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SUMMER-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-a	**Factors affecting the rate of a chemical reaction** : 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 6. Surface area available. 7. Intensity of light if reaction is light sensitive.	1 mark each for any 4 points.	4
1A-b	**Internal energy(U):** It is the energy stored in the system by virtue of the configuration and motion of the molecules constituting the system. **Unit:** Joules, Calories **Enthalpy**: Enthalpy(H) is a measure of the total heat content of the substance or system. **Unit:** Joules, Calories	1 1 1 1	4
1A-c	**Autocatalytic reaction:** A reaction in which one of the products of the reaction acts as a catalyst is called autocatalytic reaction. **Eg** $CH_3COOC_2H_5 + H_2O \rightarrow CH_3COOH + C_2H_5OH$ Here CH_3COOH acts as catalyst	2 2	4

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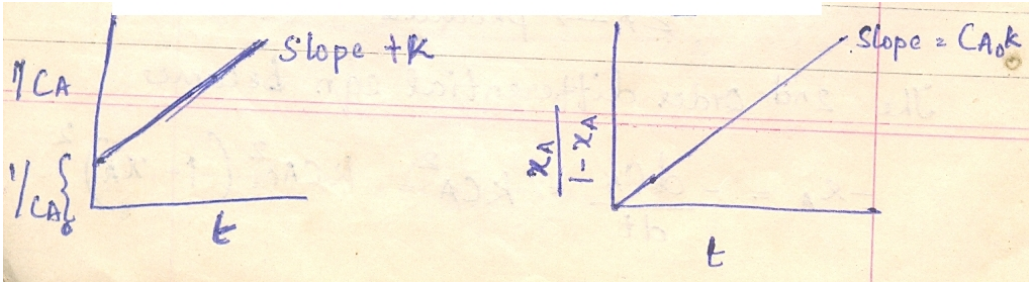
1A-d	**Difference between batch and continuous reactors:**		1 mark each for any 4 points	4
	Batch reactor	Continuous reactor		
	1.Reactants are fed at beginning, left to react for a certain time &products are discharged after that time.	Feeding of the reactants, chemical reaction &removal of product mixture occur simultaneously in a continuous manner.		
	2.Used when relatively small amount of material are to be treated	used for higher production rates		
	3.Poor quality control of products	Good quality control of products		
	4. Simple in construction	Complicated.		
	5. Needs less supporting equipments	Needs more supporting equipments		
	6 initial cost is relatively low and operating cost is high.	Initial cost is relatively high and operating cost is low.		
	7.Considerable time is required to empty, clean and refill.	No such problem		
1B-a	**Derivation:**			6

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	$2A \rightarrow$ product **In terms of concentration** $-r_A = -dc_A/dt = kC_A{}^2$ $-dc_A/C_A{}^2 = kdt$ On integration $K = 1/t(1/C_A - 1/C_{A0})$ **In terms of conversion** $-r_A = -dc_A/dt = kC_A{}^2$ $C_A = C_{A0}(1-X_A)$ $d_{CA} = -C_{A0}.d_{XA}$ $-d_{CA} = C_{A0}.d_{XA}$ $C_{A0}(d_{XA}/dt) = k.C_{A0}{}^2(1-X_A)^2$ On integrating $1/C_{A0}\{ X_A/(1-X_A)\} = kt$ **Graphical representation:** 	2 2 2	
1B-b	$k_1 = 1.6 * 10^{-3} \ S^{-1}$ $k_2 = 1.625 * 10^{-2} \ S^{-1}$ $T_1 = 10^{\circ}c = 283 \ K$ $T_2 = 30^{\circ}c = 303 \ K$ $\ln\frac{k_2}{k_1} = \frac{-E}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$	2 2	6

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	$\ln\frac{1.625 * 10-2}{1.6 * 10-3} = \frac{-E}{1.987}(\frac{1}{303} - \frac{1}{283})$ E= **19748.18 cal/mol**	2	
2-a	**Arrhenius law**		8

