are the rate constants for the first and second reactions. Show what happens it $K_1 = K_2$.
- 3. a) Distinguish between elementary and non elementary reactions.
 - b) Show that the following scheme

$$N_2O_5 \longrightarrow NO_2 + NO_3^*$$

 $NO_2 + NO_3^* \rightarrow NO^* + O_2 + NO_2$ $NO^* + NO_3^* \rightarrow 2NO_2$

is consistent with and explain the observed first order decomposition of N₂O₅.

- 4. Pure gaseous reactant A with $C_{Ao} = 100$ millimole/liter is fed at steady rate into a mixed reactor, where it dimerizes, 2 A \nvDash R with rate equation, $-r_A=2$ (liter/m.m.hr) C_A^2 . 60 % conversion takes place in this reactor, all else remaining unchanged. What will be the conversion if this reactor is changed with, (i) mixed reactor, 5 times as large (ii) plug flow reactor of equal size.
- 5. 100 liters/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 liters each. In passing through this system, how much has the activity decayed?
- 6. a) Describe the different types of catalysts with examples.
 - b) Explain the three mechanisms by which a reactant adsorbed onto the catalyst surface is capable of reacting to form the product.
- 7. Derive the expression for effectiveness factor in a single cylindrical pore for a first order reaction.
- 8. Write short notes on:
 - a) Batch and flow reactors b) Law of mass action.

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1. The following multiple chemical reactions occur in the reduction of carbon C(s)

- +2H₂(g) CH₄(g); K_{P1} =0.132 and C(s)+CO₂(g) 2CO(g); K_{P2} =1.072. The feed consists of 70% hydrogen and 30% carbon monoxide, and the reactions occur at 700°C temperature and 1atm. pressure. Calculate the equilibrium composition.
- 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?
 - b) Write a note on excess reactant and stoichiometric proportion methods.
- 3. Experiment shows that the homogeneous decomposition of ozone proceed with a rate $\overline{r_{o_3}} = K [O_3]^2 [O_2]^{-1}$. Suggest a two step mechanism to explain this rate and explain how would you further test this mechanism?
- 4. At $600 \, {}^{\circ}\text{K}$ the gas phase reaction,

$$C_2H_4 + Br_2 \xrightarrow{k_1} C_2H_4Br_2$$

has rate constants $k_1 = 500 \text{ m}^3$ / (K mole.hr) and $k_2 = 0.032 \text{ hr}^{-1}$. If a plug flow reactor is to be fed 600 m³/hr of gas containing 60 % Br2, 30 % C2H4 and 10 % inerts by volume at 600°K and 1.5 atm., calculate the volume of reaction vessel required to obtain 60% conversion of ethylene.

- 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.
- 6. For a gaseous reaction A R+S taking place on a porous catalyst, derive the rate expression if the adsorption of A controls the overall reaction.
- 7. Obtain the expression for steady state energy balance for a CSTR under nonisothermal conditions.
- 8. Write brief notes on:

a)

Series and parallel reactions b) Multiple reactor network.

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b)

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- **1**. a) What are the variables affecting the reaction rate. List out the different forms of definition of reaction rate.
 - 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 interms of molar concentration of A?
- 2. The gas reaction 2A → 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
 - the fractional increase in volume at that time.
- 3. A reaction $2A + B \longrightarrow A_2B$ 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.
- 4. The homogeneous gas reaction A ∠ 3 R follows second order kinetics. For a feed rate of 4m³/hr of pure A at 5 atm and 350^o C, an experimental reactor consisting of 0.025 m I.D. pipe and 2 m long gives 60 % conversion of feed. A commercial plant is to treat 300 m³/hr of feed at 25 atm and 350^oC to obtain 80% conversion of A. Find out the required volume of the reactor.
- 5. The kinetics of the aqueous-phase decomposition of A is investigated in two mixed reactors in series, the second having twice the volume of the first reactor. At steady state with a feed concentration of 1 mol A/liter and mean residence time of 96 sec in the first reactor, the concentration in the first reactor is 0.5 mol A/liter and in the second is 0.25 mol A/liter. Find the kinetic equation for the decomposition?
- 6. For the following gas phase solid catalyzed reaction: A+B R+S. Obtain the expression for the rate of reaction if surface reaction is the controlling step. The reaction takes place between adsorbed A and adsorbed B.
- 7. Obtain the expression for steady state energy balance for a PFR under nonisothermal conditions.

Set No:

- 8. Write a short note on:
 - a) Integral and differential methods
 - b) Total volume and total pressure methods.

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- 1. a) Calculate the conversion of pure methanol to dimethyle ether by the reaction: $2CH_3OH(CH_3)_2O + H_2O$ when pure methanol is allowed to come to equilibrium at 500° K and 1 atm. The standard Gibb's free energy for the reaction at 500° K is -2.95 kcal/gmole.
 - b) For the following vapor phase reaction occurring simultaneously A R; K_{P1} =4; A S ; K_{P2} =1. Calculate the composition of the reaction mixture at the equilibrium starting with pure A.
- 2. a) Briefly discuss the various methods of interpretation of kinetic data.
 - b) The first order reversible liquid phase reaction $A \leftrightarrow R$, CA0 = 0.5 mole/lit, CR0 = 0 takes place in a batch reactor. After 8 minutes conversion of A is 33.3% while equilibrium conversion is 66.7%. Find the rate equation for this reaction.
- 3. a) What is a chain reaction? Define chain length.
 - b) Thermal decomposition of acetaldehyde is postulated to proceed by the chain mechanism.

 $\begin{array}{c} CH_3 \ CHO & \longrightarrow \ CH_3^* + CHO^* \\ CH_3 \ CHO + CH_3^* & \longrightarrow \ CH_4 + CO + CH_3^* \\ 2CH_3^* & \longrightarrow \ C_2H_6 \end{array}$

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

$$\frac{-\mathrm{d}[\mathrm{CH}_{3}\mathrm{CHO}]}{\mathrm{d}t} = \mathrm{K}[\mathrm{CH}_{3}\mathrm{CHO}]^{1.5} .$$

- 4. A homogeneous liquid phase reaction $A \nvDash R$, $(-r_A) = k C_A^2$ 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.
- 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?

Contd...2

- 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.
- 7. a) Give a qualitative discussion about product distribution for reactions in parallel.
 - b) With suitable figures illustrate the methods of contacting two reacting fluids in continuous and non continuous operations that keep the concentrations of these components both high, both low, one high and the other low.
- 8. Write a short note on:
 - a) Half life period method
 - b) Excess reactant and stoichimetric proportions methods.

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