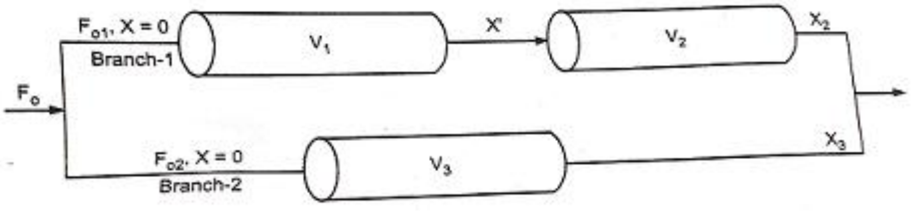
WINTER-19 EXAMINATION

Model Answer

Subject title: Chemical Reaction Engineering Subject code 22512

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.

Q No.		Answer	Marking scheme
1		**Attempt any FIVE of the following**	**10**
1	a	**Definition of activation energy:** It is the minimum energy that the reactant molecules must acquire before reaction takes place to give the product.	2
1	b	**Definition of fractional change in volume ε_A:** It is defined as the change in volume of the system between no conversion and complete conversion of reactant A.	2
1	c	**Relation between C_A and X_A** **i) Constant density (volume) System** $C_A=C_{A0}(1-X_A)$ **ii) Changing density (volume) system** $\frac{C_A}{C_{A0}}=\frac{(1-X_A)}{(1+\varepsilon_A X_A)}$	1 1
1	d	**Diagram of plug flow reactors connected in series-parallel arrangement** 	2
1	e	**Application of** **Fluidized bed reactor(any two)** Used when good temperature control is required, when catalyst regeneration	½ mark

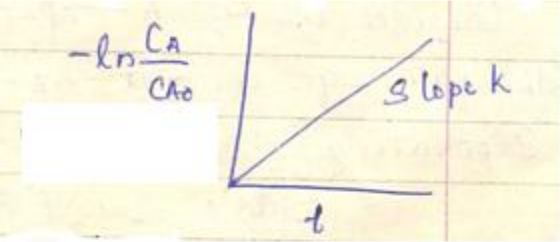
		has to be done on a continuous basis without shutting down the reactor. Used in the production of pthalic anhydride, vinyl acetate, polyethylene, polypropylene, maleic anhydride, in the incineration of solid waste, catalytic cracking of petroleum naphtha **Packed bed reactor (any two)** Used when high conversion rate per catalyst weight is required. Used in ammonia synthesis, methanol manufacture, ethylene oxide production, sulphuric acid production, styrene production, steam reforming of natural gas etc.	each ½ mark each
1	f	**Autocatalytic reactions**: A reaction in which one of the products of the reaction acts as a catalyst is known as an autocatalytic reactions. Eg1. $CH_3COOC_2H_5 + H_2O \rightarrow CH_3COOH + C_2H_5OH$ Here CH_3COOH acts as catalyst 2. Oxidation of a solution of oxalic acid by an acidified solution of $KMnO_4$. $2MnO_4^- + 6H^+ + 5(COOH)_2 \rightarrow 2Mn^{2+} + 10CO_2 + 8\,H_2\,O$ Oxalic acid 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.	1 1 mark for any 1 example
1	g	**Application of Batch reactor (any 4)**: These are used when relatively small amount of material are to be treated. Also to produce different products using same reactor, for testing new products, for the study of reaction kinetics of complex reactions. etc.Used in the production	½ mark each

