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WINTER-18 EXAMINATION

Model Answer

Subject Name: 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	Sub	Answer	Marks
No.	Q		
	No.		
1A		Attempt any THREE	12
1A	a	Factors affecting the rate of a chemical reaction :	1 mark
		1. In homogeneous system temperature, pressure and composition are the	each for
		variables.	any four
		2. In heterogeneous system, since more than one phase is involved, material	factors.
		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.	
1A	b	Gibb's free energy:	
		Gibb's free energy is the energy actually available to do useful work. It	2
		predicts the feasibility and equilibrium conditions for chemical reactions at	
		constant temperature and pressure.	
		Feasibility of a chemical reaction from Gibbs free energy change:	
		At chemical equilibrium $\Delta G^0 = 0$. For a chemical reaction at equilibrium at a	
		given temperature & pressure, the free energy must be minimum.	2
		If $\Delta G^0 < 0$ i.e. it is negative, the reaction can take place spontaneously	
		(reaction is possible under the given set of conditions).For spontaneous	



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		reaction, there should be decrease in Gibb's free energy change.	
		If ΔG^0 is positive ,the reaction cannot take place under the given conditions	
1A	c	Definition:	
		Fractional change in volume ε_A :	
		It is defined as the change in volume of the system between no conversion	1.5
		and complete conversion of reactant A.	
		Fractional conversion x _A :	
		Fractional conversion x_A of reactant A is defined as the fraction of A that is	1.5
		converted into product.	
		Mathematical expression:	
		$\varepsilon_{\rm A} = \frac{V_{XA=1}-V_{XA=0}}{V_{XA=0}}$	1
1A	d	Space time:	
		It is the time required to process one reactor volume of feed measured at	1
		specified condition.	
		$\tau = \frac{1}{s} = \frac{C_{A0} v}{F_{A0}}$	
		Unit	1
		Unit is unit of time (seconds, minute, etc)	1
		Space velocity	
		It is the number of reactor volume of feed at specified conditions which can	
		be treated in unit time.	1
		$\mathbf{S} = \frac{1}{\tau} = \frac{F_{A0}}{C_{A0V}}$	
		Unit	
		Unit is $time^{-1}$ ($second^{-1}$, $minute^{-1}$ etc)	1



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1B		Attempt any ONE	6
1B	a	Differential method of analysis of data	
		1)Assume a mechanism and from it obtain a rate equation of the form	
		$-r_A = \frac{-dC_A}{dt} = kf(c)$	
		2) From experiment obtain concentration-time data and plot them.	
		3) Draw a smooth curve through this data.	
		4) Determine the slope of this curve at suitably selected concentration	
		values. These slopes $\left(\frac{-dC_A}{dt}\right)$ are the rates of reaction at these composition.	
		5) Evaluate $f(c)$ for each composition.	
		6) Plot $\frac{-dC_A}{dt}$ vs $f(c)$ for each composition. If we get a straight line through	4
		origin; the rate equation is consistent with the data. If not, then another rate	
		equation should be tested.	
		$C_{A} -R_{A}$ $C_{A};Slope(-d_{CA})$ $C_{A};Slope(-d_{CA})$ $F(c)$	
		Merits (any one):	1
		1. It is useful for testing more complicated rate equations.	1
		2. It can be used to evolve or develop the rate equation to fit the data	



