Polymer Reaction Engineering
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Lecture - 26
Problem Solving - II

Welcome to the next stage of problem-solving session of this polymer reaction engineering. Now, let us start with the problem number 1.

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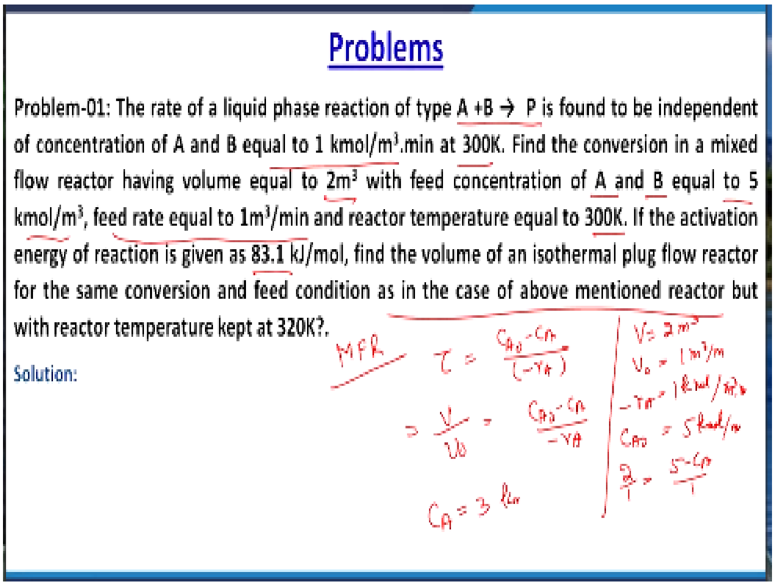

Problems

Problem-01: The rate of a liquid phase reaction of type A +B → P is found to be independent of concentration of A and B equal to 1 kmol/m³.min at 300K. Find the conversion in a mixed flow reactor having volume equal to 2m³ with feed concentration of A and B equal to 5 kmol/m³, feed rate equal to 1m³/min and reactor temperature equal to 300K. If the activation energy of reaction is given as 83.1 kJ/mol, find the volume of an isothermal plug flow reactor for the same conversion and feed condition as in the case of above mentioned reactor but with reactor temperature kept at 320K?.

Solution:

MFR

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

$$= \frac{V}{v_0} = \frac{C_{A0} - C_A}{-r_A}$$

$C_A = 3$ k

$V = 2\ m^3$

$v_0 = 1\ m^3/m$

$-r_A = 1$ kmol/m³.m

$C_{A0} = 5$ kmol/m

$$\frac{2}{1} = \frac{5 - C_A}{1}$$

Here, the rate of liquid phase reaction which is having the type of A + B is equal to P is found to be the independent of concentration of A and B which is equal to 1 kilo mole per metre cube minute at 300 Kelvin. Now, you need to find the conversion in a mixed flow reactor which is having the volume equal to 2 metre cube with the feed concentration of A and B both are equal to 5 kilo moles per metre cube.

And feed rate is equal to 1 metre cube per minute. The reactor temperature is equal to 300 Kelvin and if the activation energy of reaction is given as 83.1 kilojoules per mole. Again, you need to find the volume of an isothermal plug flow reactor for the same conversion and the feed conditions as in the case of above-mentioned reactor, but with the reactor temperature which is maintained at 320 Kelvin.

So, let us try to attempt this particular problem. Now, for mixed flow reactor, the tau is equal to $C_{A0} - C_A$ upon $-r_A$ and which can be represented as V upon V_0 $C_{A0} - C_A$ upon $-r_A$. Now, here the given parameters are V is equal to 2 metre cube, V_0 is equal to 1 metre cube per minute, $-r_A$ is equal to 1 kilo mole per metre cube minute, C_{A0} is equal to 5 kilo mole per metre cube and 2 upon 1 is equal to 5 – C_A upon 1. So, if we write that C_A, what is the value of C_A? That is C_A is equal to 3 kilo mole per metre cube.

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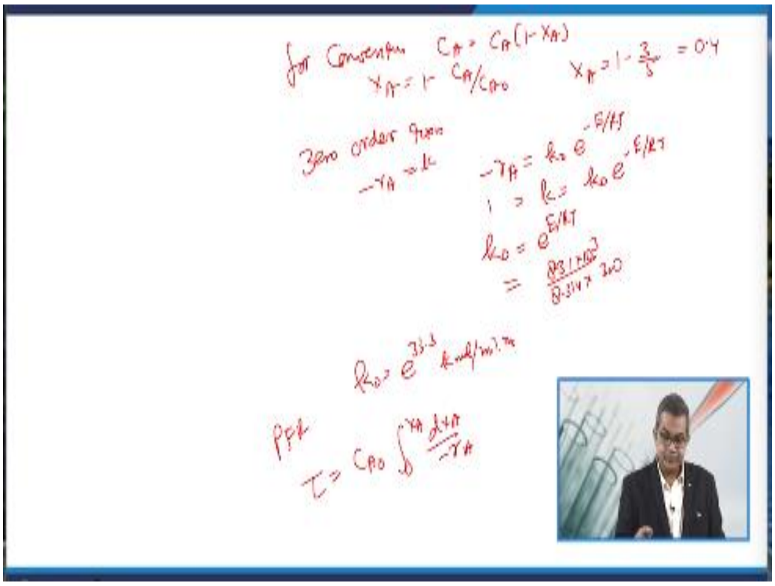