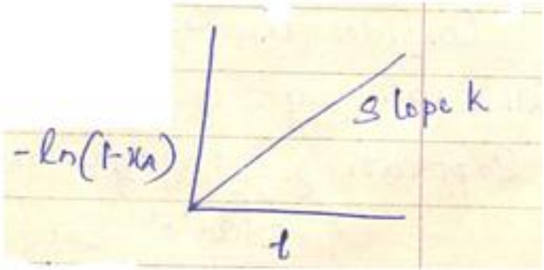
<table>
<tr><td></td><td></td><td>of pharmaceuticals, dyes, dye intermediates etc</td><td></td></tr>
<tr><td>2</td><td></td><td>Attempt any THREE of the following</td><td>12</td></tr>
<tr><td>2</td><td>a</td><td>Difference between order and molecularity of reaction.(4 points)
<table>
<tr><th>Sr.No.</th><th>Molecularity</th><th>Order of reaction</th></tr>
<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 equation.</td></tr>
<tr><td>2</td><td>Molecularity always have an integer value 1,2,3…</td><td>Order of reaction can have a fractional value.</td></tr>
<tr><td>3</td><td>Shows the elementary mechanism or separate steps of a complicated process</td><td>Shows the kinetic dependence of the rate on the concentration of the reactants.</td></tr>
<tr><td>4</td><td>Depending upon the value of molecularity, reaction can be unimolecular ,bimolecular etc.</td><td>Depending upon the value of order, the reactions are termed as first order, second order reactions</td></tr>
<tr><td>5</td><td>Molecularity is a theoretical quantity</td><td>Order of reaction is entirely an experimental value.</td></tr>
</table></td><td>1 mark each</td></tr>
<tr><td>2</td><td>b</td><td>For first order reaction, $- \ln(1-x_A) = kt$</td><td></td></tr>
</table>

		When x_A =0.5 and t = 5 minutes - ln(1-0.5) = k *5 **K = 0.1386 minutes^{-1}** When x_A =0.75 - ln(1-0.75) = 0.1386 *t **t = 10 minutes**	 2 2
2	c	**Space time:** It is the time required to process one reactor volume of feed measured at specified condition. **Mathematical expression:** $\tau = \frac{1}{s} = \frac{C_{A0\,V}}{F_{A0}}$ **Unit** Unit is unit of time (seconds, minute, etc) **Space velocity** It is the number of reactor volume of feed at specified conditions which can be treated in unit time. **Mathematical expression:** **S = $\frac{1}{\tau} = \frac{F_{A0}}{C_{A0\,V}}$** **Unit** Unit is $time^{-1}$ ($second^{-1}$, $minute^{-1}$ etc)	1 ½ ½ 1 ½ ½
2	d	**Comparison of MFR and PFR (8 points)** 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.	½ mark each

		2) For low values of conversion, reactor size is only slightly affected by type of flow. As conversion approaches zero, volume / size ratio of 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 $\tau_m . C_{A0}^{n-1} = \left(\frac{C_{A0}V}{F_{A0}}\right)_m = \frac{X_A(1+\varepsilon_A . X_A)^n}{k(1-X_A)^n}$ For PFR $\tau_p . C_{A0}^{n-1} = \left(\frac{C_{A0..}^{n} . V}{F_{A0}}\right)_p = \frac{1}{K}\int_0^{XA} \frac{(1+ \varepsilon AXA)^n}{(1-X_A)^n} . dX_A$ **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.	
3		**Attempt any THREE of the following**	**12**
3	a	**Important properties of catalyst** 1. Porosity: Porosity is defined as the ratio of volume of voids to the total volume of catalyst. A catalyst should be highly porous. 2. Large surface area: It should have a large surface area per unit mass. 3. Selectivity: Selectivity or specificity of a catalyst refers to the property	1 mark each for any four points