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		Demerits (any one):	1
		1. Differential method is not that much easy, is complicated & time	
		consuming.	
		2. It is used only when more accurate & large amount of data are	
		available.	
1B	b	Arrhenius equation	
		The temperature dependency of the reaction rate constant k, is given by	
		$\mathbf{k} = \mathbf{k}_0 \boldsymbol{e}_{RT}^{-E}$	
		Where k_0 - frequency factor or pre exponential factor	3
		E - activation energy in J/ mol or cal/ mol	
		R – universal gas constant	
		T – temperature in Kelvin	
		$T_1 = 400 \text{ K}$	
		$T_2 = 500 K$	
		$k_2 = 10 k_1$	
		From Arrhenius law	
		$\ln\frac{k_2}{k_1} = \frac{-E}{R} \left(\frac{1}{T_2} - \frac{1}{T_1}\right)$	2
		$\ln 10 = (-E / 1.987) * (\frac{1}{500} - \frac{1}{400}) = 2.52 * 10^{-4}E$	1
		E = 9150.47 cal	1
2		Attempt any TWO	16
2	a	Derivation for temperature dependency of rate constant from collision	
		theory	
		The collision rate of molecules in a gas is found from the kinetic theory of	
		gases.	
		For the bimolecular collision of like molecules A,	



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$Z_{AA} = \sigma_A^2 n_A^2 \sqrt{\frac{4\pi kT}{M_A}}$	
$= \sigma_{\rm A}^2 \frac{N^2}{10^6} \sqrt{\frac{4\pi kT}{M_A}} C_{\rm A}^2 \dots (i)$	
= number of collisions of A with A / sec.cm ^{3}	
Where σ = diameter of molecule, cm	
M = (molecular weight) / N, mass of a molecule, gm	
N = Avogadro's number	
C_A = concentration of A, mol / liter	
$n_A = NC_A / 10^3$, number of molecules of A / cm ³	
k = Boltzmann constant	
For the bimolecular collision of unlike molecules in a mixture of A and B,	
kinetic theory gives	
$Z_{AB} = \left\{ \left(\left. \sigma_A + \left. \sigma_B \right) \right. / 2 \right\} \right.^2 n_A n_B \sqrt{8\pi kT \left(\frac{1}{M_A} + \frac{1}{M_B} \right)}$	
$= \{ (\sigma_{\rm A} + \sigma_{\rm B}) / 2 \}^{2} \frac{N^{2}}{10^{6}} \sqrt{8\pi kT \left(\frac{1}{M_{A}} + \frac{1}{M_{B}}\right)} C_{\rm A} C_{\rm B} \dots \dots \dots (ii)$	4
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 $E >> RT$.	



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		Thus the rate of reaction is given by		
		$-\mathbf{r}_{\mathrm{A}} = -\frac{1}{V} \frac{dN_{A}}{dt} = \mathbf{k} \ \mathbf{C}_{\mathrm{A}} \mathbf{C}_{\mathrm{B}} \ \dots \dots (\mathrm{i}\mathrm{i}\mathrm{i}\mathrm{i})$		2
		= (collision rate, mole / liter.sec)* (fraction of		
		collision involving energies in excess of E)		
		$= Z_{AB} \frac{10^3}{N} e^{-E/RT}$		
		$= \{ (\sigma_{A} + \sigma_{B}) / 2 \}^{\frac{2}{N}} \sqrt{8\pi kT \left(\frac{1}{M_{A}} + \frac{1}{M_{B}}\right)} e^{-E/RT} C_{A} C_{B} \dots (iv)$		2
		Comparing iii and iv, $\mathbf{k} \propto T^{1/2} e^{-\mathbf{E} / \mathbf{R}T}$		2
2	b	Data:		
		Reactor is Mixed flow reactor		
		$X_{\rm A} = 0.5$		
		Reaction $A \rightarrow R$		
		$-r_A = \mathbf{k} \ C_A^2$		
		The performance equation of MFR is		
		$\frac{V}{F_{A0}} = \frac{X_A}{(-r_A)}$		2
		$\frac{V}{F_{A0}} = \frac{X_A}{(\mathrm{k}\ C_A^2)}$		
		$C_A = C_{A0}(1 - X_A)$		
		$\frac{V}{F_{A0}} = \frac{X_A}{(k C_A^2)} = \frac{.(0.5)}{k C_{A0}^2 (1 - 0.5)^2}$		
		$\frac{V}{F_{A0}} = -\frac{2}{k.c_{A0}^2}$		



