



WINTER-17 EXAMINATION
Model Answer

Subject Title: Chemical Reaction Engineering

Subject code

17562

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Important Instructions to examiners:

- 1) The answers should be examined by key words and not as word-to-word as given in the model answer scheme.
- 2) The model answer and the answer written by candidate may vary but the examiner may try to assess the understanding level of the candidate.
- 3) The language errors such as grammatical, spelling errors should not be given more Importance (Not applicable for subject English and Communication Skills).
- 4) While assessing figures, examiner may give credit for principal components indicated in the figure. The figures drawn by candidate and model answer may vary. The examiner may give credit for any equivalent figure drawn.
- 5) Credits may be given step wise for numerical problems. In some cases, the assumed constant values may vary and there may be some difference in the candidate's answers and model answer.
- 6) In case of some questions credit may be given by judgement on part of examiner of relevant answer based on candidate's understanding.
- 7) For programming language papers, credit may be given to any other program based on equivalent concept.



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Q No.	Answer	Marks															
1A	Attempt any THREE of the following	12															
1A-a	<p>Comparison of collision and transition theories:</p> <table> <tr> <th>Sr.No.</th><th>Transition State Theory</th><th>Collision Theory</th></tr> <tr> <td>1</td><td>Prediction of reaction rates is more accurate with experiment.</td><td>Prediction of reaction rates is less accurate with experiment.</td></tr> <tr> <td>2</td><td>The theory is based on statistical mechanics</td><td>The theory is based on kinetic theory of gases.</td></tr> <tr> <td>3</td><td>The theory views that the formation of activated complex is very rapid & decomposition of activated complex is slow.</td><td>The theory views that the decomposition of activated complex is very rapid & formation of activated complex is slow.</td></tr> <tr> <td>4</td><td>Temperature Dependency is $k \propto T \cdot e^{-E/RT}$</td><td>Temperature Dependency is $k \propto T^{1/2} \cdot e^{-E/RT}$</td></tr> </table>	Sr.No.	Transition State Theory	Collision Theory	1	Prediction of reaction rates is more accurate with experiment.	Prediction of reaction rates is less accurate with experiment.	2	The theory is based on statistical mechanics	The theory is based on kinetic theory of gases.	3	The theory views that the formation of activated complex is very rapid & decomposition of activated complex is slow.	The theory views that the decomposition of activated complex is very rapid & formation of activated complex is slow.	4	Temperature Dependency is $k \propto T \cdot e^{-E/RT}$	Temperature Dependency is $k \propto T^{1/2} \cdot e^{-E/RT}$	1 mark each
Sr.No.	Transition State Theory	Collision Theory															
1	Prediction of reaction rates is more accurate with experiment.	Prediction of reaction rates is less accurate with experiment.															
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3	The theory views that the formation of activated complex is very rapid & decomposition of activated complex is slow.	The theory views that the decomposition of activated complex is very rapid & formation of activated complex is slow.															
4	Temperature Dependency is $k \propto T \cdot e^{-E/RT}$	Temperature Dependency is $k \propto T^{1/2} \cdot e^{-E/RT}$															
1A-b	<p>Definition:</p> <p>Internal energy (U): It is the energy stored in the system by virtue of the configuration and motion of the molecules constituting the system.</p> <p>Chemical Potential: It is defined as the change in free energy of a substance when one mole of it is added to such a large quantity of the system that there is no appreciable change in overall composition of the system at constant temperature & pressure.</p>	<p>1</p> <p>1</p>															



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	<p>Entropy: Entropy(s) is the measure of the total disorder or randomness of the system or it is a measure of the unavailable energy to perform useful work.</p> <p>Fugacity: It is a kind of fictitious pressure used for real gases. ie it is a measure of pressure for real gases.</p>	1
		1
1A-c	<p>Autocatalytic reactions: A reaction in which one of the products of the reaction acts as a catalyst is known as an autocatalytic reactions.</p> <p>Eg1. $\text{CH}_3\text{COOC}_2\text{H}_5 + \text{H}_2\text{O} \rightarrow \text{CH}_3\text{COOH} + \text{C}_2\text{H}_5\text{OH}$</p> <p>Here CH_3COOH acts as catalyst</p> <p style="text-align: center;">OR</p> <p>2. Oxidation of a solution of oxalic acid by an acidified solution of KMnO_4.</p> $2\text{MnO}_4^- + 6\text{H}^+ + 5(\text{COOH})_2 \rightarrow 2\text{Mn}^{2+} + 10\text{CO}_2 + 8\text{H}_2\text{O}$ <p style="text-align: center;">Oxalic acid</p> <p>The reaction is very slow at room temp. The reaction is catalyzed by manganese ions (Mn^{2+}) that are not present at start of reaction, hence the rate of reaction is extremely slow. Once reaction starts, Mn^{2+} ions are formed and the rate of reaction speeds up.</p>	2
		2
1A-d	<p>Space time:</p> <p>It is the time required to process one reactor volume of feed measured at specified condition.</p> <p>Equation and unit</p> $\tau = \frac{1}{s} = \frac{C_{A0} V}{F_{A0}}$ <p>Unit is unit of time (seconds, minute, etc)</p> <p>Space velocity</p> <p>It is the number of reactor volume of feed at specified conditions which can be treated in unit time.</p> <p>Equation and unit</p>	1
		1
		1