		of catalyst to speed up the main reaction in the presence of several side reactions. A catalyst should have high selectivity 4. Activity: Activity is a measure of the accelerating effect that the catalyst has on the rate of given reaction. Activity of catalyst is measured by finding the ratio between the rate constant of a catalysed and uncatalysed reaction. A catalyst should have high activity. 5. Kindling point : Kindling point of a substance is the lowest temperature at which it spontaneously ignites in normal atmosphere without an external source of ignition, such as a flame or spark. A catalyst should have a low kindly point because then only less energy has to be spend to preheat the reaction mixture. 6. Accessibility: The catalyst should be highly accessible. 7. Life and regenerability : A good catalyst should have a long life and it should be regenerable. 8. Thermal / mechanical strength: A catalyst should have adequate thermal / mechanical strength in reaction conditions. 9. Toxicity and cost: A catalyst should be non -toxic and cheap.	
3	b	CA0'=0.1 mol/l $t_{1/2}' = 1152$ min CA0'' = 0.2 mol/l $t_{1/2}'' = 568$ min $t_{1/2} = \frac{C_{A0}^{1-n}}{k(n-1)}[(2^{n-1})-1]$ $(t_{1/2}' / t_{1/2}'') = (C_{A0}' / C_{A0}'')^{1-n}$ Taking log and rearranging $n = 1-(\log(t_{1/2}'/t_{1/2}'') / \log(C_{A0}'/C_{A0}''))$ n = 1-(log (1152/568)/(log (0.1/0.2)) n= 1 +1.02 = 2.02	2

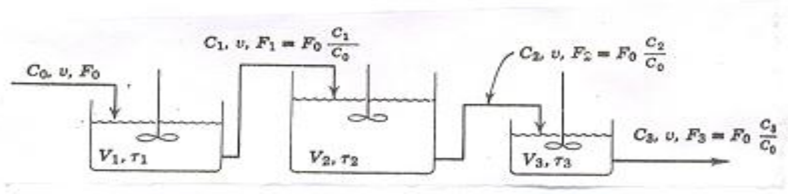
		Order of the reaction is 2	2
3	c	**Integrated rate expression for irreversible unimolecular first order reaction:** Consider the reaction A →B The rate equation is $-r_A = -dC_A / dt = kC_A$….(1) **In terms of concentration** Rearranging $-\frac{dC_A}{C_A} = k\,dt$ Integrating between appropriate limits $-\int_{C_{AO}}^{C_A} \frac{dC_A}{C_A} = k\int_0^t dt$ $-(\ln C_A / C_{A0}) = kt$  **In terms of conversion** $C_A = C_{A0}(1-x_A)$ $dC_A = -C_{A0}dx_A$ Substituting in (1) and rearranging and integrating $\int_{x_{A0}}^{x_A} (dx_A / (1-x_A) = k \int_0^t dt$ $-\ln(1-x_A) = kt$	2 2



3 d

Procedure to find conversion when MFR's of different sizes are connected in series:

Consider three MFR's in series with volume, feed rates, concentrations, space times and volumetric flow rates as shown in the figure. Graphical procedure is utilized for finding the outlet composition.

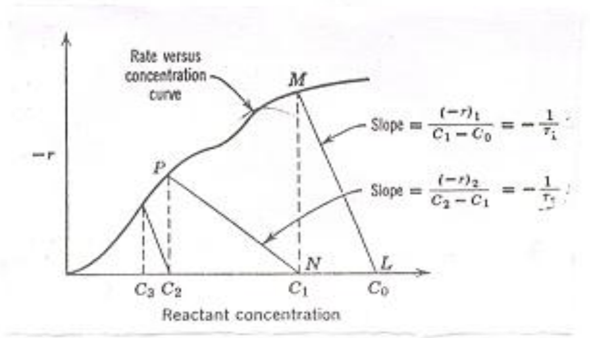


For the 1st MFR, $\tau_1 = \frac{C_0 - C_1}{(-r_1)}$

$\frac{-1}{\tau_1} = \frac{-r_1}{C_1 - C_0}$ 1

Similarly for ith reactor, $\frac{-1}{\tau_i} = \frac{-r_i}{C_i - C_{i-1}}$

Plot concentration versus rate curve for component A and suppose it is as shown in the figure.



