



WINTER-15 EXAMINATION
Model Answer

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	Total marks
1A	Attempt any THREE		12
1A-a	Rate of a reaction: It is defined as change in the moles of any reactant / product of the reaction per unit time per unit volume of reacting fluid. Rate constant: Rate constant of a chemical reaction is a measure of the rate of the reaction when all the reactants are at unit concentration. For the reaction $A \rightarrow B$, For the reactant A. $-r_A = kC_A$ For the product B $r_B = kC_A$	1 1 1 1	4
1A-b	Definition: 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. Mathematical equation: $\mu = \mu_{i0} + RT \ln p_i$ Fugacity: It is a kind of fictitious pressure used for real gases. ie it is a measure of pressure for real gases Mathematical equation: $\lim_{P \rightarrow 0} \frac{f}{P} = 1$	1 1 1	4
1A-c	Half life: It is the time required to reduce the concentration of the reactant to half of its original value. Expression for half-life for nth order reaction. For first order chemical reaction ($n=1$), $t_{1/2} = \frac{0.693}{k}$ k=rate constant of chemical reaction	2 2	4



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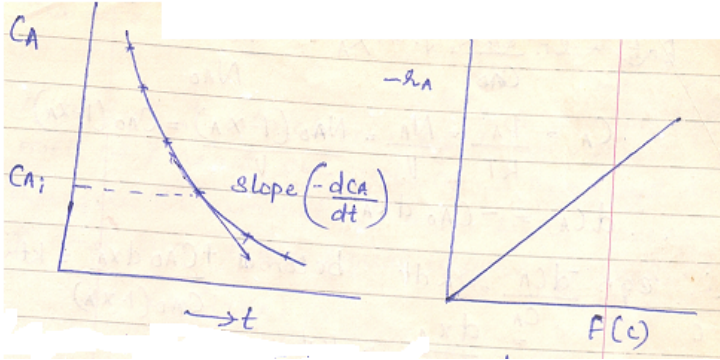
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	<p>For chemical reaction with $n \neq 1$, half-life is</p> $t_{1/2} = \left(\frac{2^{n-1} - 1}{k'(n-1)} \right) C_{A_0}^{1-n}$ <p>Where $t_{1/2}$ = half life period C_{A_0} = Initial concentration of reactant A n = Order of reaction k' = Rate constant of reaction .</p>		
1A-d	<p>Relation between C_A and X_A</p> <p>Constant volume System</p> $C_A = C_{A_0}(1 - X_A)$ <p>Variable volume system</p> $\frac{C_A}{C_{A_0}} = \frac{(1 - X_A)}{(1 + \epsilon_A X_A)}$	2 2	4
1B	<p>Attempt any ONE</p>		6
1B-a	<p>Steps for differential method of analysis of data:</p> <ol style="list-style-type: none">1. Assume a mechanism and from it obtain a rate equation of the form $-r_A = -dC_A / dt = kf(c)$2. From experiment obtain concentration-time data and plot them3. Draw a smooth curve through this data.4. Determine the slope of this curve at suitably selected concentration values. These slopes ($-dC_A/dt$) are the rates of the reaction at these composition.5. Evaluate $f(c)$ for each composition.6. Plot ($-dC_A/dt$) versus $f(c)$ for each composition. If we get a straight line passing through origin, the rate equation is consistent with the data. If not, then another rate equation should be tested.	6	6



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1B-b	<p>Activation energy: Activation energy is the minimum energy that the reactants must acquire before reaction takes place to give the product.</p> <p>$K_1 = 1 \times 10^{-3} \text{ min}^{-1}$ $K_2 = 2 \times 10^{-3} \text{ min}^{-1}$</p> <p>$T_1 = 27^\circ\text{C} = 300\text{K}$ $T_2 = 37^\circ\text{C} = 310\text{K}$</p> <p>$R = 1.987 \text{ cal / gmole K}$</p> <p>$\ln(k_1 / k_2) = -(E / R) (1/T_1 - 1/T_2)$</p> <p>Activation energy $E = 12809.2 \text{ calories.}$</p> <p>$\ln k_1 = \ln k_0 - (E / R T_1)$</p> <p>Frequency factor $k_0 = 2148434.7$</p>	2 2 2	6
2	Attempt any TWO		16
2-a	<p>Derivation for temperature dependency of rate constant from collision theory</p> <p>The collision rate of molecules in a gas is found from the kinetic theory of gases.</p> <p>For the bimolecular collision of like molecules A ,</p> $Z_{AA} = \sigma_A^2 n_A^2 \sqrt{\frac{4\pi kt}{M_A}}$ $= \sigma_A^2 \frac{N^2}{10^6} \sqrt{\frac{4\pi kt}{M_A}} C_A^2 \dots\dots(i)$	2	8