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	$S = \frac{1}{\tau} = \frac{F_{A0}}{C_{A0} V}$ <p>Unit is $time^{-1}$ ($second^{-1}$, $minute^{-1}$ etc)</p>	1
1B	Attempt any ONE of the following	6
1B-a	<p>Integrated rate equation for irreversible Second order reaction $A+B \rightarrow$ Products</p> <p>Reaction is $A+B \rightarrow$ Products</p> <p>The rate law for the reaction can be written as</p> $-r_A = -\frac{dC_A}{dt} = kC_A \cdot C_B \quad \text{eq.I}$ <p>Let C_{A0} and C_{B0} be initial concentrations of A and B respectively.</p> <p>Let $M = \frac{C_{B0}}{C_{A0}}$</p> <p>Let C_A and C_B be the concentrations of A and B at any time t.</p> <p>Let X_A and X_B be the fractional conversions of A and B respectively at time t.</p> <p>From the reaction stoichiometry, the amount of A and B reacted at any time t are equal & given by</p> $X_A \cdot C_{A0} = X_B \cdot C_{B0} \text{eq.II}$ <p>$C_A = C_{A0}(1 - X_A)$ and $C_B = C_{B0}(1 - X_B)$</p> <p>Therefore on differentiating $dC_A = -C_{A0}dX_A$</p> <p>By putting values of C_A, C_B and $-dC_A$ Eq.I becomes</p> $-r_A = \frac{C_{A0}dX_A}{dt} = kC_{A0}(1 - X_A) \cdot C_{B0}(1 - X_B)$ $-r_A = \frac{C_{A0}dX_A}{dt} = kC_{A0}(1 - X_A)(C_{B0} - C_{B0} \cdot X_B) \quad \text{eq III}$ <p>As $X_A \cdot C_{A0} = X_B \cdot C_{B0}$ and $C_{B0} = M \cdot C_{A0}$, eq III becomes</p> $\frac{C_{A0}dX_A}{dt} = kC_{A0}(1 - X_A)(C_{B0} - C_{A0} \cdot X_A)$ $\frac{C_{A0}dX_A}{dt} = kC_{A0}(1 - X_A)(M \cdot C_{A0} - C_{A0} \cdot X_A)$	2



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$$\frac{C_{A0} dX_A}{dt} = k C_{A0} (1 - X_A) C_{A0} (M - X_A)$$

$$\frac{C_{A0} dX_A}{dt} = k C_{A0}^2 (1 - X_A) (M - X_A)$$

$$\frac{dX_A}{dt} = k C_{A0} (1 - X_A) (M - X_A) \quad \text{eq IV}$$

Rearranging the Eq.IV, we get

$$\frac{dX_A}{(1 - X_A)(M - X_A)} = k C_{A0} dt \quad \text{eq.V}$$

Integrating the equation within the limits

At $t = 0$, $X_A = 0$

At $t = t$, $X_A = X_A$

$$\int_0^{X_A} \frac{dX_A}{(1 - X_A)(M - X_A)} = k C_{A0} \int_0^t dt$$

$$\int_0^{X_A} \frac{dX_A}{(1 - X_A)(M - X_A)} = k C_{A0} t$$

Breaking the L.H.S. of the above equation into partial fractions & then integrate it

$$\frac{A}{(1 - X_A)} + \frac{B}{(M - X_A)} = \frac{1}{(1 - X_A)(M - X_A)}$$

$$\frac{A(M - X_A) + B(1 - X_A)}{(1 - X_A)(M - X_A)} = \frac{1}{(1 - X_A)(M - X_A)}$$

Equating the numerator, $A(M - X_A) + B(1 - X_A) = 1$

Put $X_A = 1$, we get $A(M - 1) = 1 \therefore A = \frac{1}{(M - 1)}$

Put $X_A = M$, we get $B = -\frac{1}{(M - 1)}$

Putting values of A and B, we get

$$\frac{1}{(M - 1)} \left[\int_0^{X_A} \frac{dX_A}{(1 - X_A)} - \int_0^{X_A} \frac{dX_A}{(M - X_A)} \right] = k C_{A0} t$$



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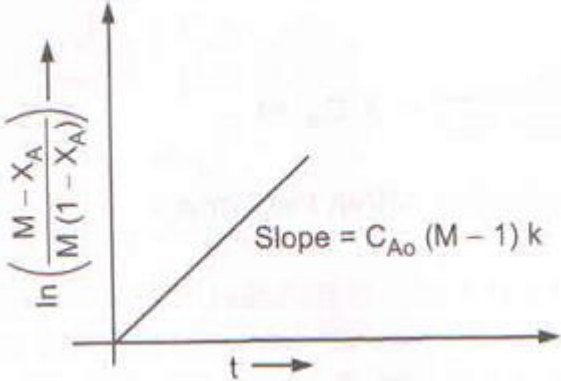
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	$\frac{1}{(M-1)} \left[-\ln(1-X_A) + \ln \frac{(M-X_A)}{M} \right] = k C_{A0} t$ $\ln \left[\frac{(M-X_A)}{M(1-X_A)} \right] = C_{A0} (M-1) k t \quad \text{Eq.VI}$ <p>EqVI is the desired integrated rate equation of irreversible second order reaction with $C_{A0} \neq C_{B0}$ in terms of conversion.</p> 	2						
1B-b	$k = 1.3 \times 10^{-3} \text{ S}^{-1}$ $T = 27^\circ\text{C} = 300 \text{ K}$ $E = 128170 \text{ cal / mol}$ $k = k_0 e^{-E/RT}$ $\ln k = \ln k_0 - (E / RT)$ $\ln k_0 = \ln k + (E / RT) = \ln(1.3 \times 10^{-3}) + (128170 / (1.987 \times 300)) = 208.36$ $k_0 = 3.11 \times 10^{90} \text{ S}^{-1}$	2						
2	Attempt any TWO of the following	16						
2-a	<p>Difference between order and molecularity of reaction.(4 points)</p> <table border="1"> <thead> <tr> <th>Sr.No.</th><th>Molecularity</th><th>Order of reaction</th></tr> </thead> <tbody> <tr> <td>1</td><td>Molecularity is the number of molecules, atoms or ions in a chemical reaction.</td><td>Order of reaction is the sum of exponents of the concentration terms involved in the rate</td></tr> </tbody> </table>	Sr.No.	Molecularity	Order of reaction	1	Molecularity is the number of molecules, atoms or ions in a chemical reaction.	Order of reaction is the sum of exponents of the concentration terms involved in the rate	2marks each
Sr.No.	Molecularity	Order of reaction						
1	Molecularity is the number of molecules, atoms or ions in a chemical reaction.	Order of reaction is the sum of exponents of the concentration terms involved in the rate						