3

Inlet concentration C_o is known (point L). To find C_1, draw a line through C_o having slope $\left(\frac{-1}{\tau_1}\right)$ until it cuts the rate curve (point M). From that point draw a perpendicular to x axis. The point where it touches the x axis is C_1 (point N). To find C_2, draw a line through C_1 having slope $\left(\frac{-1}{\tau_2}\right)$ until it touches the rate curve (point P). Perpendicular drawn from that point gives C_2. Repeat same the procedure to find C_3. Knowing Concentration, conversion can be calculated using the relation $C_A = C_{A0}(1 - X_A)$ for constant volume system.

4 **Attempt any THREE of the following** **12**

4 a **Given:**

$X_A = 0.70$, $t = 13$ min

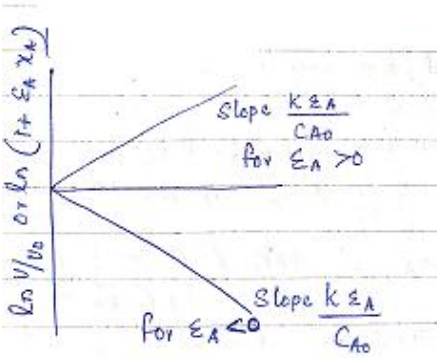
For constant volume batch reactor,

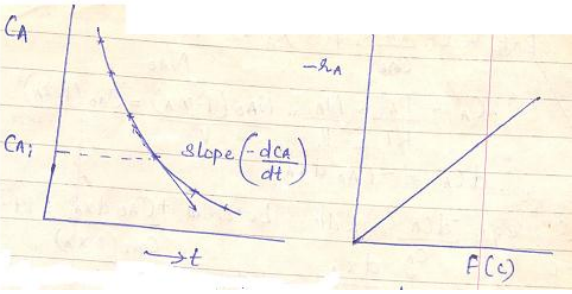
$$t = CAO \int_0^{X_A} \frac{dX_A}{-r_A}$$

First order chemical reaction is taking place

$-r_A = k.C_A = k.C_{A0}(1 - X_A)$

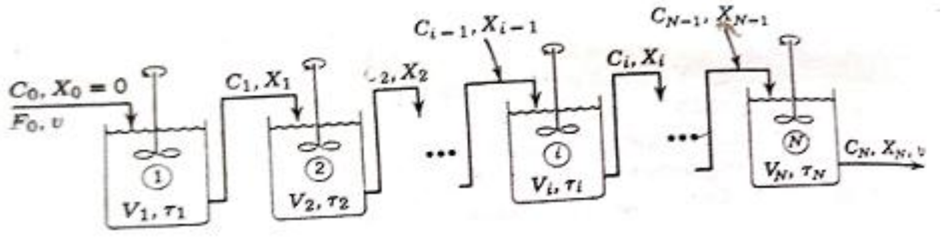
		$$t = CAO\int_0^{X_A}\frac{dX_A}{\mathrm{k.CA0\,(1-XA)}}$$ $-\ln(1 - X_A) = kt$ $-\ln(1-0.70) = k * 13$ k **= 0.0926 min^{-1}** **For Plug flow reactor** (constant –density system): $$\frac{V}{F_{A0}} = \int_0^{X_A}\frac{dX_A}{-r_A} = \frac{\tau}{C_{A0}}$$ $$\tau = C_{A0}\int_0^{X_A}\frac{dX_A}{k.C_{A0}.(1-X_A)}$$ $$\tau = \int_0^{X_A}\frac{dX_A}{k.(1-X_A)}$$ Space time $\tau = \frac{1}{k}(-\ln(1-X_A)) = \frac{1}{0.0926}(-\ln(1-0.7)) =$ $\mathbf{13\ \boldsymbol{min}}$. 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 $\tau = \frac{0.70}{0.0926(1-0.7)}$ **= 25.2 min.** Space velocity = s = 1/ τ = 1/25.2 = **0.03968 min^{-1}**	1 1.5 1.5
4	b	**Integrated form of rate expression for variable volume zero order reaction** Rate equation is $-r_A = -\frac{1}{v}\frac{dN_A}{dt} = \frac{C_{AO}}{1+\varepsilon_A X_A}\frac{dX_A}{dt} = k$ $$\frac{C_{AO}}{1+\varepsilon_A X_A}\frac{dX_A}{dt} = k$$ Rearranging and integrating	