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		$K = \frac{2.F_{A0}}{VC_{A0}^2} \dots 1$	2
		Now the original reactor is replaced by PFR of equal size	
		$\frac{V}{F_{A0}} = \int_{0}^{X_{A}} \frac{dX_{A}}{-r_{A}}$ But $-r_{A} = k C_{A}^{2}$ and $C_{A} = C_{A0}(1 - X_{A})$ $\frac{V}{T_{A}} = \int_{0}^{X_{A}} \frac{dX_{A}}{x_{A}} = \int_{0}^{X_{A}} \frac{dX_{A}}{x_{A}^{2}} \frac{dX_{A}}{x_{A}^{2}} \frac{dX_{A}}{x_{A}^{2}} \frac{dX_{A}}{x_{A}^{2}}$	
		$F_{A0} = \frac{1}{KC_{A0}^2} * \frac{X_A}{1 - X_A}$	
		Substituting the value of K from equation 1	2
		$\frac{V}{F_{A0}} = \frac{VC_{A0}^2 X_A}{2F_{A0}C_{A0}^2(1 - X_A)}$ $2 = \frac{X_A}{(1 - X_A)}$ $2 - 2X_A = X_A; 2 = 3 X_A;$	2
		$X_A = 2 / 3 = 0.667$ Conversion in PFR will be 66.7%	
2	c	Methods of catalyst Preparation:	2 marks
		1. Precipitation	each for
		2. Gel formation	explaining
		3. Simple mixing	the
		4. Impregnation method	methods
		1.Precipitation method : This method produces catalyst in porous form. It consists of adding a	with eg
		precipitating agent to the solution of the desired component. The	
		precipitation is followed by washing, drying, calcinations & activation(or	



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Page pretreatment) Eg. Magnesium oxide catalyst is prepared by this method. It is prepared by	9 of 27
pretreatment)Eg. Magnesium oxide catalyst is prepared by this method. It is prepared by	
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.	
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 heating in an oven to decompose the nitrate to nickel oxide. The final	
step is activation in which nickel oxide is reduced to nickel.	



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		Any other appropriate preparation method should also be given due	
		consideration	
3		Attempt any FOUR	16
3	a	Number of moles $(n) = 2$	
		$V_1 = 801$	
		$V_2 = 140 l$	
		$T_1 = 50^0 C = 323 K$	
		$T_2 = 200^0 C = 473 K$	
		$C_v = 7.8 \text{ cal} / \text{mol K}$	
		$\Delta \mathbf{S} = \mathbf{n} \mathbf{C}_{\mathbf{V}} \ln \frac{T_2}{T} + \mathbf{n} \mathbf{R} \ln \frac{V_2}{V}$	2
		$\Delta S = 2 \times 7.8 \times \ln (473/323) + 2 \times 1.987 \times \ln (140/80) = 8.1744 \text{ cal / K}$	2
3	b	Integrated form of rate expression for zero order reaction	
		Rate equation is $-r_A = -\frac{dC_A}{dt} = C_{A0}\frac{d_{xA}}{dt} = k$	
		In terms of concentration	
		$-\frac{dC_A}{dt} = \mathbf{k}$	
		Integrating between appropriate limits	2
		$\int_{CA_0}^{CA} - \mathrm{dCA} = \mathrm{k} \int_0^t dt$	
		$C_{A0} - C_A = kt$ for $t < \frac{c_{A0}}{k}$	