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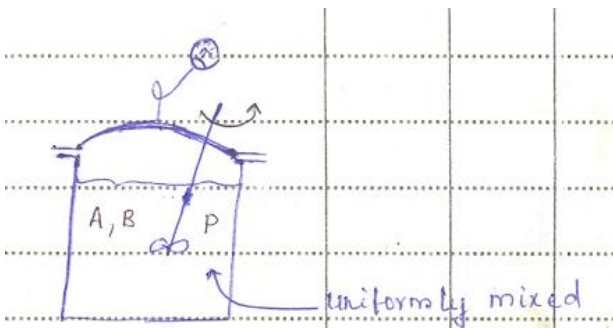
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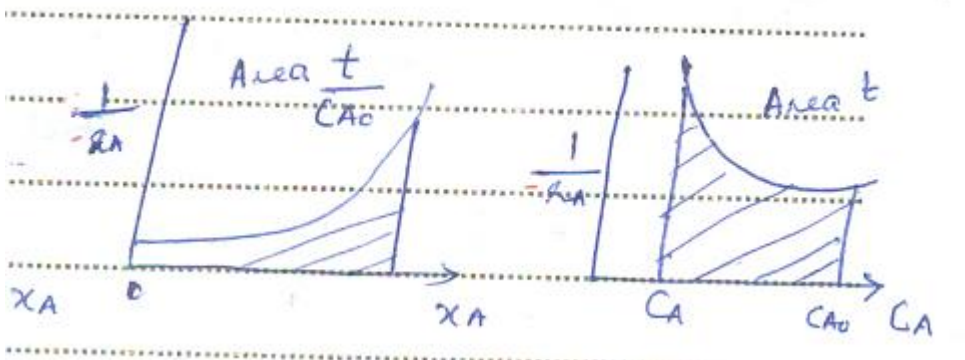
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			equation.	
	2	Molecularity always have an integer value 1,2,3...	Order of reaction can have a fractional value.	
	3	Shows the elementary mechanism or separate steps of a complicated process	Shows the kinetic dependence of the rate on the concentration of the reactants.	
	4	Depending upon the value of molecularity, reaction can be unimolecular ,bimolecular etc.	Depending upon the value of order, the reactions are termed as first order, second order reactions	
	5	Molecularity is a theoretical quantity	Order of reaction is entirely an experimental value.	
2-b	Performance equation for constant volume batch reactor with first order kinetics			
				



	<p>Writing the material balance for any component A.</p> <p>Rate of reactant A in = Rate of reactant A out + Rate of loss of reactant A due to chemical reaction + Rate of accumulation of reactant A within the reactor.</p> <p>In a batch reactor, no fluid enters or leaves the reaction mixture during the reaction. Therefore Rate of reactant A in = Rate of reactant A out = 0</p> <p>Material balance equation then becomes</p> <p>Rate of loss of reactant A due to chemical reaction = - Rate of accumulation of reactant A within the reactor----- (1)</p> <p>Rate of loss of reactant A due to chemical reaction = $-r_A V$</p> <p>Rate of accumulation of reactant A within the reactor = $\frac{dN_A}{dt} = -N_{A0} \frac{dx_A}{dt}$</p> <p>Substituting in equation (1)</p> $-r_A V = N_{A0} \frac{dx_A}{dt}$ <p>Rearranging and integrating</p> $\int_0^t dt = N_{A0} \int_0^{x_A} \frac{dx_A}{V (-r_A)}$ $t = N_{A0} \int_0^{x_A} \frac{dx_A}{V (-r_A)}$ <p>For constant volume system, the equation becomes</p> $t = \frac{N_{A0}}{V} \int_0^{x_A} \frac{dx_A}{(-r_A)} = C_{A0} \int_0^{x_A} \frac{dx_A}{(-r_A)} = - \int_{C_{A0}}^{C_A} \frac{dC_A}{(-r_A)}$ <p>For first order reaction $-r_A = kC_A = kC_{A0} (1 - X_A)$</p> $t = C_{A0} \int_0^{x_A} \frac{dx_A}{kC_{A0} (1 - X_A)} = - \int_{C_{A0}}^{C_A} \frac{dC_A}{kC_A}$ $t = \frac{-\ln(1 - X_A)}{k} = - \frac{\ln \frac{C_A}{C_{A0}}}{k}$ <p>Graphical representation for constant volume batch reactor</p>	<p>2</p> <p>3</p> <p>2</p>
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		1
2-c	<p>Methods of catalyst Preparation:</p> <ol style="list-style-type: none">1. Precipitation2. Gel formation3. Simple mixing4. Impregnation method <p>1. Precipitation method : This method produces catalyst in porous form. It consists of adding a precipitating agent to the solution of the desired component. The precipitation is followed by washing, drying, calcinations & activation (or pretreatment) Eg. Magnesium oxide catalyst is prepared by this method. It is prepared by precipitating $MgCO_3$ from magnesium nitrate solution by adding sodium carbonate. The magnesium carbonate precipitate is washed, dried & calcined to obtain magnesium oxide.</p> <p>2. Gel formation: If the precipitate formed in the above method is colloidal, then gel is formed. Eg Catalyst containing silica and alumina are suitable for gel formation because their precipitates are colloidal in nature.</p> <p>3. Simple mixing: Some porous materials are obtained by mixing the components with water, milling to the desired grain size, drying and calcining. Such materials may be ground and sieved to obtain the particle size.</p>	2 marks each for explaining the methods with eg

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	<p>Eg Mixed Mg and Ca oxide catalyst is prepared by this method</p> <p>4. Impregnation method:</p> <p>This method is used for the preparation of expensive catalysts like platinum, palladium, silver etc. A catalyst carrier provides a means of obtaining a large surface area with a small amount of catalyst. The steps in the preparation of a catalyst impregnated on a carrier include evacuating the carrier, contacting the carrier with the impregnating solution, removing the excess solution, drying, calcining and activation.</p> <p>Eg Nickel catalyst is prepared on alumina by soaking the evacuated alumina particles with nickel nitrate solution, draining to remove the excess solution and heating in an oven to decompose the nitrate to nickel oxide. The final step is activation in which nickel oxide is reduced to nickel.</p> <p><i>Any other appropriate preparation method should also be given due consideration</i></p>	
3	Attempt any FOUR of the following	16
3-a	<p>Definition</p> <p>(i) Chemical Potential:</p> <p>It is defined as the change in free energy of a substance when one mole of it is added to such a large quantity of the system that there is no appreciable change in overall composition of the system at constant temperature & pressure.</p> <p>(ii) Chemical equilibrium :</p> <p>It is the state when the rate of forward reaction is equal to the rate of backward reaction. At chemical equilibrium, the net change in the concentration of reactants and products will be zero.</p>	<p>2</p> <p>2</p>
3-b	<p>Integrated form of rate expression for zero order reaction</p> <p>Rate equation is $-r_A = -\frac{dC_A}{dt} = C_{A0}\frac{d_{xA}}{dt} = k$</p>	



