



**WINTER-19 EXAMINATION**  
**Model Answer**

Subject title: Chemical Reaction Engineering

Subject code

17562

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**Important Instructions to examiners:**

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



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Q No.	Answer	Marking scheme																					
<b>1 a</b>	<b>Attempt any THREE of the following</b>	<b>12</b>																					
1a	<b>i</b> <b>Difference between elementary and non-elementary reaction ( 4 points):</b>	1 mark each																					
	<table border="1"><thead><tr><th>Sr no.</th><th>Elementary reactions</th><th>Non-elementary reactions</th></tr></thead><tbody><tr><td>1</td><td>These are single steps reactions.</td><td>These are multistep reactions.</td></tr><tr><td>2</td><td>Simple in nature</td><td>Complex in nature</td></tr><tr><td>3</td><td>Order of each reactant is identical with stoichiometric coefficient of that species..</td><td>Not identical.</td></tr><tr><td>4</td><td>For these reactions, order must be an integer</td><td>Order may be an integer or fractional value.</td></tr><tr><td>5</td><td>If <math>2A \rightarrow R</math>, the rate law is <math display="block">-r_A = kC_A^2</math></td><td>For non-elementary reaction <math>2B \rightarrow S</math>, the rate law may be <math display="block">-r_B = kC_B^\alpha</math> Where <math>\alpha \neq 2</math></td></tr><tr><td>6</td><td>Ex <math>C_2H_5OH + CH_3COOH \rightarrow</math> <math>CH_3COOC_2H_5 + H_2O</math></td><td>Ex. <math>H_2 + Br_2 \rightarrow 2HBr</math></td></tr></tbody></table>	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 integer	Order may be an integer or fractional value.	5	If $2A \rightarrow R$ , the rate law is $-r_A = kC_A^2$	For non-elementary reaction $2B \rightarrow S$ , the rate law may be $-r_B = kC_B^\alpha$ Where $\alpha \neq 2$	6	Ex $C_2H_5OH + CH_3COOH \rightarrow$ $CH_3COOC_2H_5 + H_2O$	Ex. $H_2 + Br_2 \rightarrow 2HBr$	
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1a	ii	<p><b>Enthalpy:</b> Enthalpy is the total heat content of a body.</p> <p><b>Mathematical equation:</b> <math>H = U + PV</math></p> <p><b>Gibb's free energy:</b> It is the energy actually available to do useful work. It predicts the feasibility and equilibrium conditions for chemical reactions at constant temperature and pressure.</p> <p><b>Mathematical equation:</b> <math>G = H - TS</math></p>	1  1  1  1
1a	iii	<p><b>Half-life :</b> Half-life period is the time required to reduce the concentration of the reactant to half of its original value.</p> <p><math>t_{1/2} = 240</math> seconds</p> <p>For the first order reaction: <math>t_{1/2} = 0.693 / k</math></p> <p><math>k = 0.693 / t_{1/2} = 0.693 / 240</math></p> <p>Rate constant <math>k = 2.89 * 10^{-3} s^{-1}</math></p>	2     2
1a	iv	<p><b>Fluidized bed reactor with catalyst regenerator:</b></p>	4











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

Rearranging, we get

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

For constant volume system

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

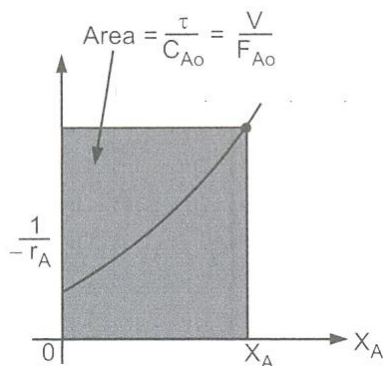
Where  $X_A$  and  $(-r_A)$  are evaluated at the exit conditions, which are same as conditions prevailing within reactor (ex .composition, temperature)

**For first order reaction**

$$-r_A = kC_A = kC_{A0}(1 - X_A)$$

$$\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \frac{X_A}{kC_{A0}(1 - X_A)} = \frac{C_{A0} - C_A}{C_{A0}(kC_A)}$$

The graphical representation of the performance equation in terms of fractional conversion is as below



The graphical representation of the performance equation in terms of concentration for constant density system is as below.