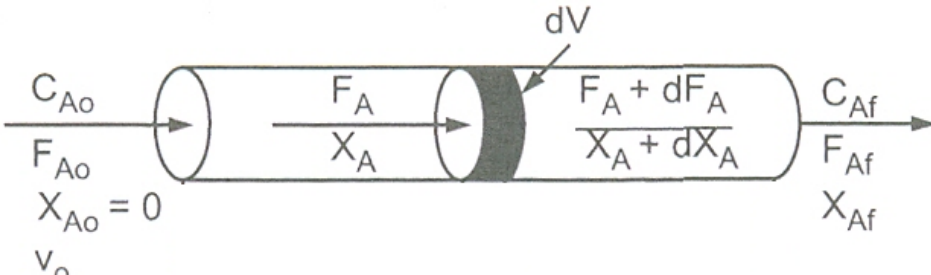


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	<p>= number of collisions of A with A / sec.cm³</p> <p>Where σ = diameter of molecule, cm</p> <p>M = (molecular weight) / N, mass of a molecule, gm</p> <p>N = Avogadro's number</p> <p>C_A = concentration of A, mol / liter</p> <p>n_A = NC_A / 10³, number of molecules of A / cm³</p> <p>k = Boltzmann constant</p> <p>For the bimolecular collision of unlike molecules in a mixture of A and B, kinetic theory gives</p> $Z_{AB} = \left\{ \left(\frac{\sigma_A + \sigma_B}{2} \right)^2 n_A n_B \sqrt{8\pi kT \left(\frac{1}{M_A} + \frac{1}{M_B} \right)} \right.$ $\left. = \left\{ \left(\frac{\sigma_A + \sigma_B}{2} \right)^2 \frac{N^2}{10^6} \sqrt{8\pi kT \left(\frac{1}{M_A} + \frac{1}{M_B} \right)} C_A C_B \dots \dots \dots (ii) \right.$ <p>If every collision between reactant molecules results in the transformation of reactants into product, these expressions give the rate of bimolecular reactions. The actual rate is much lower than that predicted and this indicates that only a small fraction of all collisions result in reaction. This suggests that only those collisions that involve energies in excess of a given minimum energy E lead to reaction. From the Maxwell distribution law of molecular energies the fraction of all bimolecular collisions that involves energies in excess of this minimum energy is given approximately by e^{-E/RT} where E \gg RT.</p> <p>Thus the rate of reaction is given by</p> $-r_A = -\frac{1}{V} \frac{dN_A}{dt} = k C_A C_B \dots \dots \dots (iii)$ <p>= (collision rate, mole / liter.sec)* (fraction of collision involving energies in excess of E)</p> $= Z_{AB} \frac{10^3}{N} e^{-E/RT}$	<p>2</p> <p>3</p>	
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	$= \left\{ \left(\frac{1}{M_A} + \frac{1}{M_B} \right) / 2 \right\}^{1/2} \frac{N}{10^3} \sqrt{8\pi kT} \left(\frac{1}{M_A} + \frac{1}{M_B} \right) e^{-E/RT} C_A C_B \dots\dots(iv)$ <p>Comparing iii and iv, $k \propto T^{1/2} e^{-E/RT}$</p>	1	
2-b	<p>Performance equation of steady state plug flow reactor:</p> <p>In PFR, the composition of the fluid varies from point to point along the flow path. So the material balance for a reaction component must be made for a differential element of volume dV.</p>  <p>Taking material balance of reactant A over the reactor, Input of A to reactor = Output of A from reactor + Disappearance of A due to chemical reaction + Accumulation of A within the reactor. For plug flow reactor, the last term is zero. Input of A to reactor = Output of A from reactor + Disappearance of A due to chemical reaction(1) Let, F_{A0} = Molar feed rate to the reactor. C_{A0} = Molar concentration of A in stream entering the reactor (moles/volume) X_A = Fractional conversion of A $F_A = F_{A0} (1 - X_A) = F_{A0} - F_{A0} X_A$ $dF_A = - F_{A0} d X_A$ For the differential volume dV</p>	2	8