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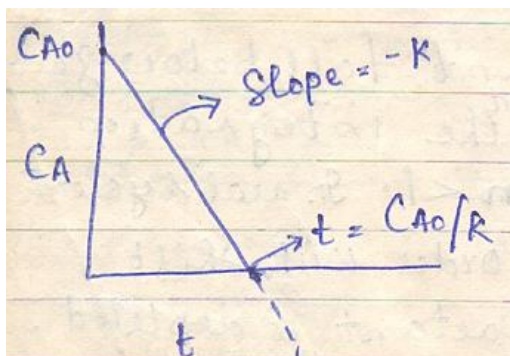
In terms of concentration

$$-\frac{dC_A}{dt} = k$$

Integrating between appropriate limits

$$\int_{C_{A0}}^{C_A} -dC_A = k \int_0^t dt$$

$$C_{A0} - C_A = kt \text{ for } t < \frac{C_{A0}}{k}$$



2

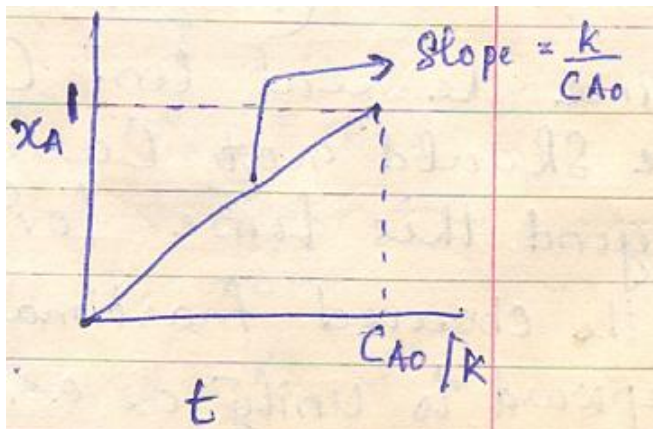
In terms of fractional conversion

$$C_{A0} \frac{dx_A}{dt} = k$$

Integrating between appropriate limits

$$C_{A0} \int_0^{x_A} dx_A = k \int_0^t dt$$

$$C_{A0} X_A = kt \text{ for } t < \frac{C_{A0}}{k}$$



2

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3-c	<p>Derivation for entropy change of an ideal gas:</p> <p>From first law of thermodynamics, $dU = dQ - dW$</p> $dQ = dU + dW \dots\dots(i)$ <p>But $dQ = TdS \dots\dots(ii)$</p> $dW = PdV \dots\dots(iii)$ <p>For ideal gas $dU = n C_v dT \dots\dots(iv)$</p> <p>Substituting ii,iii and iv in i</p> $TdS = n C_v dT + PdV$ $dS = \frac{n C_v dT}{T} + \frac{PdV}{T}$ <p>For ideal gas $P = \frac{nRT}{V}$</p> $\text{Substituting } dS = \frac{n C_v dT}{T} + \frac{nRdV}{V}$ <p>Integrating between limits</p> $\int_{S_1}^{S_2} dS = nC_v \int_{T_1}^{T_2} \frac{dT}{T} + nR \int_{V_1}^{V_2} \frac{dV}{V}$ $\Delta S = nC_v \ln \frac{T_2}{T_1} + nR \ln \frac{V_2}{V_1} \dots\dots(v)$ <p>For constant volume process , $v_1 = v_2$ and the equation becomes</p> $\Delta S = nC_v \ln \frac{T_2}{T_1}$	2 2
3-d	<p>Factors affecting the rate of a chemical reaction (4 factors) :</p> <ol style="list-style-type: none"> 1. In homogeneous system temperature, pressure and composition are the variables. 2. In heterogeneous system, since more than one phase is involved, material have to move from phase to phase during reaction, hence the rate of mass transfer is important. 3. rate of heat transfer 4. Catalyst 5. Nature of reactants 	1 mark each



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	6. Surface area available. 7. Intensity of light if reaction is light sensitive.	
3-e	<p>Catalyst regeneration.</p> <p>Catalyst gets poisoned due to the presence of impurities present either in the reactant stream or produced as a result of chemical reaction. Regeneration is the methods adopted for regaining the activity of poisoned catalysts.</p> <p>Methods for regeneration of catalyst (any three)</p> <ol style="list-style-type: none">1. Volatile poison may be removed from the catalyst surface by passing current of pure gas or liquid or by raising the temperature.2. Coke deposited on the catalyst is removed by roasting the coke by atmospheric oxygen at 550-700 °C.3. Metallic catalysts like nickel are regenerated by washing with alcohol or acid and other solvents. Irreversibly poisoned catalyst like platinum on silica support, silver and vanadium pentoxide are regenerated by extracting platinum, silver and vanadium from them using acids and alkalies.4. Magnetic methods are also used for regenerating the activity of catalyst.5. Metals concentrate on the surface of cracking catalyst and they can be removed by the abrasion of surface bed.6. Alumino silicate cracking catalyst gets poisoned due to the deposition of metal on them. The poison is converted to a form which is highly volatile or readily soluble in water and the catalyst is treated with aqueous solution of organic acid, alkalies and gases.	<p>1</p> <p>1 mark each</p>
4A	Attempt any THREE of the following	12
4-A-a	Graph of concentration term with time (i) For first order reaction	



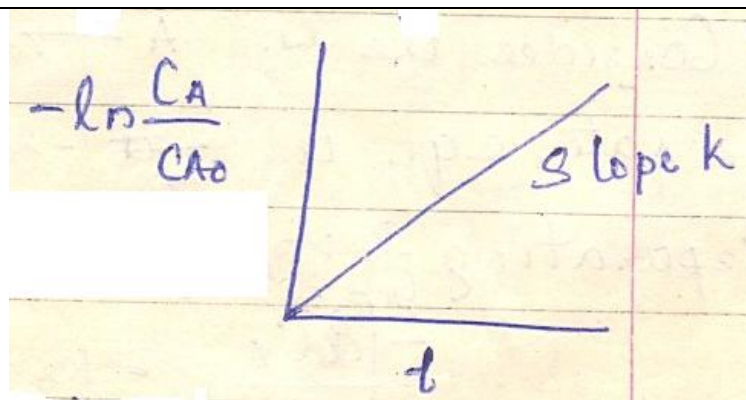
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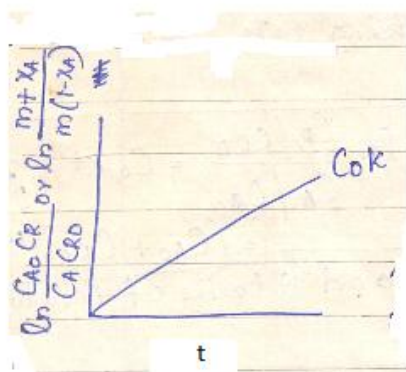
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Slope is k