1

2











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3	e	<p><b>Comparison between fluidized bed and packed(fixed) bed reactor (any four):</b></p> <table border="1" data-bbox="383 590 1219 1478"> <thead> <tr> <th></th> <th>Fluidized bed</th> <th>Fixed bed</th> </tr> </thead> <tbody> <tr> <td>(i) Recovery units</td> <td>Catalyst loss is there, so recovery units are required</td> <td>Catalyst loss is not there, so recovery units are not required</td> </tr> <tr> <td>(ii) Catalyst regeneration</td> <td>Easily done</td> <td>Difficult</td> </tr> <tr> <td>(iii) isothermal condition:</td> <td>Can maintain isothermal conditions</td> <td>Difficult to maintain</td> </tr> <tr> <td>(iv) size of catalyst</td> <td>Can use small size of catalyst</td> <td>Cannot use very small size of catalyst because of plugging and high pressure drop</td> </tr> <tr> <td>(v) Type of flow</td> <td>Flow is complex</td> <td>Plug flow</td> </tr> </tbody> </table>		Fluidized bed	Fixed bed	(i) Recovery units	Catalyst loss is there, so recovery units are required	Catalyst loss is not there, so recovery units are not required	(ii) Catalyst regeneration	Easily done	Difficult	(iii) isothermal condition:	Can maintain isothermal conditions	Difficult to maintain	(iv) size of catalyst	Can use small size of catalyst	Cannot use very small size of catalyst because of plugging and high pressure drop	(v) Type of flow	Flow is complex	Plug flow	1 mark each
	Fluidized bed	Fixed bed																			
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4 a		<b>Attempt any THREE of the following</b>	<b>12</b>																		
4a	i	<p>Second order reaction of the form <math>A + B \rightarrow \text{product}</math>            Since <math>C_{A0} = C_{B0} = 0.03 \text{ mol/l}</math>, the reaction reduces to the form  <math>2A \rightarrow \text{Product}</math>            For second order reaction of the form <math>2A \rightarrow \text{Product}</math> :</p> $k = \frac{1}{t} \left[ \frac{1}{C_A} - \frac{1}{C_{A0}} \right]$ <p><math>k = 6.5 \text{ l / (mol minute)}</math></p>	2																		



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		$t = 10 \text{ min}$ $6.5 = \frac{1}{10} \left[ \frac{1}{C_A} - \frac{1}{0.03} \right]$ $C_A = 0.01017 \text{ mol / l}$ $\text{Proportion of ester hydrolyzed} = \frac{C_{AO} - C_A}{C_{AO}} = \frac{0.03 - 0.01017}{0.03} = 0.661 = \mathbf{66.1\%}$	2
4a	ii	<p><b>Desired properties of catalyst ( any four)</b></p> <ol style="list-style-type: none"><li>1. Porosity</li><li>2. Large surface area</li><li>3. High selectivity</li><li>4. High activity</li><li>5. Low kindling point</li><li>6. High accessibility</li><li>7. Long life and regenerability</li><li>8. Adequate thermal / mechanical strength in reaction conditions</li><li>9. Non toxic and cheap</li></ol> <p><b>Definition (any two)</b></p> <p><b>Activity</b> 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.</p> <p><b>Selectivity or specificity</b> of a catalyst refers to the property of catalyst to speed up the main reaction in the presence of several side reactions.</p> <p><b>Porosity</b> is defined as the ratio of volume of voids to the total volume of catalyst.</p> <p><b>Kindling point</b> 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.</p>	<p>½ mark each</p> <p>1 mark each</p>