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Input of A in moles/time = F_A

Output of A from reactor in moles/time = $F_A + dF_A$

Disappearance of A due to chemical reaction in moles/ time = $(-r_A) dV$

Substituting all the terms in the material balance equation (1)

$$F_A = F_A + dF_A + (-r_A) \cdot dV$$

$$- dF_A = (-r_A) dV$$

$$F_{A0} \cdot dX_A = (-r_A) dV$$

$$\frac{dV}{F_{A0}} = \frac{dX_A}{-r_A}$$

This is the equation accounting for A in the differential section of the reactor of volume dV . For the whole reactor, the equation must be integrated.

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

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

Where X_A and $(-r_A)$ are evaluated at the exit conditions

For constant volume system :

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

For first order reaction $-r_A = kC_A = kC_{A0}(1-X_A)$

$$\text{Therefore } \frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \frac{-1}{C_{A0}} \int_{C_{A0}}^{C_A} \frac{dC_A}{kC_A} = \int_0^{x_A} \frac{dX_A}{kC_{A0}(1-X_A)}$$

$$\tau = \frac{V}{F_{A0}} = \frac{-1}{k} \ln \frac{C_A}{C_{A0}} = \frac{-\ln(1-x_A)}{k}$$

Graphical representation:

2

2



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	<p>Area = $\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}}$</p> <p>Area = $\tau = \frac{C_{A0}V}{F_{A0}}$</p> <p>r - C curve</p>	2	
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>	2 marks each	8

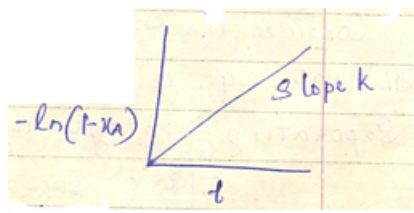


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	<p>3. Simple mixing: Some porous materials are obtained by mixing the components with water, milling to the desired grain size, drying and calcining. Such materials may be ground and sieved to obtain the particle size. Eg Mixed Mg and Ca oxide catalyst 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 method should also be given due consideration.</i></p>		
3	Attempt any FOUR		16
3-a	<p>$C_p(\text{ice}) = 9 \text{ cal / g mole K}$ $C_p(\text{water}) = 18 \text{ cal / g mole K}$ Molar enthalpy of fusion = 1437 cal / g mole</p> <ol style="list-style-type: none"> Entropy change when 1 mole of ice is heated from -10°C to 0°C $\Delta S_1 = nC_{p(\text{ice})} \int_{T_1}^{T_2} d \ln T = nC_{p(\text{ice})} \ln \frac{T_2}{T_1} = 1 * 9 * \ln (273 / 263) = 0.335 \text{ cal / K}$ Entropy change when 1 mole of ice at 0°C is converted to water at 0°C $\Delta S_2 = n\Delta H_{\text{fusion}} / T_{\text{fusion}} = 1 * 1437 / 273 = 5.2637 \text{ cal / k}$ Entropy change when 1 mole of water is heated from 0°C to 10°C $\Delta S_3 = nC_{p(\text{water})} \int_{T_1}^{T_2} d \ln T = 1 * 18 * \ln (283 / 273) = 0.64755 \text{ cal / k}$ 	1 1 1	4