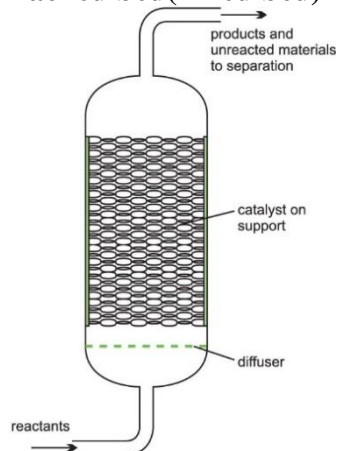
(ii) For autocatalytic reaction:



Slope is C_0k

4A-b

Packed bed(Fixed bed) reactor



Explanation: Fixed bed reactors normally consist of one or more tubes packed



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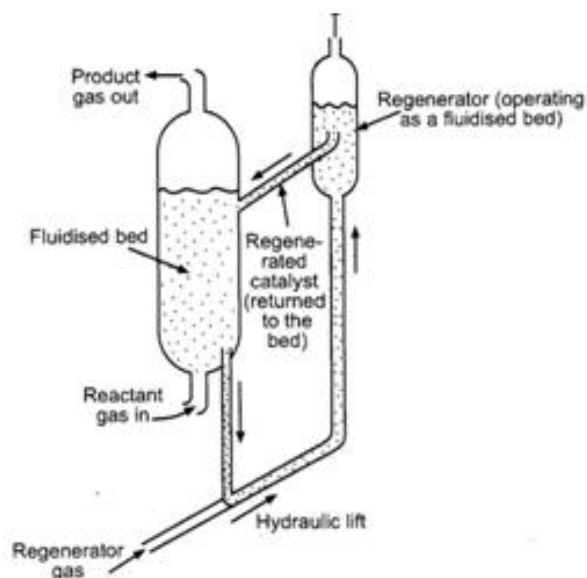
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with catalyst particles and are generally operated in vertical position. The catalyst particles may be of a variety of sizes and shapes – granular, pelleted, cylinder, spheres etc. Wires of metals are made into screens in the case of expensive catalysts.

Chances of hot spot formation are there in fixed bed reactor. In order to prolong the time between regeneration and shut down, the reactor tube may be made longer than required. The problem of regeneration of catalyst is a serious issue in this type of reactor.

Fluidized bed reactor with regenerator:



Explanation:

Consider a bed of fine particles and gases passing upward through them. On increasing the flow rate, a point is reached when the solids become suspended in the gas stream. In this state the bed is said to be fluidized and the particular inlet gas velocity is called minimum fluidizing velocity. If the gas velocity is



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	much larger than this minimum, the bed takes the appearance of a violently boiling liquid with solids in vigorous motion and large bubbles rising rapidly through the bed. In this case we have the bubbling fluidized bed. Industrial reactors particularly for solid catalyzed gas phase reactions often operate as bubbling beds with gas velocities equal to 9 to 30 times minimum fluidizing velocity.	
4A-c	<p>Relation between C_A & C_{A0}</p> <p>Consider the reaction $A \rightarrow R$</p> <p>Let</p> <p>N_{A0} represent the number of moles of A present initially ($t = 0$).</p> <p>N_A represent the number of moles of A present at time t.</p> <p>X_A be the fractional conversion of A at time t</p> <p>Moles of A reacted at any time $t = N_{A0} X_A$</p> <p>At time t, moles of A present $N_A = N_{A0} - N_{A0} X_A$</p> <p>Divide throughout by V, $(N_A / V) = (N_{A0} / V) - (N_{A0} X_A / V)$</p> <p>But concentration = moles / l</p> <p>Therefore $C_A = C_{A0} - C_{A0} X_A$;</p> <p>$C_A = C_{A0} (1 - X_A)$</p>	2
4A-d	<p>Relation between K_p and K_c (Derivation)</p> <p>Consider the reaction $aA + bB + \dots \rightarrow rR + sS \dots$</p> <p>$K_c = (C_R^r \cdot C_S^s) / (C_A^a \cdot C_B^b)$</p> <p>For ideal gas $C_i = p_i / RT$</p> <p>Where R is the ideal gas constant</p> <p>T the absolute temperature in K</p> <p>P is the pressure in atm</p> <p>Therefore $K_c = \{ (p_R / RT)^r \cdot (p_S / RT)^s \} / \{ (p_A / RT)^a \cdot (p_B / RT)^b \}$</p> <p>$= (p_R^r \cdot p_S^s) / (p_A^a \cdot p_B^b) \cdot (1 / RT)^{(r+s+\dots-(a+b+\dots))}$</p>	2



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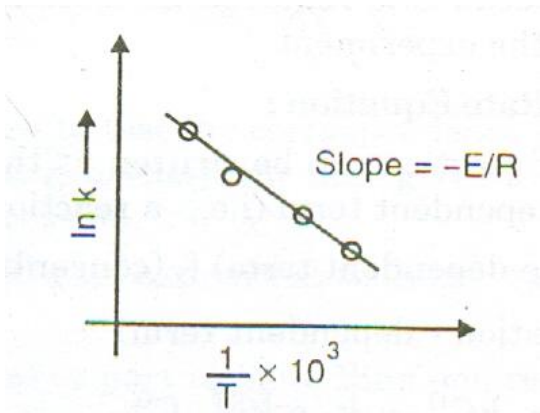
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	<p>Ie $K_c = K_p \cdot (1/RT)^{\Delta n}$ where $K_p = (p_R^r \cdot p_S^s) / (p_A^a \cdot p_B^b)$</p> <p>And $\Delta n = (r + s + \dots - (a + b + \dots))$ is the difference in the number of moles of product and reactant</p> <p>Or $K_p = K_c \times (RT)^{\Delta n}$</p>	2
4B	Attempt any ONE of the following	6
4B-a	<p>Arrhenius law</p> <p>The temperature dependency of the reaction rate constant k, is given by $k = k_0 e^{-E/RT}$</p> <p>Where k_0 - frequency factor or pre exponential factor</p> <p>E - activation energy in J/ mol or cal/ mol</p> <p>R – universal gas constant</p> <p>T – temperature in Kelvin</p> <p>The activation energy is determined experimentally by carrying out the reaction at different temperatures. A plot of $\ln k$ vs $\frac{1}{T}$ should give a straight line with slope equal to $-\frac{E}{R}$.</p>  <p>Alternatively, if the rate is known at two different temperatures T_1 and T_2, then we can evaluate E with the help of equation</p> $\ln \frac{k_2}{k_1} = \frac{-E}{R} \left(\frac{1}{T_2} - \frac{1}{T_1} \right)$	2