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	At equil $(r \mu_R + s)$	ibrium there is no Gibb's μ_S) -(a μ_A + b μ_B) = 0	free energy change, $\Delta G = 0$		2
	$(r \mu_R + s)$ But $\mu_i =$ Therefore	$\mu_{S} = (a \ \mu_{A} + b \ \mu_{B})$ = $\mu_{i}^{0} + RT \ lnp_{i}$ re $r(\ \mu_{B}^{0} + RT \ lnp_{B}) + si$	$(\mu_{s}^{0} + RT \ln p_{s}) = a(\mu_{A}^{0} + RT \ln p_{A}) +$		
		rs	$b(\mu_B^0 + RT \ln p_B)$		
	RT ln $\left(\frac{p}{p}\right)$	$\frac{\frac{R}{a}}{\frac{p_S}{p_B}} = (a \ \mu_A^0 + b \ \mu_B^0)$	$-(r \mu_{\rm R}^0 + s \mu_{\rm S}^0)$		
		$= - (\Delta G \text{ product} -$ $= - \Delta G \text{ reaction.}$	· Δ G reactant)		2
	$\ln \left(\frac{p_R^r}{p_A^a} \frac{p_S^s}{p_B^b}\right)$	$-\Delta G reaction = \frac{-\Delta G reaction}{RT}$ Bu	t $\left(\frac{p_R^r p_S^s}{p_A^a p_B^b}\right) = \mathbf{K}_p$		
2	Therefor	$re \Delta G = - RT \ln K_p$			- montr
5	points):	rison between elementar	y and non elementary reaction (4		each
	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 each reactant is identical with stoichiometric coefficient of that species	Not identical.		
	4	For these reactions, order must be an	Order may be an integer or fraction value.	al	



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		integer					
		5 If $2A \rightarrow R$, the rate law For nonelementary reaction					
		is $2B \rightarrow S$, the rate law may be					
		$-r_{\rm A} = kC_{\rm A}^2 \qquad -r_{\rm B} = kC_{\rm B}^{\alpha}$					
		Where $\propto \neq 2$					
		$6 \qquad Ex C_2H_5OH + \qquad Ex. H_2 + Br_2 \rightarrow 2HBr$					
		$CH_3COOH \rightarrow$					
		$CH_3COOC_2H_5 + H_2O$					
3	e	Steps involved in solid catalyzed gas phase reactions	4				
		1. Diffusion of the reactant from bulk fluid phase to external surface of					
		catalyst					
		2. Diffusion of reactant tfrom pour mouth into catalyst pores					
		3. Adsorption of reactant into catalyst surface					
		4. Chemical reaction to form product					
		5. Deadsorption of product					
		6. Diffusion of deadsorped product from interior of catalyst pores to					
		surface					
		7. Diffusion of product to the bulk of fluid phase					
4A		Attempt any THREE	12				
4A	a	Derivation of integrated rate expression for irreversible second order					
		reaction $2A \rightarrow Products:$					
		$2A \rightarrow \text{product}$					
		In terms of concentration					



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Fluidized bed Fixed bed	each
(i) Recovery Catalyst loss is there, Catalyst loss is not	
units so recovery units are there, so recovery	
required units are not required	
(ii) Catalyst Easily done Difficult	
regeneration	
(iii) Can maintain Difficult to maintain	
isothermal isothermal conditions	
condition:	
(iv) size of Can use small size of Cannot use very small	
catalyst catalyst size of catalyst	
because of plugging	
and high pressure	
drop	
4A c Half life period : Half life period is the time required to reduce the	1
concentration of the reactant to half of its original value	1
Mathematical expression:	
For first order chemical reaction($n=1$) the half life is independent of initial	
concentration of the reactant & is calculated as	
0.693	1
$t_{1/2} = \frac{1}{k}$	-
k=rate constant of chemical reaction	
For chemical reaction with $n \neq 1$, half life is	