	The temperature dependence of the reaction rate constant k is given by
	
	 $k = k_0 e_{RT}^{-E}$
	
	 Where k_0 - frequency factor or pre exponential factor
	
	           E - activation energy in J/ mol or cal/ mol
	
	           R – universal gas constant
	
	           T – temperature in Kelvin
		4	

	Finding out activation energy graphically Activation energy of a reaction can be determined if rate constant is measured at a number of different temperatures. $k = k_o e^{-E}/_{RT}$ Taking ln, $\ln k = \ln k_o - (E / RT)$ Plot a graph with $(1 / T)$ on x axis and $\ln k$ on y axis. Slope is $-E / R$ and y	2	
	   intercept is $\ln k_o$. Activation energy = slope * R	2	

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2-b	**Given:** $X_A = 0.70$, $t = 13$ min For batch reactor, in which first order chemical reaction is taking place $-r_A = k.C_A$ $-\ln(1 - X_A) = kt$ $-\ln(1-0.70) = k * 13$ $k = 0.0926$ min^{-1} **For Plug flow reactor** (constant –density system): $$\frac{V}{F_{A0}} = \int_0^{X_A} \frac{dX_A}{-r_A} = \frac{\tau}{C_{A0}}$$ $$\tau = C_{A0} \int_0^{X_A} \frac{dX_A}{k.C_{A0}.(1-X_A)}$$ $$\tau = \int_0^{X_A} \frac{dX_A}{k.(1-X_A)}$$ Space time $\tau = \frac{1}{k}(-\ln(1-X_A)) = \frac{1}{0.0926}(-\ln(1-0.7)) = \textbf{13 } \textit{min}.$ **Space velocity = s = 1/ τ = 1/13 = 0.07692 min^{-1}** **For Mixed flow reactor** : $$\tau = \frac{C_{A0}.X_A}{(-r_A)}$$ $$\tau = \frac{C_{A0}.X_A}{-r_A} = \frac{C_{A0}.X_A}{kC_{A0}(1-X_A)}$$ **Space time $\tau = \frac{0.70}{0.0926(1-0.7)} = \textbf{25.2 min.}$** **Space velocity = s = 1/ τ = 1/25.2 = 0.03968 min^{-1}**	2 2 1 2 1		8
2-c	**Methods of catalyst Preparation:** 1. Precipitation 2. Gel formation	2		8

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3. Simple mixing	
4. Impregnation method	
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.	3marks each for any 2 methods.
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.	
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	
4. Impregnation method: 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. Eg Nickel catalyst is prepared on alumina by soaking the evacuated alumina particles with nickel nitrate solution, draining to remove the excess solution and	

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	heating in an oven to decompose the nitrate to nickel oxide. The final step is activation in which nickel oxide is reduced to nickel. *Any other appropriate method should also be given due consideration.*		
3-a	1. Thermodynamics tells whether a given process or a chemical reaction is feasible /possible or not, under the given set of condition (e.g. temperature, pressure etc.) 2. Thermodynamic provides information regarding how far a given process may proceed and also gives the maximum possible extent to which a given process can proceed. 3. It gives the degree to which the energy present in a system can be utilized to cause a given process to occure /takes place. 4. It help to make the preliminary choice of the process variable. 5. It helps to find out the effect of process variable on the extent of a reaction. 6. It give the thermal effect involved in a chemical process or reaction .	1mark each for any 4 points	4
3-b	**i) Constant volume System** $C_A = C_{A0}(1-X_A)$ **ii) Variable volume system** $\dfrac{C_A}{C_{A0}} = \dfrac{(1-X_A)}{(1+\mathcal{E}_A X_A)}$	2 2	4
3-c	for the reaction: $$CO_2 + H_2 \rightleftharpoons CO + H_2O$$ K_p is given by		4

$$K_p = \frac{P_{CO} \times P_{H_2O}}{P_{CO_2} \times P_{H_2}}$$

Equilibrium partial pressures are:

$$P_{CO} = 0.272 \text{ atm}, \quad P_{CO_2} = 0.218 \text{ atm}$$

$$P_{H_2} = 0.258 \text{ atm}$$

1

$$P_{H_2O} = P - (P_{CO} + P_{H_2} + P_{CO_2})$$
$$= 1.02 - (0.272 + 0.258 + 0.218)$$
$$= 0.272 \text{ atm}$$