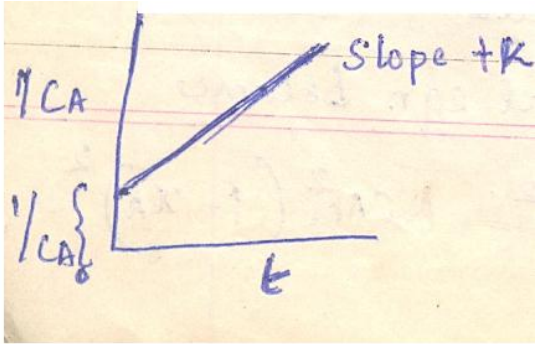
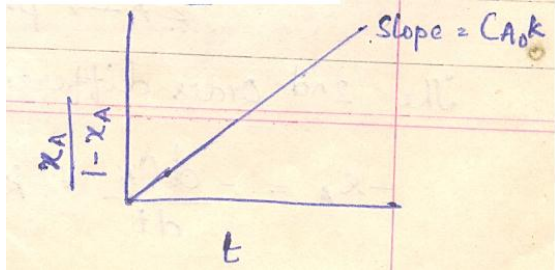
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4a	iii	<p><b>Graphical representation of integrated rate equation for second order reaction <math>2A \rightarrow \text{Product}</math>:</b></p> <p><b>In terms of concentration:</b></p>  <p><b>In terms of conversion:</b></p> 	2
4a	iv	<p><b>Feasibility of a chemical reaction from Gibbs free energy change:</b></p> <p>At chemical equilibrium <math>\Delta G^0 = 0</math>. For a chemical reaction at equilibrium at a given temperature &amp; pressure, the free energy must be minimum.</p> <p>If <math>\Delta G^0 &lt; 0</math> i.e. it is negative, the reaction can take place spontaneously (reaction is possible under the given set of conditions). For spontaneous reaction, there should be decrease in Gibb's free energy change.</p> <p>If <math>\Delta G^0</math> is positive, the reaction cannot take place under the given conditions.</p>	4
<b>4b</b>		<b>Attempt any ONE of the following</b>	<b>06</b>
4b	i	From Arrhenius law, $k = k_0 e^{-E/RT}$	



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		<p><math>E_1 = 17982 \text{ cal / mol}</math>                      <math>E_2 = 11980 \text{ cal / mol}</math></p> <p><math>T = 25^\circ\text{C} = 298\text{K}</math></p> <p>For Un catalyzed reaction, <math>k_1 = k_0 e^{-E_1 / RT}</math> and</p> <p>For catalyzed reaction <math>k_2 = k_0 e^{-E_2 / RT}</math></p> <p><math>\ln k_1 = \ln k_0 - \frac{E_1}{RT} \dots\dots(1)</math></p> <p><math>\ln k_2 = \ln k_0 - \frac{E_2}{RT} \dots\dots(2)</math></p> <p>(2) - (1) gives <math>\ln \frac{k_2}{k_1} = \frac{E_1 - E_2}{RT} = \frac{17982 - 11980}{1.987 * 298} = 10.136</math></p> <p><math>\frac{k_2}{k_1} = 25,244</math></p> <p><math>k_2 = 25,244 k_1</math></p> <p><b>ie Catalyzed reaction is 25,244 times faster than un catalyzed reaction</b></p>	<p>2</p> <p>2</p> <p>2</p>
4b	ii	<p><b>Relation between <math>K_p</math>, <math>K_y</math> and <math>K_c</math></b></p> <p>Consider the reaction <math>aA + bB + \dots \rightarrow rR + sS \dots\dots</math></p> <p><math>K_c = (C_R^r \cdot C_S^s) / (C_A^a \cdot C_B^b)</math></p> <p>For ideal gas <math>C_i = p_i / RT</math></p> <p>Therefore <math>K_c = \{ (p_R / RT)^r \cdot (p_S / RT)^s \} / \{ (p_A / RT)^a \cdot (p_B / RT)^b \}</math></p> <p><math>= (p_R^r \cdot p_S^s) / (p_A^a \cdot p_B^b) \cdot (1 / RT)^{(r+s+\dots-(a+b+\dots))}</math></p> <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 <math>K_c = K_p \cdot (1 / RT)^{\Delta n}</math> where <math>K_p = (p_R^r \cdot p_S^s) / (p_A^a \cdot p_B^b)</math></p> <p><math>\Delta n = (r + s + \dots - (a + b + \dots))</math> is the difference in the number of moles of product and reactant</p> <p><b>Or <math>K_p = K_c \times (RT)^{\Delta n}</math></b></p> <p><math>K_p = (p_R^r \cdot p_S^s) / (p_A^a \cdot p_B^b)</math></p>	<p>3</p>