		$C_{AO}\int_0^{x_A}\frac{dX_A}{1+\varepsilon_A X_A}$ = kt $\frac{C_{AO}}{\varepsilon_A}$ ln $(1+\varepsilon_A X_A)$ = kt = $\frac{C_{AO}}{\varepsilon_A}$ ln$\frac{V}{V_0}$ 	2 2
4	c	**Stepwise procedure for differential method of analysis of kinetic 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($\frac{-dC_A}{dt}$) 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 origin; the rate equation is consistent with the data. If not, then another rate equation should be tested.	4



4 d **Expression to represent conversion as a function of number of equal size CSTR's series**

Consider N equal size MFR in series



For constant volume MFR , $\tau = \frac{C_0 - C}{(-r)}$

For 1st MFR, , $\tau_1 = \frac{C_0 - C_1}{(-r_1)}$ But $-r_1 = kC_1$

$$\tau_1 = \frac{C_0 - C_1}{(kC_1)}$$

$$\tau_1 * kC_1 = C_0 - C_1$$

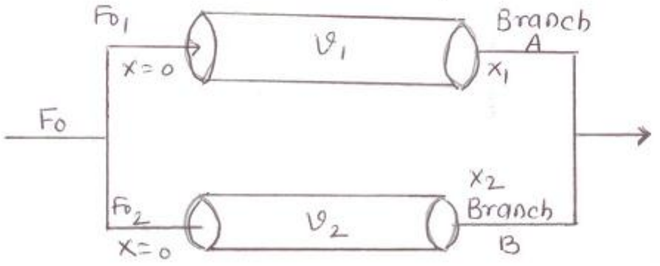
$$C_0 = \tau_1 * kC_1 + C_1 = C_1 (1 + k\tau_1)$$

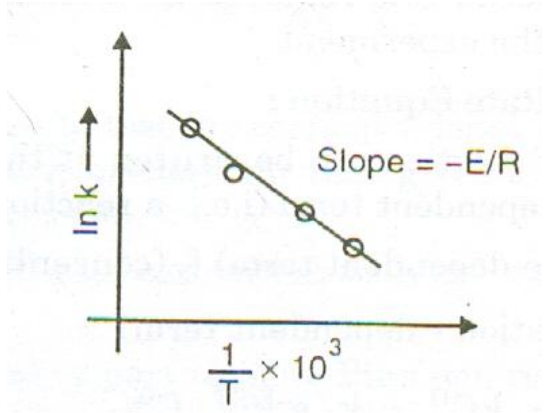
$$\frac{C_1}{C_0} = \frac{1}{(1 + k\tau_1)}$$

$$C_1 = \frac{C_0}{1 + k\tau_1} \ldots\ldots\ldots(1)$$

2

		For 2nd MFR , $\frac{C_2}{C_1} = \frac{1}{(1+k\tau_2)}$ $C_2 = \frac{C_1}{1+k\tau_2}$……..(2) Substituting C_1 from equation (1) into equation (2) $C_2 = \frac{C_0}{1+k\tau_1} * \frac{1}{(1+k\tau_2)}$ …….(3) Since all the MFR's are of equal size, $\tau_1 = \tau_2 = \tau_i = \tau_N = \tau$ Therefore equation (3) becomes $C_2 = \frac{C_0}{1+k\tau} * \frac{1}{(1+k\tau)} = \frac{C_0}{(1+k\tau)^2}$ $\frac{C_2}{C_0} = \frac{1}{(1+k\tau)^2}$ For Nth reactor $\frac{C_N}{C_0} = \frac{1}{(1+k\tau)^N}$ ……..(4) $C_N = C_0 (1 - X_{AN})$ $\frac{C_N}{C_0} = 1 - X_{AN}$ ……..(5) Substituting (5) in (4) $1 - X_{AN} = \frac{1}{(1+k\tau)^N}$ $\mathbf{X_{AN} = 1 - \frac{1}{(1+k\tau)^N}}$	2
4	e	**Method of feeding when PFR's are connected in parallel** Consider PFRs are connected as shown in the figure.	