1

$$\therefore \quad K_p = \frac{(0.272 \text{ atm}) \times (0.272 \text{ atm})}{(0.218 \text{ atm}) \times (0.258 \text{ atm})}$$

2

$$= 1.32$$

3-d	**Difference between molecularity and order:**		1 mark each for any 4 points	4
	ORDER OF A REACTION	**MOLECULARITY OF A REACTION**		
	1. It is sum of the concentration terms on which the rate of reaction actually depends or it is the sum of the exponents of the concentrations in the rate law equation.	It is the number of atoms, ions or molecules that must collide with one another simultaneously so as to result into a chemical reaction.		
	2. It need not be a whole number i.e. it can be fractional as well as zero.	It is always a whole number.		
	3. It can be determined	It can be calculated by simply adding		

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	experimentally only and cannot be calculated.	the molecules of the slowest step.		
	4. It is for the overall reaction and no separate steps are written to obtain it.	The overall molecularity of a complex reaction has no significance. It is only slowest step whose molecularity has significance for the overall reaction.		
	5. Even the order of a simple reaction may not be equal to the number of molecules of the reactants as seen from the unbalance equation.	For simple reactions, the molecularity can usually be obtained from the Stoichiometry of the equation.		
3-e	**Catalyst Deactivation** 1. Deactivation by Fouling 2. Chemical Deactivation - Poisoning 3. Deactivation by Thermal Degradation and Sintering **Deactivation by Fouling** Generally fouling covers all phenomena where the surface is covered with a deposit. The most widely known form of fouling of catalysts is coke formation. There are many reactions and mechanisms of coke formation depending on the nature of the catalyst therefore it is not clearly defined. But one can say that for the most part coke formation arises as a result of carbonaceous residues covering the active sites of a heterogeneous catalyst surface, subsequently decreasing the active surface area of the catalyst. In addition the deposition of rust and scale from elsewhere in the catalytic system is not uncommon. Coke-forming processes also involve chemisorption of different kinds of carbons or condensed hydrocarbons that may act as catalyst		1 3	4

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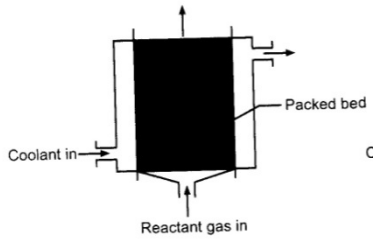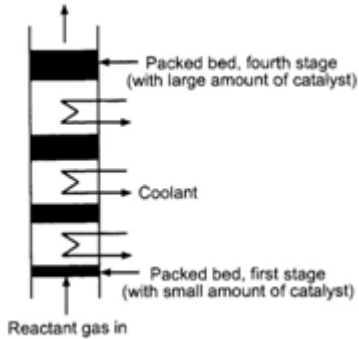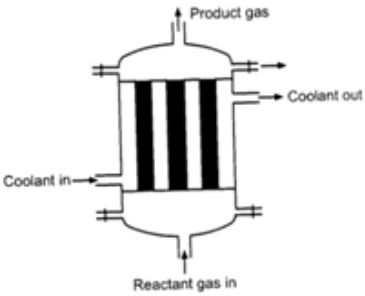|			
	poisons causing the chemical deactivation of the catalyst. The fouling of zeolite catalysts occurs in the form of coke molecules limiting the access of the reactant to the active sites of a cavity or a pore intersection of the zeolite. The pores in which the hexane molecules are rearranged to form the desired products end up being filled with the coke molecules resulting in the zeolite's deactivation. *Note: Description of the other two types should also be considered*		
4A-a	$$N_2O_5 \longrightarrow N_2O_4 + \frac{1}{2}O_2$$ $$N_2O_5 \longrightarrow Products$$ Let, $N_2O_5 = A$, $\therefore$ A $\longrightarrow$ Products for a first order reaction, we have $$-\ln\left[\frac{C_A}{C_{A_0}}\right] = k \cdot t$$ 1) $C_A = 0.113$ mol/l , at $C_{A_0} = 0.16$; $t = 1$ min. $$k = \frac{-\ln(C_A/C_{A_0})}{t} = \frac{-\ln(0.113/0.160)}{1} = 0.3478 \text{ min}^{-1}$$ 2) $C_A = 0.08$ mol/l at $t = 2$ min $$k = \frac{-\ln(0.08/0.160)}{2} = 0.3466 \text{ min}^{-1}$$ 3) $C_A = 0.056$ mol/l at $t = 3$ min $$k = \frac{-\ln(0.056/0.160)}{3} = 0.3499 \text{ min}^{-1}$$ 4) $C_A = 0.040$ mol/l at $t = 4$ min $$k = \frac{-\ln(0.040/0.160)}{4} = 0.3466 \text{ min}^{-1}$$	1 2	4