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Subject Name: Chemical Reaction Engineering Subject Code: 17562 Page 16 of 27 $t_{1/2} = \left(\frac{2^{n-1}-1}{k'(n-1)}\right) C_{A_0}^{1-n}$ 1 Where t 1/2=half life period $C_A o =$ Initial concentration of reactant A 1 n= Order of reaction, k' = Rate constant of reaction. Relation between K_p and K_v(derivation) 4Ad Consider the reaction $aA + bB \rightarrow rR + sS$ $K_{p} = (p_{R}^{r} \cdot p_{S}^{s}) / (p_{A}^{a} \cdot p_{B}^{b})$ But $p_A = P \cdot y_A$ Where p_A - partial pressure of A, P- total pressure 2 y_A – mole fraction of A. $K_{p} = (p_{R}^{r} \cdot p_{S}^{s}) / (p_{A}^{a} \cdot p_{B}^{b})$ $= \{(Py_R)^r . (Py_S)^s\} / \{(Py_A)^a . (Py_B)^b\}$ $= (y_{R}^{r} \cdot y_{S}^{s}) / (y_{A}^{a} \cdot y_{B}^{b}) \cdot P^{(r+s+...)-(a+b+...))}$ $K_p = K_y \cdot P^{\Delta n}$ where $K_y = (y_R^r \cdot y_S^s) / (y_A^a \cdot y_B^b)$ and 2 $\Delta n = (r + s + ...) - (a + b + ...)$ is the difference in the number of moles of product and reactant 4BAttempt any ONE 6 4B1.5 marks **Types of intermediates in non- chain reaction:** a 1. Free radicals. Free atoms or larger fragments of stable molecules for each which contain one or more unpaired electrons are called free radicals. The point unpaired electron is designated by a dot in the chemical symbol for the substance. Eg. CH₃ $C_2 \dot{H}_5$ 2. Ions and polar substances. Electrically charged atoms, molecules or fragments of molecules such as Na⁺, OH⁻ , NH4⁺are called ions. They



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	may act as intermediates in reac	tion.		
	3. Molecules: Consider the cons	ecutive reaction		
	$A \rightarrow R \rightarrow S$			
	This is a multiple reaction. If the	product R is highly reactive, its		
	concentration in the reaction mix	ture can become too small to measu	ire. In	
	such a situation, R is not observe	ed and can be considered to be a reac	tive	
	intermediate.			
	4. Transition complexes. The coll	lision between reactant molecules re	sult in	
	a wide distribution of energies an	nong the individual molecules. This	can	
	result in strained bonds, unstable	form of molecules or unstable assoc	iation	
	of molecules which can then either	er decompose to give products or by	further	
	collision return to molecules in th	he normal state. Such unstable forms	are	
	called transition complexes.			
4B t	Relation between conversion an	nd equilibrium constant for second	l order	
	reversible reaction			
	Reaction is $A + B \leftrightarrow R + S$			
	Let 1 mole of A and 1 mo	ble of B is present initially.		
	x_A mole of A reacts	s at equilibrium		
	P is the total pressure	е.		
	When 1 mole of A reacts, 1mole	e of B also reacts. Then 1mole of R	and 1	2
	mole of S is produced			



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	А	В	R	S	Total	
					moles	
Moles present initially	1	1	-	-		
Moles reacted / produced at equilibrium	X _A	x _A	X _A	x _A		2
Moles present at equilibrium	1- x _A	1- x _A	x _A	X _A	2	
Mole fraction	1- x _A /2	$1 - x_A/2$	x _A / 2	x _A / 2		
Partial pressure	P(1- x _A) /2	P(1- x _A) / 2	P x _A / 2	P x _A / 2		
$K_{p} = \frac{P\left(\frac{X_{A}}{2}\right)F}{P\left(\frac{1-X_{A}}{2}\right)F}$ $K_{p} (1-x_{A})^{2} = x_{A}^{2}$	$\frac{p\left(\frac{X_A}{2}\right)}{p\left(\frac{1-X_A}{2}\right)} =$	$\frac{x_A^2}{(1-x_A)^2}$				
$K_p (1-2x_A + x_A^2) =$ $K_p - 2 K_p x_A + K_p$	$= x_A^2$ $x_A^2 = x_A^2$					
$(K_{p} - 1) x_{A}^{2} - 2 K_{p}$ $x_{A} = \frac{2K_{P} \pm \sqrt{(4K_{P} + $	$x_{A} + K_{p} = 0$ $b^{2} - 4(K_{P} - 1)$ $k_{P} - 1)$) <i>K</i> _P)				2
Attempt any TWO						16