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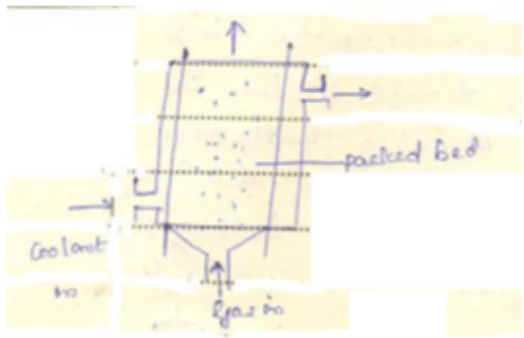
	Total entropy change $\Delta S = \Delta S_1 + \Delta S_2 + \Delta S_3 = 6.246 \text{ cal /K}$	1							
3-b	<p>Integrated form of rate expression for first order irreversible reaction in terms of fractional conversion</p> <p>Consider the reaction $A \rightarrow B$</p> <p>The rate equation is $-r_A = -dC_A / dt = kC_A \dots (1)$</p> <p>But $C_A = C_{A0}(1-x_A)$ and $dC_A = -C_{A0}dx_A$</p> <p>Substituting in (1) and rearranging and integrating</p> $\int_{x_{A0}}^{x_A} \frac{dx_A}{(1-x_A)} = k \int_0^t dt$ $-\ln(1-x_A) = kt$ <p>Graphical representation</p> 	3	4						
3-c	<p>Decrease in temperature is not desirable for endothermic reaction:</p> <p>Van't Hoff equation is $\frac{d \ln K}{dT} = \frac{\Delta H}{RT^2}$</p> <p>For endothermic reaction, ΔH is positive. When temperature is decreased, dT is negative; the overall equation is negative, which means $\ln K$ is negative. When $\ln K$ is negative, the value of K is low which denotes lower concentration of products. Therefore temperature decrease is not desirable for endothermic reaction.</p>	4	4						
3-d	<p>Difference between order and molecularity of reaction</p> <table border="1" data-bbox="186 1822 1183 1864"> <thead> <tr> <th>Sr.No.</th> <th>Molecularity</th> <th>Order of reaction</th> </tr> </thead> <tbody> <tr> <td> </td> <td> </td> <td> </td> </tr> </tbody> </table>	Sr.No.	Molecularity	Order of reaction				1 mark each for any four	4
Sr.No.	Molecularity	Order of reaction							



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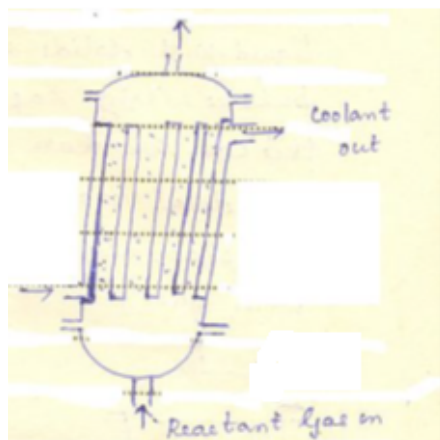
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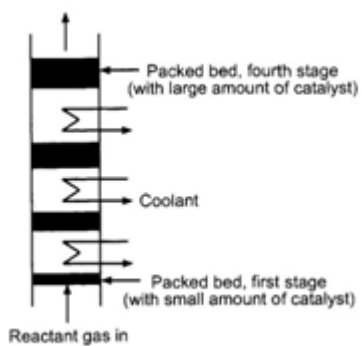
	1	Molecularity is the number of molecules, atoms or ions in a chemical reaction.	Order of reaction is the sum of exponents of the concentration terms involved in the rate equation.	points	
	2	Molecularity always have an integer value 1,2,3...	Order of reaction can have a fractional value.		
	3	Molecularity refers only to an elementary reactions	Order of reaction refers to an empirically found rate expression.		
	4	Molecularity has no meaning for overall reaction specially in complex reactions. Reaction can be unimolecular ,bimolecular etc.	Order of reaction can be one,two ,three & has definite meaning for overall reaction.		
	5	Molecularity is a theoretical quantity	Order of reaction is entirely an experimental value.		
3-e	Diagrams of (i) Packed bed reactor  (ii) Multitubular packed bed reactor			1 mark each	4



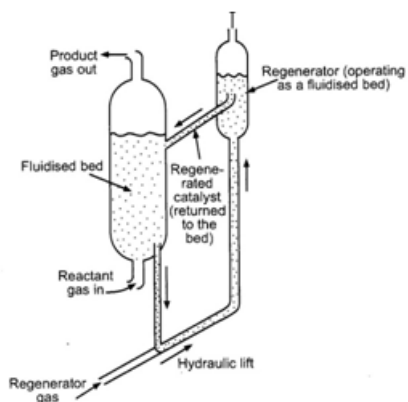
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(iii) Multibed packed bed reactor



(iv) Fluidised bed reactor with regenerator:





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4	Attempt any THREE		12
4A-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> $t_1 = \frac{0.693}{k} \quad - (1)$ <p>When $x_A = 0.75$ $-\ln(1-0.75) = kt_2$</p> $t_2 = \frac{1.386}{k} \quad - (2)$ <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>	1 1 1 1	4
4A-b	<p>Methods for regeneration of catalyst (any four)</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 $550-700^\circ\text{C}$.3. Metallic catalyst 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	1 mark each	4



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	<table border="1"> <thead> <tr> <th></th> <th>A</th> <th>R</th> <th>Total moles</th> </tr> </thead> <tbody> <tr> <td>Moles present initially</td> <td>1</td> <td>--</td> <td></td> </tr> <tr> <td>Moles reacted / produced at equilibrium</td> <td>x_A</td> <td>x_A</td> <td></td> </tr> <tr> <td>Moles present at equilibrium</td> <td>$1 - x_A$</td> <td>x_A</td> <td>1</td> </tr> <tr> <td>Mole fraction</td> <td>$1 - x_A$</td> <td>x_A</td> <td></td> </tr> <tr> <td>Partial pressure</td> <td>$P(1 - x_A)$</td> <td>$P x_A$</td> <td></td> </tr> </tbody> </table> <p> $K_p = \frac{P x_A}{P(1-x_A)} = \frac{x_A}{1-x_A}$ $K_p (1 - x_A) = x_A$ $K_p - K_p x_A = x_A$ $K_p = x_A (1 + K_p)$ $x_A = \frac{K_p}{1 + K_p}$ </p>		A	R	Total moles	Moles present initially	1	--		Moles reacted / produced at equilibrium	x_A	x_A		Moles present at equilibrium	$1 - x_A$	x_A	1	Mole fraction	$1 - x_A$	x_A		Partial pressure	$P(1 - x_A)$	$P x_A$		2	
	A	R	Total moles																								
Moles present initially	1	--																									
Moles reacted / produced at equilibrium	x_A	x_A																									
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Partial pressure	$P(1 - x_A)$	$P x_A$																									
4B	Attempt any one		6																								
4B-a	<p>Types of intermediates formed in a non-chain reaction</p> <p>1. Free radicals. Free atoms or larger fragments of stable molecules which contain one or more unpaired electrons are called free radicals. The unpaired electron is designated by a dot in the chemical symbol for the substance. Eg. $CH_3\cdot$, $C_2H_5\cdot$ Etc</p> <p>2. Ions and polar substances. Electrically charged atoms, molecules or fragments of molecules such as Na^+, OH^-, NH_4^+ are called ions. They may act as intermediates in reaction.</p> <p>3. Molecules: Consider the consecutive reaction $A \rightarrow R \rightarrow S$ This is a multiple reaction. If the product R is highly reactive, its concentration</p>	1½ marks each	6																								



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5-a	<p>Integrated form of rate equation for first Order Reversible Reaction:</p> <p>For first order unimolecular reaction: $A \rightleftharpoons B$</p> <p>Where k_1 is rate constant for forward reaction and k_2 rate constant for backward reaction</p> <p>The net rate of disappearance of A</p> $-r_A = k_1 C_A - k_2 C_B$ <p>The</p> $\frac{-dC_A}{dt} = k_1 C_A - k_2 C_B$ <p>Let initial mole ratio of B to A to be M</p> $M = \frac{C_{B0}}{C_{A0}}$ <p>When 1 mole of A reacts, 1 mole of B is produced, therefore $C_{A0} X_A = C_{B0} X_B$</p> <p>Concentration of A at time t is $C_A = C_{A0}(1 - X_A)$</p> <p>Therefore on differentiating $-dC_A = C_{A0} dX_A$</p> <p>Concentration of B at time t is $C_B = C_{B0} + C_{A0} X_A$</p> $-\frac{dC_A}{dt} = C_{A0} \frac{dX_A}{dt} = k_1 C_{A0}(1 - X_A) - k_2(C_{B0} + C_{A0} X_A)$ <p>The reaction is composed of two elementary reaction</p> $\frac{dC_A}{dt} = C_{A0} \frac{dX_A}{dt} = C_{A0}[k_1(1 - X_A) - k_2(M + X_A)] \text{eq. I}$ <p>At equilibrium, net rate is zero, therefore $\frac{-dC_A}{dt} = 0$ and</p> $X_A = X_{Ae} \text{ (fractional conversion)}$ $0 = C_{A0}[k_1(1 - X_{Ae}) - k_2(M + X_{Ae})]$ $k_1(1 - X_{Ae}) = k_2(M + X_{Ae}) \text{eq.II}$	2	8
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$$K_C = \frac{C_{Re}}{C_{Ae}} = \frac{k_1}{k_2} = \frac{(M+X_{Ae})}{(1-X_{Ae})} \text{eq.III}$$