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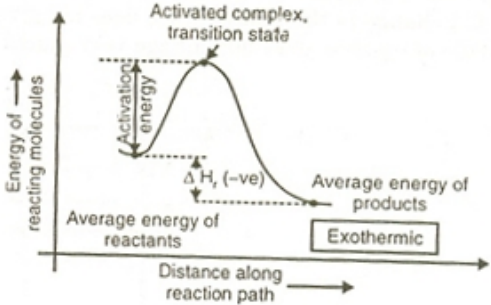|			
	As the value of K is constant , the given reaction is of first order. Value of rate constant k= 0.3479 min^{-1}	1	
4A-b	i) Packed bed reactor: ii) Multibed reactor: iii) Multi tube fixed bed reactor: 	1 mark each	4

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	iv) Fluidised bed reactor: (a) Without regenerator (b) With regenerator		
4A-c	**Rate of reaction:** Rate of a reaction is defined as change in 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. **Unit of Rate constant** **for Zero order reaction :** (Mol/lit) / sec OR concentration /time **For First order reaction :** $(Second)^{-1}$ OR $(time)^{-1}$	1 1 1 1	4
4A-d	**Feasibility of a chemical reaction from Gibbs free energy change:**	4	4

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|			
	At chemical equilibrium $\Delta G^0 = 0$. For a chemical reaction at equilibrium at a given temperature &pressure ,the free energy must be minimum.		
	If $\Delta G^0 < 0$ i.e.it is negative ,the reaction can take place spontaneously.(reaction is possible under a given set of reactions).For spontaneous reaction,there should be decrease in Gibb's free energy change .		
	If ΔG^0 is positive ,the reaction cannot take place under these conditions.		
4B-a	**Activation energy**: Activation energy is the minimum energy that the reactants must acquire before reaction takes place to give the product.	2	6
	For exothermic reaction		
		1	
	For endothermic reaction:		

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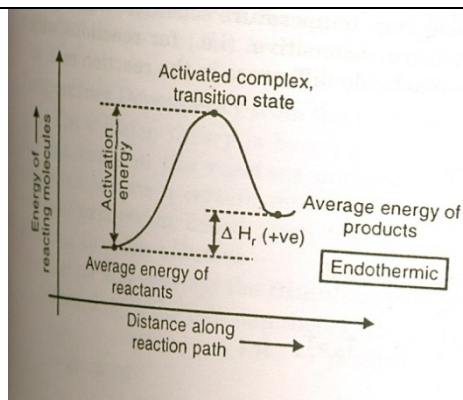
		1	

Role of Activation energy in Chemical reaction : Activation energy can be considered as a potential energy barrier. Only those molecules that have sufficient energy to reach the top of the barrier and form activated complex react. Smaller the activation energy (low barrier), greater will be the number of activated molecules and faster will be the rate of reaction. It will help to find out the nature of the reaction.(endothemic or exothermic). It will give the difference between activated complex and energy of reactant.