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	Lower the value of activation energy, higher will be the rate at which reaction will proceed as the considerable part of collisions between the molecules result in a reaction and higher the value of activation energy, lower will be the rate at which the reaction proceeds.	2
4B-b	<p>Number of moles (n)= 4/4 =1</p> <p>$P_1 = 1 \text{ atm}$</p> <p>$P_2 = 0.1 \text{ atm}$</p> <p>$T = 30^0\text{C} = 303 \text{ K}$</p> <p>$\Delta S = nC_p \ln \frac{T_2}{T_1} + nR \ln \frac{P_1}{P_2}$</p> <p>For isothermal operation, $\Delta S = nR \ln \frac{P_1}{P_2}$</p> <p>$\Delta S = 1 \times 1.987 \times \ln (1/ 0.1) = \mathbf{4.575 \text{ cal / K}}$</p>	3
5	Attempt any TWO of the following	16
5-a	<p>For first order reaction, $-\ln(1-x_A) = kt$</p> <p>When $x_A = 0.5$ $-\ln(1-0.5) = kt_1$</p> <p>$t_1 = \frac{0.693}{k}$ - (1)</p> <p>When $x_A = 0.75$ $-\ln(1-0.75) = kt_2$</p> <p>$t_2 = \frac{1.386}{k}$ - (2)</p> <p>From equation (1) and (2) $t_2 = 2 t_1$</p> <p>Therefore the time required for 75% conversion is double the time required for 50% conversion.</p>	3
5-b	<p>Comparison of size of MFR and PFR for first order reaction</p> <p>The performance or design equation for MFR is</p> <p>$V / F_{AO} = \tau / C_{AO} = X_A / -r_A$</p> <p>$\tau_m = \left(\frac{C_{AO} V}{F_{AO}} \right)_m = C_{AO} X_A / -r_A$</p>	2



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For constant volume MFR, where first order reaction is taking place

$$\tau_m = \left(\frac{C_{A0}V}{F_{A0}} \right)_m = C_{A0} X_A / -r_A = X_A / K(1-X_A) \dots \dots \dots (i)$$

The performance or design equation for PFR is

$$\frac{V}{F_{A0}} = \int_0^{x_A} \frac{dX_A}{-r_A} = \frac{\tau}{C_{A0}}$$

$$\tau_P = \left(\frac{C_{A0}V}{F_{A0}} \right)_P = C_{A0} \int_0^{x_A} \frac{dX_A}{-r_A}$$

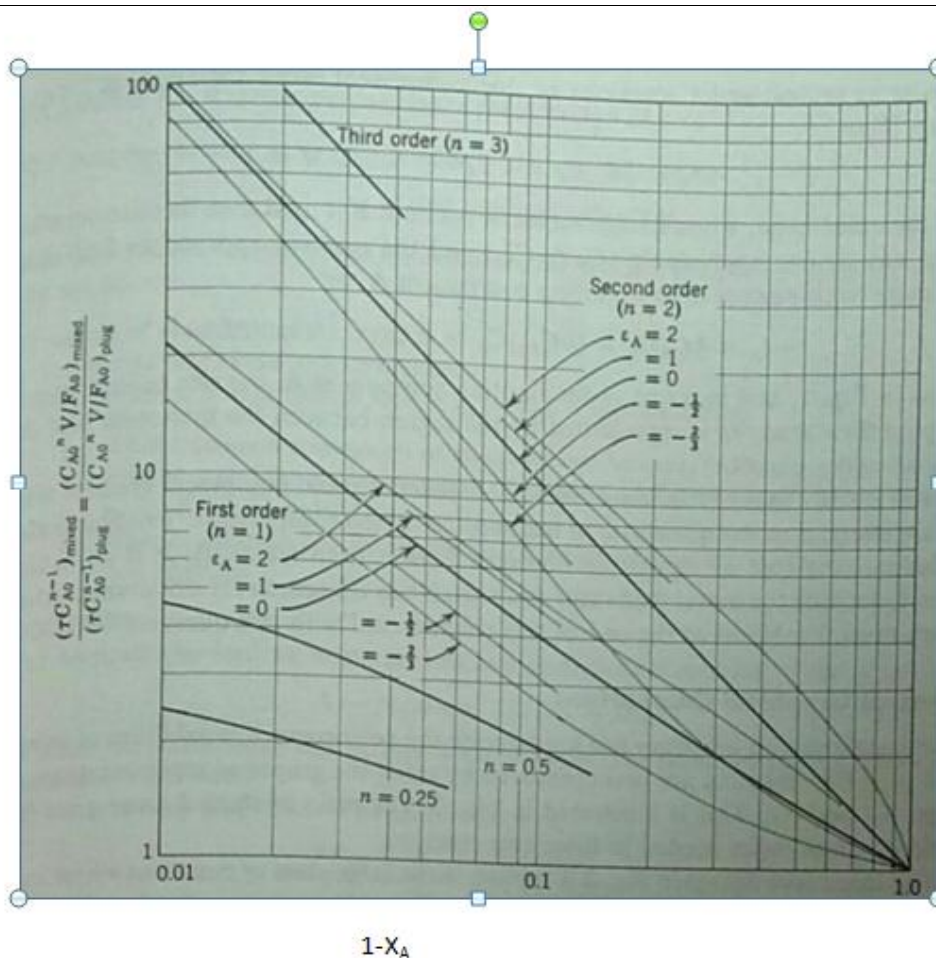
For constant volume PFR, where first order reaction is taking place

$$\tau_P = \left(\frac{C_{A0}V}{F_{A0}} \right)_P = C_{A0} \int_0^{x_A} \frac{dX_A}{-r_A} = \frac{1}{k} \int_0^{x_A} \frac{dX_A}{(1-X_A)} = -\ln (1 - X_A) / k \dots \dots \dots (ii)$$