From eq. I, we have

$$\frac{dX_A}{dt} = [k_1(1 - X_A) - k_2(M + X_A)]$$

Substituting the value of k_2 from eq.III in above equation2

$$\frac{dX_A}{dt} = k_1(1 - X_A) - \frac{k_1(1 - X_{Ae})}{(M + X_{Ae})}(M + X_A)$$

$$\frac{dX_A}{dt} = k_1 \left[\frac{(1 - X_A)(M + X_{Ae}) - (1 - X_{Ae})(M + X_A)}{(M + X_{Ae})} \right]$$

$$\frac{dX_A}{dt} = k_1 \left[\frac{(1 - X_A)(M + X_{Ae}) - (1 - X_{Ae})(M + X_A)}{(M + X_{Ae})} \right]$$

$$\frac{dX_A}{dt} = k_1 \left[\frac{M + X_{Ae} - MX_A - X_A X_{Ae} - M - X_A + MX_{Ae} + X_A X_{Ae}}{(M + X_{Ae})} \right]$$

Collecting the terms,we get

$$\frac{dX_A}{dt} = \frac{k_1[X_{Ae}(M + 1) - X_A(M + 1)]}{(M + X_{Ae})}$$

$$\frac{dX_A}{dt} = \frac{k_1(M + 1)}{(M + X_{Ae})}(X_{Ae} - X_A)$$

$$\int_0^{X_A} \frac{dX_A}{X_{Ae} - X_A} = \frac{k_1(M + 1)}{(M + X_{Ae})} \int_0^t dt$$

$$-\ln \left(\frac{X_{Ae} - X_A}{X_{Ae}} \right) = \frac{(M+1)}{(M+X_{Ae})} k_1 \cdot t$$

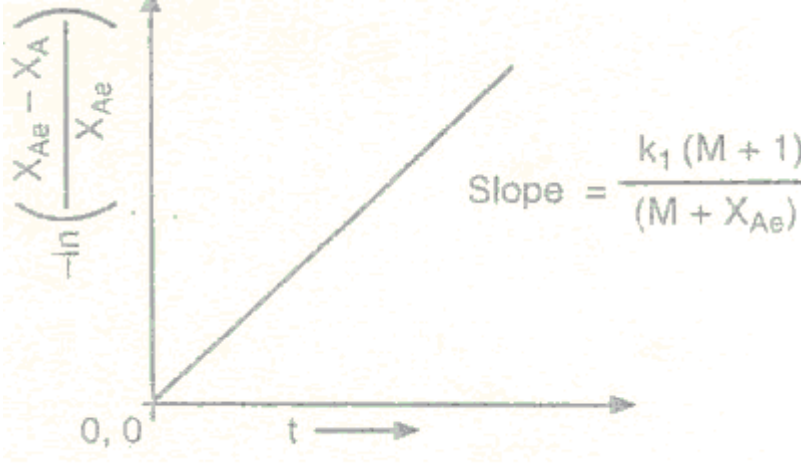
eq. IV

2

1



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	<p style="text-align: right;">eq.V</p> 		
5-b	<p>Comparison of mixed flow reactor(CSTR/ MFR) & plug flow reactor(PFR):</p> <ol style="list-style-type: none">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	1 mark each for any four points	8