4B-b	**Relation between Gibb's free energy and equilibrium constant**		6

we will consider a homogeneous chemical reaction of the form

$$A+B \rightleftharpoons C+D$$
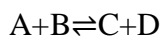
$\Delta G = \sum G°f, \text{ products} - \sum G°f, \text{ reactants}$

$G_A = G°_A + RT \ln P_A$

The free energy change for the reaction is sum of the free energies of the products, minus the sum of free energies of the reactants:

$\Delta G = G_C + G_D - G_A - G_B$

$\Delta G = (G°_C + RT \ln P_C) + (G°_D + RT \ln P_D) - (G°_B + RT \ln P_B) - (G°_A + RT \ln P_A)$

We can now express the G° terms collectively as $\Delta G°$, and combine the

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logarithmic pressure terms into a single fraction

$\Delta G = \Delta G° + RT\ln(P_C P_D / P_A P_B)$

which is more conveniently expressed in terms of the reaction quotient Q

$\Delta G = \Delta G° + RT\ln Q$

$\Delta G = \Delta G° + RT\ln Q$

As the reaction approaches equilibrium, ΔG becomes less negative and finally

reaches zero. At equilibrium $\Delta G = 0$ and $Q = K$,

$\Delta G° = -RT\ln K_p$

in which K_p, the equilibrium constant expressed in pressure units, is the special

value of Q that corresponds to the equilibrium composition.

OR

Consider the reaction $aA + bB \rightarrow rR + sS$

ΔG reaction = ΔG product - ΔG reactant.

$\qquad = (r\,\mu_R + s\,\mu_S) - (a\,\mu_A + b\,\mu_B)$.

At equilibrium there is no Gibb's free energy change, $\Delta G = 0$

$(r\,\mu_R + s\,\mu_S) - (a\,\mu_A + b\,\mu_B) = 0$

$r(\mu_R^0 + RT\ln p_R) + s(\mu_S^0 + RT\ln p_S) = a(\mu_A^0 + RT\ln p_A) +$

$\qquad\qquad\qquad\qquad\qquad b(\mu_B^0 + RT\ln p_B)$

$RT\ln\left(\dfrac{p_R^r\, p_S^s}{p_A^a\, p_B^b}\right) = (a\,\mu_A^0 + b\,\mu_B^0) - (r\,\mu_R^0 + s\,\mu_S^0$

$\qquad\qquad = -(\Delta G \text{ product} - \Delta G \text{ reactant})$

$\qquad\qquad = -\Delta G \text{ reaction}.$

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	$\ln \left(\dfrac{p_R^r \, p_S^s}{p_A^a \, p_B^b}\right) = \dfrac{-\Delta G \text{ reaction}}{RT}$ But $\left(\dfrac{p_R^r \, p_S^s}{p_A^a \, p_B^b}\right) = K_p$ Therefore $\Delta G = -RT \ln K_p$		
5-a	**Integrated form of rate expression For reversible first order reaction** $A \rightleftharpoons B$ **(Derivation)** $\dfrac{dC_A}{dt} = C_{A0}\dfrac{dX_A}{dt} = C_{A0}[k_1(1 - X_A) - k_2(M + X_A)]$ ...... eq. **I** At equilibrium ,net rate is zero ,therefore $\dfrac{-dC_A}{dt} = 0$ and	2	8

In the handwritten derivation:

Given reaction is $A \underset{k_2}{\overset{k_1}{\rightleftharpoons}} B$.

k_c = equilibrium Constant = $\dfrac{k_1}{k_2}$

The rate equation is $-\dfrac{dC_A}{dt} = \dfrac{dC_B}{dt} = k_1 C_A - k_2 C_B$.