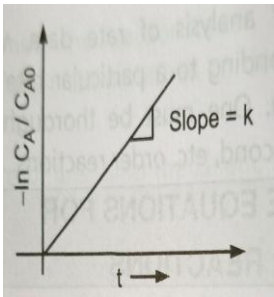
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		<p>But <math>p_A = P \cdot y_A</math> Where <math>p_A</math> - partial pressure of A, <math>P</math> - total pressure <math>y_A</math> - mole fraction of A.</p> $K_p = (p_R^r \cdot p_S^s) / (p_A^a \cdot p_B^b)$ $= \{ (P y_R)^r \cdot (P y_S)^s \} / \{ (P y_A)^a \cdot (P y_B)^b \}$ $= (y_R^r \cdot y_S^s) / (y_A^a \cdot y_B^b) \cdot P^{(r+s+\dots)-(a+b+\dots)}$ <p><math>K_p = K_y \cdot P^{\Delta n}</math> where <math>K_y = (y_R^r \cdot y_S^s) / (y_A^a \cdot y_B^b)</math> and <math>\Delta n = (r + s + \dots) - (a + b + \dots)</math> is the difference in the number of moles of product and reactant</p> $K_c = K_p (1/RT)^{\Delta n} = K_y (P/RT)^{\Delta n}$	3
5		<b>Attempt any TWO of the following</b>	<b>16</b>
5	a	<p><b>Integrated rate expression for constant volume irreversible unimolecular first order reaction (derivation):</b></p> <p>Consider the reaction <math>A \rightarrow B</math></p> <p><b>In terms of concentration</b></p> <p>The rate equation is <math>-r_A = -dC_A / dt = kC_A \dots (1)</math></p> <p>Rearranging - <math>\frac{dC_A}{C_A} = k dt</math></p> <p>Integrating between appropriate limits</p> $-\int_{C_{A0}}^{C_A} \frac{dC_A}{C_A} = k \int_0^t dt$ <p><math>-(\ln C_A / C_{A0}) = kt</math></p> 	2
			2







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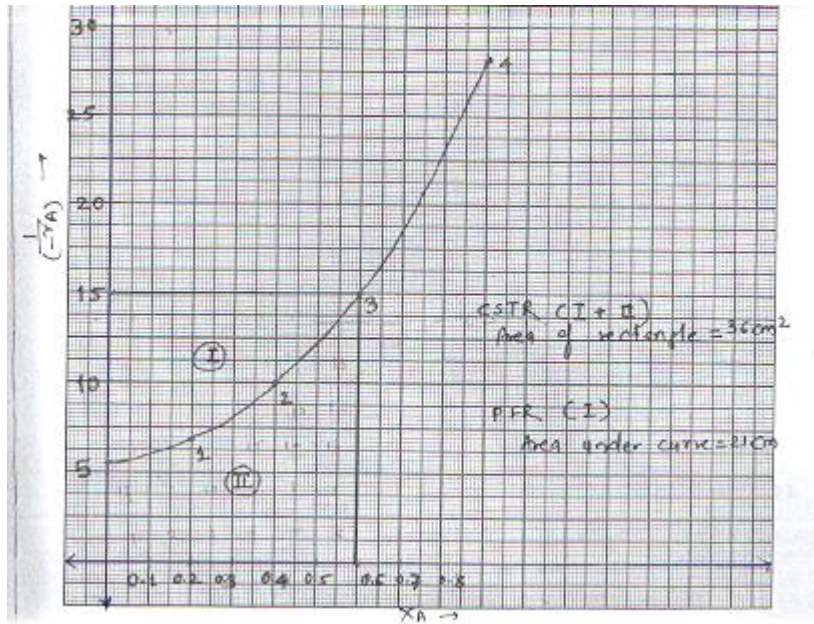
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$$\frac{V}{F_{A0}} = \frac{X_A}{-r_A}$$

For a plug flow reactor

$$\frac{V}{F_{A0}} = \int_0^{X_A} \frac{dX_A}{(-r_A)} = \int_0^{X_A} \frac{1}{(-r_A)} dX_A \text{ where } X_A = 0.6$$

Construct a plot of  $1/(-r_A)$  vs  $X_A$



3

For a mixed flow reactor, refer the graph

$\frac{V}{F_{A0}}$  is the rectangular area upto  $X_A = 0.6$

Area of CSTR =  $36 \text{ cm}^2$

$$\frac{V}{F_{A0}} = \text{Area} \times (\text{Scale on } X\text{-axis}) \times (\text{Scale on } Y\text{-axis})$$

$$\frac{V}{F_{A0}} = 36 \text{ cm}^2 * \frac{5 (\text{l.sec/mol})}{2 \text{ cm}} * \frac{0.1}{1 \text{ cm}}$$