From eqn (i) and (ii), for constant density system

$$\tau_m / \tau_P = \left(\frac{C_{A0}V}{F_{A0}} \right)_m / \left(\frac{C_{A0}V}{F_{A0}} \right)_P = \{ X_A / (1-X_A) \}_m / \{ -\ln (1 - X_A) \}_P$$

2



2

- 1) For any given duty & for all positive reaction orders , **size** of MFR is always larger than that of PFR.the volume ratio V_m / V_p increases with reaction order.
- 2) For low values of conversion, the reactor performance is only slightly affected by type of flow, the volume ratio approaching unity as conversion approaches zero. The size ratio increases very rapidly at high values of conversion.
- 3) Design of reactor is affected by **density variation** during reaction. Expansion(density decrease) during reaction increases the size ratio, but

4



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	decreases, the effectiveness of CSTR with respect to PFR. The density increase during reaction has the opposite effect.	
5-c	<p>$A \rightarrow 1.6 R$</p> <p>$V = 1.5 V_0$</p> <p>$t = 4$ minutes</p> <p>$C_A = \frac{V_{XA=1} - V_{XA=0}}{V_{XA=0}} = (1.6 - 1) / 1 = 0.6$</p> <p>$V = V_0 (1 + C_A X_A)$</p> <p>$1.5 V_0 = V_0 (1 + 0.6 X_A)$</p> <p>$X_A = \mathbf{0.8333}$</p> <p>For first order reaction $-\ln(1 - X_A) = kt$</p> <p>$-\ln(1 - 0.8333) = k \times 4$</p> <p>$k = \mathbf{0.4478 \text{ min}^{-1}}$</p>	<p>2</p> <p>3</p> <p>3</p>
6	Attempt any FOUR of the following	16
6-a	<p>Derivation of performance equation / design equation of mixed flow reactor:</p> <p>In MFR, the composition of the reactants is uniform throughout the reactor.</p> <p>Taking material balance of reactant A over the reactor as a whole,</p> <p>Rate of input of A to the reactor = Rate of output of A from the reactor + Rate of disappearance of A due to chemical reaction + Rate of accumulation of A within the reactor.</p> <p>For mixed flow reactor at steady state the last term is zero. Therefore the material balance equation becomes</p> <p>Rate of input of A to the reactor = Rate of output of A from the reactor + Rate of disappearance of A due to chemical reaction + Rate of accumulation of A within the reactor.(i)</p> <p>Let, F_{A0} = Molar feed rate to the reactor</p>	



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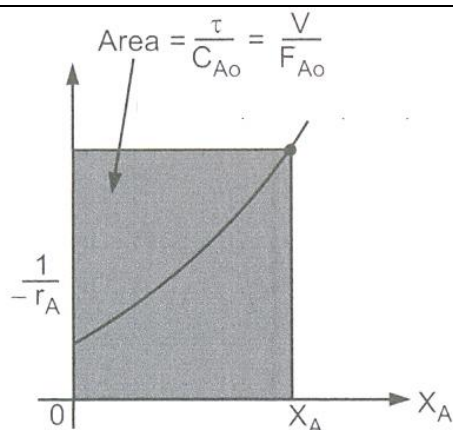
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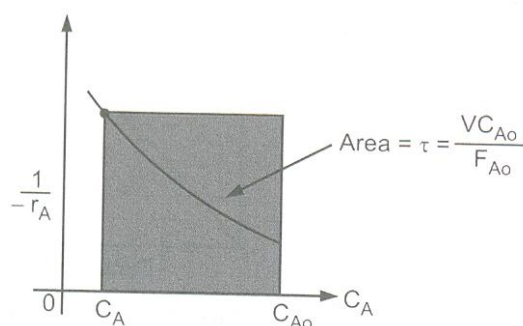
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	<p>V = Volume of reactor</p> <p>C_{A0} = Molar concentration of A in stream entering the reactor (moles/volume)</p> <p>v_0 = Volumetric flow rate(volume/time)</p> <p>X_A = Fractional conversion of A</p> <p>$F_{A0} = C_{A0} \cdot v_0$</p> <p>Input of A to the reactor in moles / time = F_{A0}.</p> <p>Disappearance of A due chemical reaction in moles / time = $(-r_A) \cdot V$</p> <p>Output of A from the reactor in moles / time = F_A</p> <p>Substituting in (i)</p> <p>$F_{A0} = F_A + (-r_A) \cdot V$ (ii)</p> <p>But $F_A = F_{A0} (1 - X_A) = F_{A0} - F_{A0} \cdot X_A$</p> <p>Equation (ii) becomes $F_{A0} = F_{A0} - F_{A0} \cdot X_A + (-r_A) \cdot V$</p> <p>$F_{A0} \cdot X_A = (-r_A) \cdot V$</p> <p>Rearranging, we get</p> $\frac{V}{F_{A0}} = \frac{X_A}{-r_A} = \frac{\tau}{C_{A0}}$ <p>For constant volume system</p> $\frac{V}{F_{A0}} = \frac{X_A}{-r_A} = \frac{\tau}{C_{A0}} = \frac{C_{A0} - C_A}{C_{A0}(-r_A)}$ <p>Where X_A and $(-r_A)$ are evaluated at the exit conditions, which are same as conditions prevailing within reactor (ex .composition,temperature)</p> <p>The graphical representation of the performance equation in terms of fractional conversion is as below</p>	<p>2</p> <p>2</p>
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The graphical representation of the performance equation in terms of concentration for constant density system is as below .



6-b

Van't Hoff equation:

$$\frac{d \ln K}{dT} = \frac{\Delta H^\circ}{RT^2}$$

Where K is the equilibrium constant.

ΔH° is the standard enthalpy change for the process.