But $C_A = C_{A0}(1 - X_A)$ and $C_B = C_{B0}(1 + X_B)$

From the reaction stoichiometry, When 1 mole of A reacts, 1 mole of B is produced. ie $C_{A0} X_A = C_{B0} X_B$

$\therefore$ Rate equation can be written as

$-\dfrac{dC_A}{dt} = k_1 C_{A0}(1 - X_A) - k_2 C_{B0}(1 + X_B)$

$= k_1 [C_{A0} - C_{A0} X_A] - k_2 [C_{B0} + C_{B0} X_B]$

$= k_1 [C_{A0} - C_{A0} X_A] - k_2 (C_{B0} + C_{A0} X_A)$

Starting with a Concentration ratio, $M = \dfrac{C_{B0}}{C_{A0}}$

$\dfrac{dC_A}{dt} = k_1 C_{A0}(1 - X_A) - k_2 C_{A0}\left(\dfrac{C_{B0}}{C_{A0}} + X_A\right)$

But $d\dfrac{C_A}{dt} = -C_{A0}\dfrac{dX_A}{dt}$.

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$X_A = X_{Ae}$ $(fractional\ conversion)$

$$0 = C_{A0}[k_1(1 - X_{Ae}) - k_2(M + X_{Ae})]$$

$$k_1(1 - X_{Ae}) = k_2(M + X_{Ae})$$

eq.II

$$K_C = \frac{C_{Be}}{C_{Ae}} = \frac{k_1}{k_2} = \frac{(M + X_{Ae})}{(1 - X_{Ae})} \qquad \text{eq.III}$$

$From\ eq.I\ ,we\ have$

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

$Substituting\ the\ value\ of\ k_2$ from eq.III in above equation

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

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

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

$$\frac{dX_A}{dt} = k_1\left[\frac{M + X_{Ae} - MX_A - X_A X_{Ae} - M - X_A + MX_{Ae} + X_A X_{Ae}}{(M + X_{Ae})}\right]$$
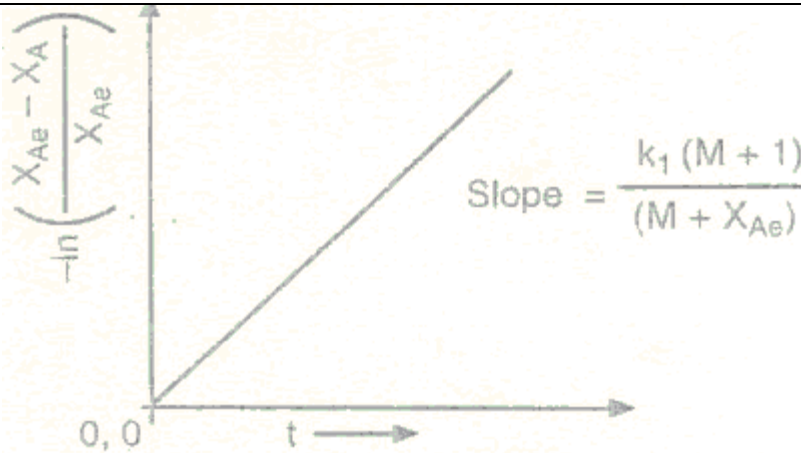
$Collecting\ the\ terms$,we get

2

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

3

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

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

$$-\ln\left(\frac{X_{Ae} - X_A}{X_{Ae}}\right) = \frac{(M+1)}{(M+X_{Ae})} k_1 t \qquad \text{eq. IV}$$

$$-\ln\left(\frac{X_{Ae} - X_A}{X_{Ae}}\right) = -\ln\left(\frac{C_A - C_{A0}}{C_{A0} - C_{Ae}}\right) = \frac{(M+1)}{(M+X_{Ae})} k_1 t \qquad \text{eq.V}$$

Eq.V is the desired integrated rate equation for reversible first order r

A plot of

$$-\ln\left(\frac{X_{Ae} - X_A}{X_{Ae}}\right) \text{ vs time gives a straight line with slope equal to}$$