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		$\frac{V}{F_{A0}} = 9 \text{ (l. sec/mol)}$ <p><math>V = 9 * F_{A0} = 9 * 10 = 90 \text{ lit.}</math> <b>Volume of CSTR = 90 lit.</b></p> <p>For a plug flow reactor <math>\frac{V}{F_{A0}}</math> is the area under the curve from <math>X_A = 0</math> to <math>X_A = 0.6</math></p> <p>Area under the curve = <math>21.5 \text{ cm}^2</math></p> $\frac{V}{F_{A0}} = \text{Area} \times (\text{Scale on } X - \text{axis}) \times (\text{Scale on } Y - \text{axis})$ $\frac{V}{F_{A0}} = 21.5 \text{ cm}^2 \times \frac{5 \text{ (l. sec/mol)}}{2 \text{ cm}} \times \frac{0.1}{1 \text{ cm}}$ $\frac{V}{F_{A0}} = 5.375$ <p><math>V = 5.375 \times F_{A0} = 5.375 \times 10 = 53.75 \text{ lit}</math> <b>Volume of PFR = 53.75 lit.</b></p> <p>Volume of PFR (53.75 lit.) is less than the volume of CSTR (90 lit.) for the same conversion. (<math>X_A = 0.6</math>)</p>	2
5	c	<b>Design equation of batch reactor</b> <p>In batch reactor, the composition is uniform throughout reaction zone at any instant of time.</p> <p>Taking material balance of a limiting reactant A, over the reactor as a whole</p> <p>Rate of reactant A in = Rate of reactant A out + Rate of loss of reactant A due to chemical reaction + Rate of accumulation of reactant A within the reactor.</p> <p>In a batch reactor, no fluid enters or leaves the reaction mixture during the</p>	2



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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 =  $\frac{dN_A}{dt} = -N_{A0} \frac{dx_A}{dt}$

Substituting in equation ( 1 )

$$-r_A V = N_{A0} \frac{dx_A}{dt}$$

Rearranging and integrating

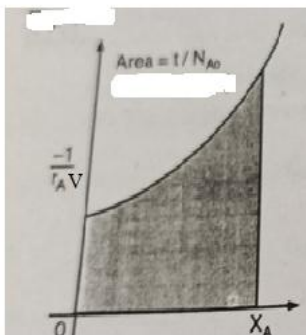
$$\int_0^t dt = N_{A0} \int_0^{x_A} \frac{dx_A}{V(-r_A)}$$

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

For constant volume system, the equation becomes

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

**Graphical representation**



General case

4

2



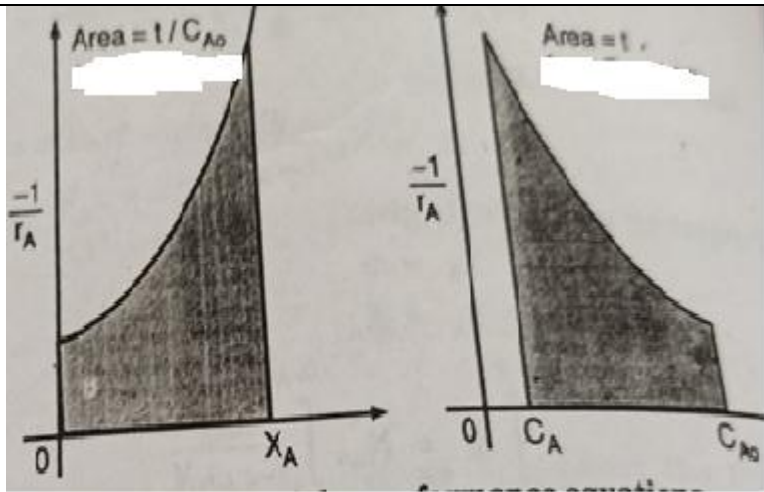
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	 <p style="text-align: center;">For constant volume system</p>	
6	<b>Attempt any FOUR of the following</b>	<b>16</b>
6	<p>a <b>Method of feeding when PFR's are connected in parallel</b></p> <p>Consider PFRs are connected as shown in the figure.</p> <p>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, <math>V/F</math> or <math>\tau</math> must be the same for each parallel line. Any other method of feeding is inefficient.</p> <p>Ie <math>\left(\frac{V}{F}\right)</math> for branch A = <math>\left(\frac{V}{F}\right)</math> for branch B</p> $\left(\frac{F_{01}}{F_{02}}\right) = \left(\frac{V_1}{V_2}\right)$ <p>For example: If <math>V_1 = 80</math> lit &amp; <math>V_2 = 40</math> lit</p>	2