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Given: 5 а $C_{A0} = 1 \text{ mol/l}$ $X_A = 0.80$ when t = 8 min. $X_A = 0.90$ when t = 18 min Let us first assume reaction is of zero order. The integrated equation for zero order reaction in terms of fractional conversion is $C_{A0}X_A = kt$ Case 1) Where $X_A = 0.80$ when t = 8 min. 2 1*0.8 = k*8 $k = 0.1 \text{ (min)}^{-1} \text{(mol / l)}$ Case 2) Where $X_A = 0.90$ when t = 18 min. 1*0.9 = k*18 $k = 0.05(min)^{-1}(mol / 1)$ Since k values are not same, the reaction is not of zero order Let us now assume reaction is of First order. The integrated equation for first order reaction in terms of fractional conversion is $\ln\left[\frac{1}{1-X_A}\right] = kt$ Case 1) Where $X_A = 0.80$ when t = 8 min. $\ln \left| \frac{1}{1-0.8} \right| = k^* 8$ $k = 0.201 \text{ (min)}^{-1}$ Case 2) Where $X_A = 0.90$ when t = 80 min. 2 $\ln \left[\frac{1}{1-0.9} \right] = k*18$ $k = 0.1279 \text{ (min)}^{-1}$ Since k values are not same, the reaction is not of first order.



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		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	
		$\frac{X_A}{1-X_A} = \mathbf{k} C_{AO} \mathbf{t}$	
		Case 1) Where $X_A = 0.80$ when $t = 8$ min. & C $_{A0} = 1$ mol/l	2
		$\frac{0.8}{1-0.8} = k * 1 * 8$	
		$k = 0.5 \text{ (mol/l)}^{-1} \text{ (min)}^{-1}$	
		Case 2) Where $X_A = 0.90$ when $t = 18$ min. & C $_{A0} = 1$ mol/l	
		$\frac{0.9}{1-0.9} = k * 1 * 18$	
		$k = 0.5 (mol/l)^{-1} (min)^{-1}$	
		since k values are same, reaction is of second order.	2
		Rate of the reaction is $-r_A = kC_A^2 = 0.5C_A^2$ (mol/l minute)	
5	b	Derivation of performance equation / design equation of mixed flow	
		reactor:	
		reactor : In MFR, the composition of the reactants is uniform throughout the reactor.	
		reactor : In MFR, the composition of the reactants is uniform throughout the reactor. Taking material balance of reactant A over the reactor as a whole,	
		<pre>reactor: In MFR, the composition of the reactants is uniform throughout the reactor. Taking material balance of reactant A over the reactor as a whole, Rate of input of A to the reactor = Rate of output of A from the reactor</pre>	
		<pre>reactor: In MFR, the composition of the reactants is uniform throughout the reactor. Taking material balance of reactant A over the reactor as a whole, 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</pre>	
		<pre>reactor: In MFR, the composition of the reactants is uniform throughout the reactor. Taking material balance of reactant A over the reactor as a whole, 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.</pre>	
		 reactor: In MFR, the composition of the reactants is uniform throughout the reactor. Taking material balance of reactant A over the reactor as a whole, 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. For mixed flow reactor at steady state the last term is zero. Therefore the 	
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$C_{A0} = Molar concentration$	of A in stream entering the reactor		
(moles/volume)			
$v_0 =$ Volumetric flow rate	e(volume/time)		
X _A = Fractional conversio	n of A		
$\mathbf{F}_{\mathbf{A}0} = \mathbf{C}_{\mathbf{A}0.} \mathbf{v}_{0}$			
Input of A to the reactor in mole	$es / time = F_{A0.}$		2
Disappearance of A due chemica	al reaction in moles / time = $(-r_A)$.V		
Output of A from the reactor	in moles / time $= F_A$		
Substituting in (i)			
$F_{A0} = F_{A+}(-r_A) .V$	(ii)		
But $F_A = F_{A0}(1 - X_A) = F_{A0} - F_{A0}$	F _{A0.} X _A		
Equation (ii) becomes $F_{A0} = F_{A0}$	$_{0}$ - $F_{A0.} X_{A} + (-r_{A}) .V$		
$F_{A0.} X_A = (-r_A) . V$			
Rearranging, we get			
$\frac{V}{F_{A0}} = \frac{X_A}{-r_A} = \frac{\tau}{C_{A0}}$			2
For constant volume system			
$\frac{V}{F_{A0}} = \frac{X_A}{-r_A} = \frac{\tau}{C_{A0}} = \frac{C_{A0-CA}}{CA0(-r_A)}$			
Where X_A and $(-r_A)$ are evaluate	ed at the exit conditions, which are same	ie as	
conditions prevailing within reac	tor (ex .composition,temperature)		
For first order reaction			
$-\mathbf{r}_{A} = \mathbf{k}\mathbf{C}_{A} = \mathbf{k}\mathbf{C}_{Ao} = \mathbf{k}\mathbf{C}_{Ao} (1-\mathbf{x}_{A})$			2
$\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \frac{X_A}{KC_{A0}(1-X_A)} = \frac{C_{A0-CA}}{CA0(kC_A)}$	$\left(\frac{A}{A}\right)$		Z
The graphical representation o	f the performance equation in term	s of	