		 For the PFRs 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 method of feeding is inefficient. Ie $\left(\frac{V}{F}\right)$ for branch A = $\left(\frac{V}{F}\right)$ for branch B $\left(\frac{F_{01}}{F_{02}}\right) = \left(\frac{V_1}{V_2}\right)$ For example: If V_1 = 80 lit & V_2 = 40 lit $\left(\frac{F_{01}}{F_{02}}\right) = \left(\frac{V_1}{V_2}\right) = \frac{80}{40} = 2$ $F_{o1} = 2F_{o2}$ Total feed $F = F_{o1} + F_{o2} = 2F_{o2} + F_{o2} = 3F_{o2}$ Fraction of feed fed to branch A = $F_{o1} / F = 2F_{o2} / 3F_{o2} = 2/3$ Fraction of feed fed to branch B = $F_{o2} / F = F_{o2} / 3F_{o2} = 1/3$	2 2
5		**Attempt any TWO of the following**	12
5	a	**Arrhenius law** The temperature dependency of the reaction rate constant k, is given by $k = k_0 e^{\frac{-E}{RT}}$	

		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 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 $\frac{-E}{R}$.  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 $\ln\frac{k_2}{k_1} = \frac{-E}{R} \left(\frac{1}{T_2} - \frac{1}{T_1}\right)$ 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 2 2
5	b	**Promoters** They are substances which do not act as catalyst but enhances the efficiency and life of the catalyst. It is a substance added during the preparation of a	1

<table>
<tr><td></td><td></td><td>catalyst which improves the activity or selectivity or stabilizes the catalytic agent so as to increase its life.
Eg Al_2O_3 is used as a promoter to iron catalyst in the manufacture of ammonia</td><td>1</td></tr>
<tr><td></td><td></td><td>Inhibitors
It is the substance which decreases the performance of the catalyst. It lessens activity, stability or selectivity of a catalyst. It is useful for reducing the activity of a catalyst for an undesirable side reaction.</td><td>1</td></tr>
<tr><td></td><td></td><td>Eg silver supported on alumina is an excellent oxidation catalyst and is used in the production of ethylene oxide from ethylene. But at the same conditions, complete oxidation to CO_2 and H_2O also occurs. So selectivity is poor. By adding halogen compounds to the catalyst inhibits the oxidation to CO_2 and H_2O and results in satisfactory selectivity.</td><td>1</td></tr>
<tr><td></td><td></td><td>Accelerators
They are substances added to the reactant streams to improve the performance of a catalyst.</td><td>1</td></tr>
<tr><td></td><td></td><td>Eg steam added to butane feed of a dehydrogenation reactor reduces the amount of coke formed and increases the yield of butadiene.</td><td>1</td></tr>
<tr><td>5</td><td>c</td><td>$C_{A0} = 0.1$ mol / l
Assume the reaction is of zero order
For zero order reaction $C_{A0} - C_A = kt$ $k = (C_{A0} - C_A) / t$
When t-= 10 minutes
$k = (C_{A0} - C_A) / t = (0.1-0.0714) / 10 = 2.86*10^{-3}$mol / (l. minute)
<table>
<tr><th>Time, min</th><th>Concentration, mol/l</th><th>k, mol / (l. minute)</th></tr>
<tr><td>0</td><td>0.1</td><td>---</td></tr>
<tr><td>10</td><td>0.0714</td><td>$2.86*10^{-3}$</td></tr>
</table></td><td></td></tr>
</table>

20	0.0556	$2.22*10^{-3}$
40	0.0385	$1.5375*10^{-3}$
100	0.02	$8*10^{-4}$
125	0.0167	$6.664*10^{-4}$