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	<p>decreases, the effectiveness of CSTR with respect to PFR. The density increase during reaction has the opposite effect.</p> <p>4) For a given space time, conversion in a PFR is higher than in MFR.</p> <p>5) The performance equation for MFR is</p> $\tau_m \cdot C_{A0}^{n-1} = \left(\frac{C_{A0} V}{F_{A0}} \right)_m = \frac{X_A (1 + \varepsilon_A \cdot X_A)^n}{k (1 - X_A)^n}$ <p>The performance equation of PFR is</p> $\tau_p \cdot C_{A0}^{n-1} = \left(\frac{C_{A0}^n \cdot V}{F_{A0}} \right)_p = \frac{1}{K} \int_0^{X_A} \frac{(1 + \varepsilon_A X_A)^n}{(1 - X_A)^n} \cdot dX_A$ <p>6) It is possible to operate MFR under isothermal conditions where as with PFR it is difficult.</p> <p>7) MFR have long residence time compared to PFR</p> <p>8) MFR is not suitable for high pressure reactions where as PFR is suitable.</p> <p>Applications of MFR/CSTR:</p> <p>Used for maintain good temperature control in reactor, operating reactor under isothermal reaction conditions, useful for liquid phase reactions.</p> <p>Applications of PFR: for high pressure reactions as it can use small diameter tubes, for reactions with high heat effects as rate of heat transfer per unit volume of reaction mixture is high, used for gas phase reactions.</p>	<p>2</p> <p>1 mark each for any two</p>	
5-c	<p>Data:</p> <p>Reactor is Mixed flow reactor</p> <p>$X_A = 0.5$</p> <p>Reaction $A \rightarrow R$</p> <p>$-r_A = k C_A^2$</p>		8

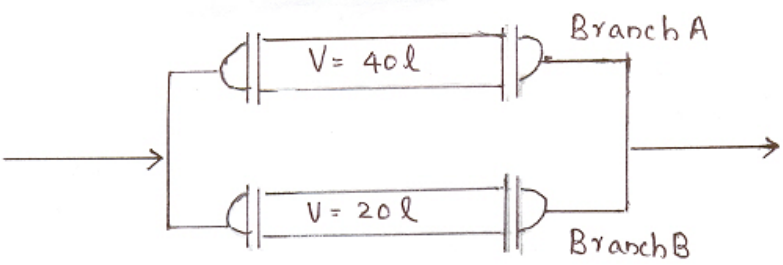


WINTER-15 EXAMINATION
Model Answer

<p>The performance equation of MFR is</p> $\frac{V}{F_{A0}} = \frac{X_A}{(-r_A)}$ $\frac{V}{F_{A0}} = \frac{X_A}{(k C_A^2)}$ $C_A = C_{A0}(1 - X_A)$ $\frac{V}{F_{A0}} = \frac{X_A}{(k C_{A0}^2 (1 - 0.5)^2)}$	2	
$\frac{V}{F_{A0}} = \frac{2 \cdot K}{k \cdot C_{A0}^2}$ $K = \frac{2 \cdot F_{A0} \cdot \dots \cdot 1}{V C_{A0}^2}$	2	
<p>As per new condition where volume of reactor is six times ($V_1 = 6V$) greater than in case of first condition (other terms kept constant), the equation can be written as</p> $\frac{V}{F_{A0}} = \frac{X_A}{(-r_A)}$ $\frac{6V}{F_{A0}} = \frac{X_A}{(K \cdot C_{A0}^2 (1 - X_A)^2)}$ <p style="text-align: center;"><i>Substituting the value of K from equation 1</i></p> $6V = \frac{X_A}{\frac{2 \cdot F_{A0} \cdot C_{A0}^2 (1 - X_A)^2}{V C_{A0}^2}}$ $6 = \frac{X_A}{2(1 - X_A)^2}$ $12 = \frac{X_A}{(1 - X_A)^2}$ $12 - 24X_A + 12X_A^2 = X_A$ $12X_A^2 - 25X_A + 12 = 0$	2	



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Model Answer

	<p>Roots of quadratic equation</p> $X_A = \frac{25 \pm \sqrt{(25^2 - 4 * 12 * (-12))}}{2 * 12}$ $X_A = \frac{25 \pm \sqrt{49}}{24}$ $X_A = \frac{25 \pm 7}{24}$ <p>$X_A = 1.33$ and 0.75 since X_A cannot be greater than 1, the value to be taken as 0.75</p>	2	
6	Attempt any FOUR		16
6-a	<p>Method of feeding when Plug flow reactors are connected in parallel:</p>  <p>For PFR's connected in parallel, the whole system can be treated as a single plug flow reactor of volume equal to total volume of the individual units if the feed is distributed in such a manner that fluid stream which meet have the same composition. Thus for reactors in parallel, V/F or τ must be the same for each parallel line. Any other way of feeding is inefficient.</p> <p>V/F should be identical if the conversion is to be the same in each branch.</p> $(V/F)_A = (V/F)_B$ <p>ie $\frac{F_A}{F_B} = \frac{V_A}{V_B} = \frac{40}{20} = 2$</p>	4	4