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	these reactors approaches unity. 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 volume ratio,		
	but decreases, the effectiveness of CSTR with respect to PFR. Density		
	increase during reaction has the opposite effect.		
	4) The performance equation for MFR is		
	$\tau_m \cdot C_{A0}^{n-1} = \left(\frac{C_{A0}V}{F_{A0}}\right)_m = \frac{X_A (1 + \varepsilon_A \cdot X_A)^n}{k(1 - X_A)^n}$		
	For PFR		
	$\tau_p. C_{A0}^{n-1} = \left(\frac{C_{A0}^n V}{F_{A0}}\right)_p = \frac{1}{K} \int_0^{XA} \frac{(1 + \varepsilon A X A)^n}{(1 - X_A)^n} dX_A$		
	5) For a given space time, conversion in a PFR is higher than in MFR.		
	6) It is possible to operate MFR under isothermal conditions whereas with		
	PFR it is difficult.		
	7) MFR has long residence time compared to PFR.		
	8) MFR is not suitable for high pressure reactions whereas PFR is		
	suitable.		
6	Attempt any FOUR		16
6	a Method of feeding when PFR's are connected in parallel		
	Consider PFRs are connected as shown in the figure.		



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Model Answer

Subject Name: Chemical Reaction Engineering Subject Code: 17562 Page 25 of 27 Temperature increase is not desirable for exothermic reaction. 4 6 b Van't Hoff equation is $\frac{dlnK}{dT} = \frac{\Delta H}{RT^2}$ For exothermic reaction, ΔH is negative. When temperature is increased, overall equation is negative, which means ln K is dT is positive; the negative. When ln K is negative, the value of K is low which denotes lower concentration of products. Therefore temperature increase is not desirable for exothermic reaction. Difference between order and molecularity of reaction.(4 points) 1 mark 6 с Sr.No. Molecularity Order of reaction each Order of reaction is the sum 1 Molecularity is the number of molecules, atoms or ions in a of exponents of the chemical reaction. concentration terms involved in the rate equation. 2 Molecularity always have an Order of reaction can have a integer value 1,2,3... fractional value. Shows the kinetic 3 Shows the elementary mechanism or separate steps of a complicated dependence of the rate on the concentration of the process reactants. 4 Depending upon the value of Depending upon the value molecularity, reaction can be of order, the reactions are unimolecular, bimolecular etc. termed as first order, second



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