$$\frac{(M + 1)}{(M + X_{Ae})} k_1.$$

1

$$\text{Slope} = \frac{k_1 (M + 1)}{(M + X_{Ae})}$$

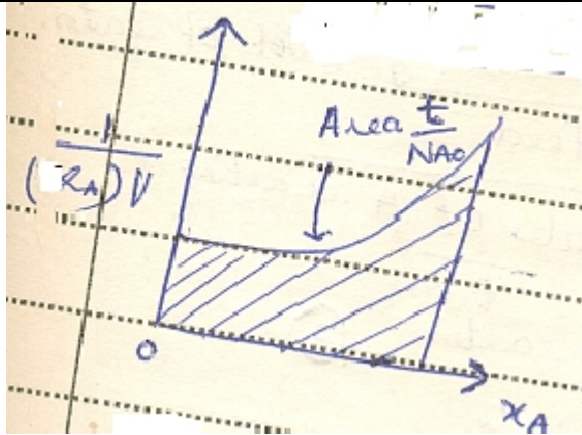| 5-b	**Design equation of batch Reactor:**		8
	In batch reactor, the composition is uniform throughout reaction zone at any instant of time.		
	Taking material balance of a limiting reactant A ,over the reactor as a whole		
	Rate of Rate of flow Rate of Rate of		
	Flow of A = of A + disappearance of A +accumulation of A		
	into reactor out of reactor by chemical reaction within the reactor		
	…………(1)		
	In batch reactor, no fluid enters or leaves from the reactor during the reaction.		
	Therefore Rate of Flow of A into reactor = Rate of flow of A out of reactor = 0		
	Eq.I becomes		
	rate of disappearance of A - Rate of accumulation of A within the	2	
	by chemical reaction = reactor …………..(2)		

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Rate of disappearance of A in moles/time in the reaction volume

$$V = (-r_A)V$$

Moles of A fed $= N_{A0}$

$N_A = N_{A0}(1 - X_A)$ where X_A is the fractional conversion of A at time t

Rate of accumulation of A within reactor (moles/time) $= \frac{dN_A}{dt}$

$$= \frac{d[N_{A0}(1-X_A)]}{dt} = = -N_{A0}\frac{dX_A}{dt}$$

Replacing the terms in eq(2)

$$(-r_A)V = \left(N_{A0}\frac{dX_A}{dt}\right)$$

Rearranging we get

$$dt = N_{A0}\frac{dX_A}{(-r_A)V} \quad .....(3)$$

Integrating eq.(3) within the limits

$$\int_0^t dt = N_{A0}\int_0^{X_A}\frac{dX_A}{(-r_A).V}$$

$$t = N_{A0}\int_0^{X_A}\frac{dX_A}{(-r_A).V} \quad ....(4)$$

Eq.(4) is the design equation for batch reactor ,which indicates the time needed

to achieve a conversion X_A . For either isothermal or non-isothermal operation,

the terms rate $-r_A$ & volume V are retained under the integral sign because they

both may change as the reaction proceeds.

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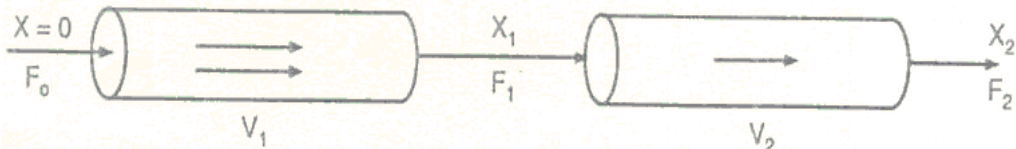
5-c	**Comparison of mixed flow reactor(CSTR/ MFR) & plug flow reactor(PFR):**	2 marks each for any 4 points	8
	1) For any given duty & for all positive reaction orders , **size** of MFR is always larger than that of PFR.the volume ratio Vm / Vp increases with reaction order.		
	2) For low values of conversion, 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 decreases, the effectiveness of CSTR with respect to PFR. The density increase during reaction has the opposite effect.		
	4) For a given **space time**, conversion in a PFR is higher than in MFR.		
	5) The **performance equation** for MFR is $$\tau_m . C_{A0}^{n-1} = \left(\frac{C_{A0}V}{F_{A0}}\right)_m = \frac{X_A (1+\varepsilon_A . X_A)^n}{k (1-X_A)^n}$$ The performance equation of PFR is		