2

Since k values are not same, reaction is not of zero order

Assume reaction is of first order

For first order reaction $-\ln(C_A / C_{A0}) = kt$

$k = -\ln(C_A / C_{A0}) / t$

At $C_{A0} = 0.1$ and $C_A = 0.0714\ at\ t = 10\ min.$

$$k = \frac{1}{10}\ ln \frac{0.1}{0.0714} = 0.0343\ \text{min}^{-1}$$

Time, min	Concentration, mol/l	k, min^{-1}
0	0.1	--
10	0.0714	0.0343
20	0.0556	0.0342
40	0.0385	0.0239
100	0.02	0.0161
125	0.0167	0.0143

2

Since k values are not same, reaction is not of first order

Assume reaction is of second order
For second order reaction:

$$k = \frac{1}{t}\left[\frac{1}{C_A} - \frac{1}{C_{A0}}\right]$$

For $C_A = 0.0556\ at\ t = 20\ min$
$$k = \frac{1}{20}\left[\frac{1}{0.0556} - \frac{1}{0.1}\right] = 0.399(l/mol)\ min^{-1}$$

Time, min	Concentration, mol/l	k, $(l/mol)\ min^{-1}$

0	0.1	--
10	0.0714	0.4
20	0.0556	0.399
40	0.0385	0.399
100	0.02	0.4
125	0.0167	0.399

2

Since the k values are same , reaction is of second order

Order of reaction is **2**

Value of rate constant(average) = $\mathbf{0.4 (l/mol)\ min^{-1}}$

6 **Attempt any TWO of the following** 12

6 a **Performance equation of batch reactor for constant volume and variable volume system:**

In batch reactor, the composition is uniform throughout reaction zone at any instant of time.

Writing the material balance for any component A.

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.

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

Material balance equation then becomes

Rate of loss of reactant A due to chemical reaction = - Rate of accumulation of reactant A within the reactor-------(1)

Rate of loss of reactant A due to chemical reaction = $-r_A V$

Rate of accumulation of reactant A within the reactor = $\frac{dN_A}{dt} = -N_{A0}\frac{dX_A}{dt}$

2

		Substituting in equation (1) $-r_AV = N_{A0}\frac{dX_A}{dt}$ Rearranging and integrating $\int_0^t dt = N_{A0}\int_0^{x_A}\frac{dx_A}{V\,(-r_A)}$ $t = N_{A0}\int_0^{x_A}\frac{dx_A}{V\,(-r_A)}$ ....(2)	2
		This 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. **For constant volume system**, the equation (2) becomes $t = \frac{N_{A0}}{V}\int_0^{x_A}\frac{dx_A}{(-r_A)} = C_{A0}\int_0^{x_A}\frac{dx_A}{(-r_A)} = -\int_{CA0}^{C_A}\frac{dC_A}{(-r_A)}$ ....(3)	1
		For variable volume reaction systems $V = V_0(1+\varepsilon_A X_A)$ Eq.2 becomes $t = N_{A0}\int_0^{X_A}\frac{dX_A}{(-r_A).V_0(1+\varepsilon_A X_A)}$ As $C_{A0} = \frac{N_{A0}}{V_0}$ $t = C_{A0}\int_0^{X_A}\frac{dX_A}{(-r_A)(1+\varepsilon_A X_A)}$ .....(4)	1
6	b	Reaction: A →3 R $-r_A = 10^{-1}C_A$ k =$10^{-1}s^{-1}$ = $0.1s^{-1}$ Let 1 mol of A be present initially. Along with 1mole of A,I mole of inert is also present (Reaction mixture contains 50 % A and 50% inerts)	