T is the temperature in K

Significance:

The Van't Hoff equation relates the change in the equilibrium constant K of a chemical reaction to the change in temperature, T , given the standard enthalpy change, ΔH° , for the process. The equation helps to find out the variation of the

2

2



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	<p>equilibrium constant, and hence equilibrium conversion with temperature.</p> <p>When ΔH^0 is positive (endothermic reaction), $\frac{d \ln K}{dT} > 0$, $K(T)$ is a <i>increasing function</i>. Therefore K increases with increase in temperature.</p> <p>When ΔH^0 is negative (exothermic reaction), $\frac{d \ln K}{dT} < 0$, $K(T)$ is a <i>decreasing function</i>. Therefore K decreases with increase in temperature.</p>	
6-c	<p>$T_1 = 400 \text{ K}$</p> <p>$T_2 = 500 \text{ K}$</p> <p>$k_2 = 10 k_1$</p> <p>From Arrhenius law</p> $\ln \frac{k_2}{k_1} = \frac{-E}{R} \left(\frac{1}{T_2} - \frac{1}{T_1} \right)$ $\ln 10 = (-E / 1.987) * \left(\frac{1}{500} - \frac{1}{400} \right) = 2.52 * 10^{-4} E$ <p>$E = 9137.2 \text{ cal}$</p>	<p>2</p> <p>2</p>
6-d	<p>Given:</p> <p>$C_{A0} = 1 \text{ mol/l}$</p> <p>$X_A = 0.80$ when $t = 8 \text{ min.}$</p> <p>$X_A = 0.90$ when $t = 18 \text{ min}$</p> <p>Let us first assume reaction is of zero order. Therefore the integrated equation for zero order reaction in terms of fractional conversion is</p> $C_{A0} X_A = kt$ <p>Case 1) Where $X_A = 0.80$ when $t = 8 \text{ min.}$</p> $1 * 0.8 = k * 8$ $k = 0.1 \text{ (min)}^{-1} (\text{mol / l})$ <p>Case 2) Where $X_A = 0.90$ when $t = 80 \text{ min.}$</p> $1 * 0.9 = k * 18$	<p>1</p>



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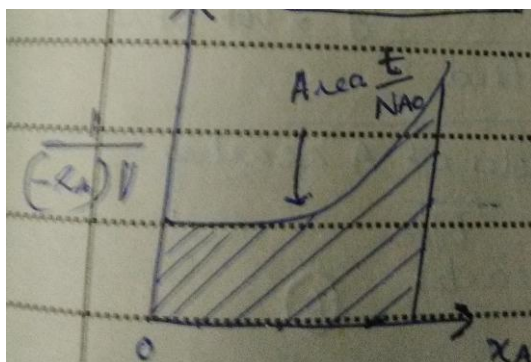
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	<p>$k = 0.05(\text{min})^{-1}(\text{mol / l})$</p> <p>Since k values are not same, the reaction is not of zero order</p> <p>Let us now assume reaction is of First order. The integrated equation for first order reaction in terms of fractional conversion is</p> $\ln \left[\frac{1}{1-X_A} \right] = kt$ <p>Case 1) Where $X_A = 0.80$ when $t = 8$ min.</p> $\ln \left[\frac{1}{1-0.8} \right] = k * 8$ $k = 0.201 (\text{min})^{-1}$ <p>Case 2) Where $X_A = 0.90$ when $t = 80$ min.</p> $\ln \left[\frac{1}{1-0.9} \right] = k * 18$ $k = 0.1279 (\text{min})^{-1}$ <p>Since k values are not same, the reaction is not of first order.</p> <p>Let us now assume it is of Second order. The integrated equation for second order reaction with respect to A in terms of fractional conversion is</p> $\left[\frac{X_A}{1-X_A} \right] = kC_{A0}t$ <p>Case 1) Where $X_A = 0.80$ when $t = 8$ min. & $C_{A0} = 1 \text{ mol/l}$</p> $\left[\frac{0.8}{1-0.8} \right] = k * 1 * 8$ $k = 0.5 (\text{mol/l})^{-1} (\text{min})^{-1}$ <p>Case 2) Where $X_A = 0.90$ when $t = 18$ min. & $C_{A0} = 1 \text{ mol/l}$</p> $\left[\frac{0.9}{1-0.9} \right] = k * 1 * 18$ $k = 0.5 (\text{mol/l})^{-1} (\text{min})^{-1}$ <p>since k values are same, reaction is of second order .</p> <p>Rate expression for the reaction is $-r_A = kC_A^2 = 0.5C_A^2$</p>	<p>1</p> <p>1</p> <p>1</p>
6-e	Graphical representation:	

Batch reactor

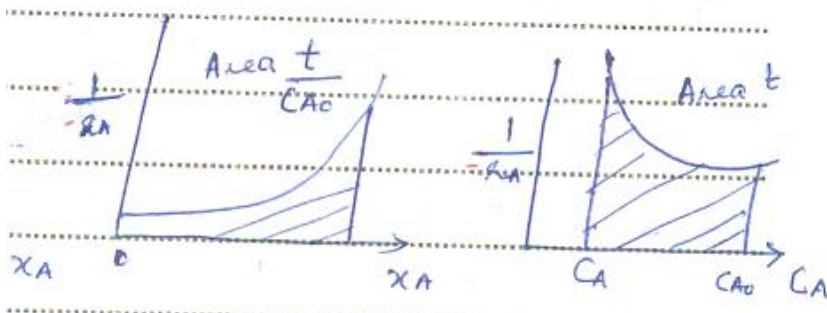
The performance or design equation is

$$t = N_{A0} \int_0^{x_A} \frac{dx_A}{V(-r_A)}$$



For constant volume system, the equation becomes

$$t = \frac{N_{A0}}{V} \int_0^{x_A} \frac{dx_A}{(-r_A)} = C_{A0} \int_0^{x_A} \frac{dx_A}{(-r_A)} = - \int_{C_A}^{C_{A0}} \frac{dC_A}{(-r_A)}$$



PFR

The performance or design equation is

$$\frac{V}{F_{A0}} = \int_0^{x_A} \frac{dx_A}{-r_A} = \frac{\tau}{C_{A0}}$$

For constant density system

$$\frac{V}{F_{A0}} = \int_0^{x_A} \frac{dx_A}{-r_A} = \frac{\tau}{C_{A0}} = \frac{-1}{C_{A0}} \int_{C_A}^{C_{A0}} \frac{dC_A}{-r_A}$$



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