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	$$\tau_p . C_{A0}^{n-1} = \left(\frac{C_{A0}^n \cdot V}{F_{A0}}\right)_p = \frac{1}{K}\int_0^{XA} \frac{(1 + \varepsilon A X A)^n}{(1 - X_A)^n} . dX_A$$ **6)** It is possible to operate MFR under **isothermal conditions** where as with PFR it is difficult. **7)** MFR have **long residence time** compared to PFR **8)** MFR is not suitable for **high pressure reactions** where as PFR is suitable			
6-a	**Plug flow reactors in Series** :Assume two PFRs are placed in series as shown below Let X_1 & X_2 be the fractional conversions of a component A leaving reactors 1 &2 . X_1 : conversion of A from first reactor X_2 : overall conversion of A from entire system The performance equation for PFR1 is $\frac{V_1}{F_0} = \int_0^{X_1} \frac{dX}{(-r)}$ The performance equation for PFR2 is $\frac{V_2}{F_0} = \int_{X_1}^{X_2} \frac{dX}{(-r)}$ Two PFRS in series $$\frac{V}{F_0} = \frac{V_1}{F_0} + \frac{V_2}{F_0} = \int_0^{X_1}\frac{dX}{(-r)} + \int_{X_1}^{X_2}\frac{dX}{(-r)} \qquad \text{EqI}$$ From eqI ,it is clear that the total volume of two PFRs in series is identical to that of one PFR(single reactor) for the same conversion.If the total volume of	2	4

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	two PFRs in series is V= $V_1 + V_2$ for X_2,then the same conversion (X_2) can be achieved using one PFR of volume V.Thus it makes no diffence if two PFRs are connected in series or one PFR of same reactor volume.	2	
6-b	**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. **Fugacity:** :It is defined as a thermodynamic property of a real gas which if substituted for the pressure or partial pressure in the equations for an ideal gas gives equations applicable to the real gas. **Gibbs Free Energy**:It is the the energy actually available to do useful work..It predicts the feasibility and equilibrium conditions for chemical reactions at constant temperature and pressure. **Entropy(s):**It is the measure of the total disorder or randomness of the system or it is a measure of the unavailable energy to perform the useful work	1mark each	4
6-c	**Elementary and non elementary reactions:**	1mark each for any 4	4

Elementary and non elementary reactions:

Sr no.	Elementary reactions	Non-elementary reactions
1	These are single steps reactions.	These are multistep reactions.
2	Simple in nature	Complex in nature
3	Order of reaction agrees with stoichiometry.	Order of reaction does not agree with stoichiometry.
4	For these reactions,order must be an integer	Order may be an integer or fractional value.

	5	If 2A→ R,the rate law is $$-r_A = kC_A^2$$	For nonelementary reaction 2B→ S ,the rate law may be $$-r_B = kC_B^{\propto}$$ Where $\propto \neq 2$		
	6	Ex $C_2H_5OH + CH_3COOH$ → $CH_3COOC_2H_5 +$ H_2O	Ex. $H_2 + Br_2 \rightarrow 2HBr$		
6-d	For second order reaction: $$k = \frac{1}{t}\left[\frac{1}{c_A} - \frac{1}{c_{A0}}\right]$$ t = 50 min $C_{A0} = 5*10^{-4}$ mol/l Gas is 40% decomposed $C_A = C_{A0}(1 - X_A) = 0.6 \times 5 \times 10^{-4} = 3*10$ mol/l $$k = \frac{1}{50}\left[\frac{1}{3*10^{-4}} - \frac{1}{5*10^{-4}}\right]$$ $k = 26.67$ l/mol.min^{-1}		1 1 2	4
6-e	**Space time (τ):** It is the time required to process one reactor volume of feed measured at specified condition. **Equation and** **unit:** Space time $\tau = $ Reactor volume/volumetric flow rate $= \frac{V}{v_0}$ Unit is unit of time (seconds, minute, etc) **Space velocity(s)** It is the number of reactor volume of feed at specified conditions which can		1 1 1	4

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	be treated in unit time. Space time = volumetric flow rate / Reactor volume **Equation and unit** Space velocity s = volumetric flow rate / Reactor volume = $\frac{v_0}{V}$ Unit is time^{-1} (ex.second^{-1} min^{-1})	1	