		Moles of R formed =3 Moles present initially = of A + moles of inerts = 1+1 = 2moles Moles present finally = moles of R + moles of inerts = 3 + 1 =4 moles $\epsilon_A = \frac{V_{XA=1}-V_{XA=0}}{V_{XA=0}} = \frac{4-2}{2} = 1$ $For\ PFR \quad \frac{V}{F_{A0}} = \int_0^{X_A}\frac{dX_A}{-r_A} = \frac{\tau}{C_{A0}}$ From the unit of rate constant, the reaction is of first order $-r_A = \frac{KC_{A0}(1-x_A)}{(1+\varepsilon_A X_A)}$ for variable volume system $\int_0^{X_A}\frac{dX_A}{-r_A} = \frac{\tau}{C_{A0}}$ $\frac{\tau}{C_{A0}} = \int_0^{X_A}\frac{(1+\varepsilon_A X_A)dX_A}{kc_{A0}(1-X_A)}$ $\frac{\tau}{C_{A0}} = \frac{1}{kc_{A0}}\int_0^{X_A}\frac{(1+\varepsilon_A X_A)dX_A}{(1-X_A)}$ $\frac{\tau}{C_{A0}} = \frac{1}{KC_{A0}}(-\ln(1-X_A) + \varepsilon_A\{-\ln(1-X_A)-X_A\}$ $= \frac{1}{KC_{A0}}\{-\ln(1-X_A) - \varepsilon_A \ln(1-X_A) - \varepsilon_A X_A\}$ $= \frac{1}{KC_{A0}}(-\ln(1-X_A)(1+\varepsilon_A) - \varepsilon_A X_A)$ $\tau = (-\ln(1-X_A)(1+\varepsilon_A) - \varepsilon_A X_A) / k$ $= (-\ln(1-0.8)(1+1) - (1*0.8)) / 0.1 = 24.19$ s **Space time τ= 24.19 s**	1 1 1 2 1
6	c	Design equation of a MFR is	

$$\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \frac{X_A}{(-r_A)}$$

Where $X_A = 0.5$;

$-r_A = \text{k}\, C_A^2$

For constant volume reaction system

$$\frac{V}{F_{A0}} = \frac{X_A}{(-r_A)}$$

$$\frac{V}{F_{A0}} = \frac{0.5}{(\text{k}\, C_A^2)}$$

As $C_A = C_{A0}(1 - X_A)$,above equation can be written as

$$\frac{V}{F_{A0}} = \frac{0.5}{(\text{k}.\, C_{A0}^2(1 - X_A)^2\,)}$$

$$\frac{V}{F_{A0}} = \frac{0.5}{(\text{k}.\, C_{A0}^2(1 - 0.5)^2\,)}$$

$$\frac{V.\,\text{k}.\, C_{A0}^2}{F_{A0}} = \frac{0.5}{((1 - 0.5)^2\,)}$$

3

$$\frac{V.\,\text{k}.\, C_{A0}^2}{F_{A0}} = 2$$

For a plug flow reactor of same size ,design equation is

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

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

$$\frac{V}{F_{A0}} = \int_0^{X_A} \frac{dX_A}{\text{k}.\, C_{A0}^2(1 - X_A)^2}$$

$$\frac{V}{F_{A0}} = \frac{1}{\mathrm{k}.C_{A0}^2}\int_0^{X_A} \frac{dX_A}{(1-X_A)^2}$$

$$\frac{V.\mathrm{k}.C_{A0}^2}{F_{A0}} = \int_0^{X_A} \frac{dX_A}{(1-X_A)^2}$$

But $\frac{V.\mathrm{k}.C_{A0}^2}{F_{A0}} = 2$

Therefore $2 = \int_0^{X_A} \frac{dX_A}{(1-X_A)^2}$

For second order reaction the integrated rate equation in terms of conversion is

$$\int_0^{X_A} \frac{dX_A}{(1-X_A)^2} = \frac{X_A}{1-X_A}$$

Therefore $\frac{X_A}{1-X_A} = 2$

$$2(1-X_A) = X_A$$

$$2 - 2X_A = X_A$$

$$2 = 3X_A$$

$$X_A = \frac{2}{3} = 0.667$$

3

Conversion in PFR is 0.667 =66.7%