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		$\left(\frac{F_{O_1}}{F_{O_2}}\right) = \left(\frac{V_1}{V_2}\right) = \frac{80}{40} = 2$ $F_{O_1} = 2F_{O_2}$ <p>Total feed <math>F = F_{O_1} + F_{O_2} = 2F_{O_2} + F_{O_2} = 3 F_{O_2}</math></p> <p>Fraction of feed fed to branch A = <math>F_{O_1} / F = 2F_{O_2} / 3 F_{O_2} = 2/3</math></p> <p>Fraction of feed fed to branch B = <math>F_{O_2} / F = F_{O_2} / 3 F_{O_2} = 1/3</math></p>	2
6	b	<p><b>Entropy change of an ideal gas:</b></p> <p>From first law of thermodynamics, <math>dU = dQ - dW</math></p> $dQ = dU + dW \dots\dots(i)$ <p>But <math>dQ = TdS \dots\dots(ii)</math></p> $dW = PdV \dots\dots(iii)$ <p>For ideal gas <math>dU = n C_v dT \dots\dots (iv)</math></p> <p>Substituting ii,iii and iv in i</p> $TdS = n C_v dT + PdV$ $dS = \frac{n C_v dT}{T} + \frac{PdV}{T}$ <p>For ideal gas <math>P = \frac{nRT}{V}</math></p> $\text{Substituting } dS = \frac{n C_v dT}{T} + \frac{nRdV}{V}$ <p>Integrating between limits</p> $\int_{S_1}^{S_2} dS = nC_v \int_{T_1}^{T_2} \frac{dT}{T} + nR \int_{V_1}^{V_2} \frac{dV}{V}$ $\Delta S = nC_v \ln \frac{T_2}{T_1} + nR \ln \frac{V_2}{V_1} \dots\dots(v)$ <p>For ideal gas <math>PV = RT</math></p> $\frac{P_2 V_2}{P_1 V_1} = \frac{T_2}{T_1}$ <p>Therefore <math>\frac{V_2}{V_1} = \frac{T_2 P_1}{T_1 P_2} \dots\dots (vi)</math></p>	2





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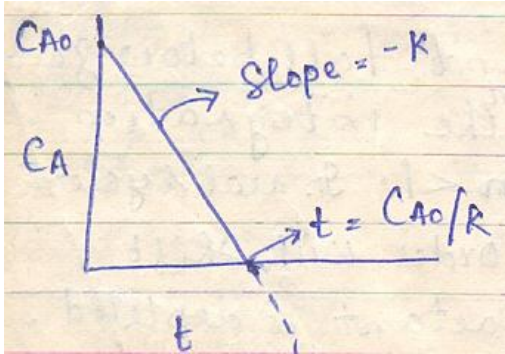
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$$C_{A0} - C_A = kt \text{ for } t < \frac{C_{A0}}{k}$$



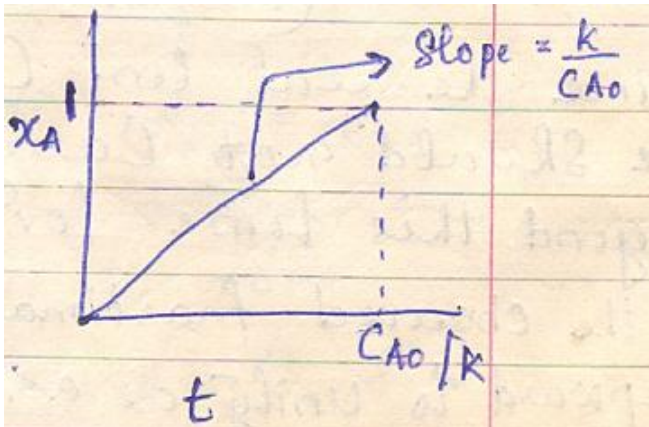
**In terms of fractional conversion**

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

Integrating between appropriate limits

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

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



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**Batch reactor**

**Advantages (2 each):**

1. Simple in construction & operation

1 mark each





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Model Answer

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	<p>2. Low equipment cost</p> <p>3. Gives highest conversion by leaving the reactants for longer periods in reactor.</p> <p>4. Requires small instrumentation &amp; less supporting equipment.</p> <p><b>Disadvantages (2 each):</b></p> <p>1. High labor costs per unit volume of production.</p> <p>2. Requires considerable time to empty, clean out &amp; refill.</p> <p>3. Poorer quality control of product.</p> <p>4. Large scale production is difficult.</p>	<p>1 mark each</p>
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