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	$F_A = 2 F_B$ $\frac{2}{3}$ rd of the feed must be fed to branch A and $\frac{1}{3}$ rd must be fed to branch B												
6-b	<p>Relation between K_p and K_c</p> <p>Consider the reaction $aA + bB + \dots \rightarrow rR + sS \dots$</p> $K_c = (C_R^r \cdot C_S^s) / (C_A^a \cdot C_B^b)$ <p>For ideal gas $C_i = p_i / RT$</p> <p>Therefore $K_c = \{ (p_R / RT)^r \cdot (p_S / RT)^s \} / \{ (p_A / RT)^a \cdot (p_B / RT)^b \}$</p> $= (p_R^r \cdot p_S^s) / (p_A^a \cdot p_B^b) \cdot (1 / RT)^{(r+s+\dots-(a+b+\dots))}$ <p>R is the ideal gas constant</p> <p>T the absolute temperature in K</p> <p>P is the pressure in atm</p> <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>$\Delta n = (r + s + \dots - (a + b + \dots))$ is the difference in the number of moles of product and reactant</p> <p>Or $K_p = K_c \times (RT)^{\Delta n}$</p>	01 01 01	4										
6-c	<p>Units of rate constant</p> <table border="1"> <thead> <tr> <th>Order of reaction</th> <th>Unit of rate constant</th> </tr> </thead> <tbody> <tr> <td>Zero</td> <td>mol/lit.sec.</td> </tr> <tr> <td>First</td> <td>sec.⁻¹</td> </tr> <tr> <td>Second</td> <td>lit/mol.sec.</td> </tr> <tr> <td>Third</td> <td>lit²/mol².sec.</td> </tr> </tbody> </table>	Order of reaction	Unit of rate constant	Zero	mol/lit.sec.	First	sec. ⁻¹	Second	lit/mol.sec.	Third	lit ² /mol ² .sec.	1 mark each	4
Order of reaction	Unit of rate constant												
Zero	mol/lit.sec.												
First	sec. ⁻¹												
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Third	lit ² /mol ² .sec.												
6-d	<p>Autocatalytic reactions: A reaction in which one of the products of the reaction acts as a catalyst is called as an autocatalytic reactions.</p> <p>Example: Oxidation of a solution of oxalic acid by an acidified solution of $KMnO_4$.</p> $2MnO_4^- + 6H^+ + 5(COOH)_2 \rightarrow 2Mn^{2+} + 10CO_2 + 8H_2O$	2	4										



WINTER-15 EXAMINATION
Model Answer

	<p>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 ,the rate of reaction speeds up.</p>	2	
6-e	<p>Classification of Reactors:</p> <p>1) Based on mode of operation:</p> <p>1) Batch reactors: Reactants added at beginning into reactor,left to react for certain time & products are withdrawn at a subsequent time.</p> <p>2) Continuous reactors:Feeding of reactants,chemical reaction & removal of product occur simultaneously,</p> <p>3) Semi batch reactor:One of the reactant added initially& the other is continuously added to a reactor over a certain time under agitation.</p> <p>2)Based on shape of reactor:</p> <p>1) Tank reactor:A cylindrical vessel with a mechanical stirrer & provision for heat transfer.</p> <p>Ex. Continuous stirred tank reactor(CSTR)</p> <p>2)Tubular reactor:A single continuous long tube or several tubes arranged in parallel.</p> <p>Ex. Plug flow reactor(PFR)</p> <p>3)Based on packing of catalyts:</p> <p>4) Fixed bed reactor:Catalyst particles are stationary & gas flows</p>	2	4



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	<p>through it.</p> <p>2) Fluidised bed reactor:Catalyst particles are suspended in gas stream.</p> <p>Material Balance Equation for any reactant A at any instant of time for Reactor:</p> <p>Rate of Flow of A into reactor = Rate of flow of A out of reactor + Rate of disappearance of A by chemical reaction + Rate of accumulation of A within the reactor</p>	2	
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