for Conversion $C_A = C_A(1-X_A)$

$X_A = 1 - C_A/C_{A0}$

$X_A = 1 - \frac{3}{5} = 0.4$

zero order rxn

$-r_A = k$

$-r_A = k_0 e^{-E/RT}$

$1 = k = k_0 e^{-E/RT}$

$k_0 = e^{E/RT}$

$= \frac{83.1\times10^3}{8.314\times300}$

$k_0 = e^{33.3}$ kmol/m³.min

PFR

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

Now, for conversion C_A is equal to C_{A0} $(1 – X_A)$ and X_A is equal to 1 – C_A upon C_{A0}. So, X_A will come out to be 1 – 3 upon 5 equals to 0.4. So, given that the rate of reaction is found to be independent of concentration of reactants A and B. So, the given reaction is a zero-order reaction. So, that is if we say that it is a zero-order reaction, then in that case – r A is equal to k.

So, for from Arrhenius law, we may have this $-r_A$ is equal to k 0 e to the power – E upon RT and that is 1 is equal to k that is equal to k_0 e to the power – E upon R T. And we can find out k_0 is equal to e to the power E upon R T and that comes out to be 83.1 into 10 to the power 3 upon 8.314 into 300. And that the k 0 comes out to be e to the power 33.3 kilo mole per metre cube per minute.

Now, for volume of plug flow reactor, the performance equation for plug flow reactor is given as tau is equal to C_{A0}, 0 to X_A dX_A upon $-r_A$.

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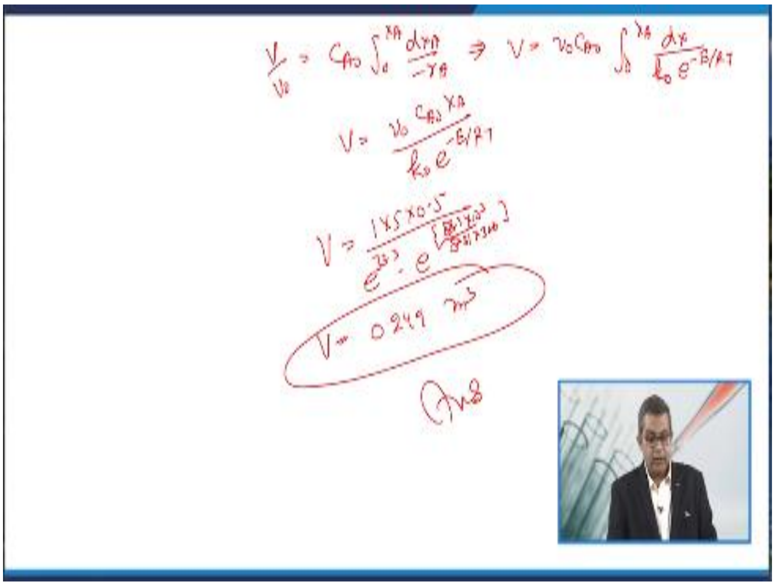

$$\frac{V}{v_0} = C_{A0}\int_0^{X_A}\frac{dX_A}{-r_A} \Rightarrow V = v_0 C_{A0}\int_0^{X_A}\frac{dX_A}{k_0 e^{-E/RT}}$$

$$V = \frac{v_0 C_{A0} X_A}{k_0 e^{-E/RT}}$$

$$V = \frac{1\times5\times0.5}{e^{33.3}\cdot e^{\left[\frac{83.1\times10^3}{8.31\times320}\right]}}$$

$$\boxed{V = 0.249\ m^3}$$

Ans

So, V upon V_0 is equal to C_{A0}, 0 to X_A dX_A upon $-r_A$ that is V is equal to V_0 C_{A0}, 0 to X_A dX_A upon k_0 e to the power – E upon R T or V is equal to V_0 C_{A0} X_A upon k_0 e to the power – E upon R T. So, if you substitute all the values, then we can find the volume of the plug flow reactor as V is equal to 1 into 5 into 0.5 if you recall the problem then divided by e to the power 33.3 into e to the power 83.1 into 10 to the power 3 upon 8.31 into 320, 320 is given.

Now, V is equal to 0.249 metre cube, this is the volume of for the plug flow reactor.

Solution:

Given

$V = 2\ m^3$

$v_o = 1 m^3/min$

$-r_A = 1\ kmol/m^3$

$C_{Ao} = 5\ kmol/m^3$

E = 83.1 KJ/mol

The performance equation for MRF can be written as;

$$\tau = \frac{V}{v_o} = \frac{C_{A_o} - C_A}{-r_A}$$

$$\frac{2}{1} = \frac{5 - C_A}{1}$$

$$C_A = 3\ \text{kmol}$$

For conversion

$$C_A = C_{A_o}(1 - X_A)$$

$$X_A = (1 - \frac{C_A}{C_{A_o}})$$

$$X_A = (1 - \frac{3}{5})$$

$$X_A = 0.4$$

For zero order reaction

$$-r_A = k$$

$$-r_A = k = k_o e^{-\frac{E}{RT}}$$

$$\Rightarrow 1 = k_o e^{-\frac{E}{RT}}$$

$$k_o = e^{\frac{E}{RT}}$$

On putting the values of all of the parameters we have

$$k_o = e^{(\frac{83.1\times10^3}{8.314\times300})}$$

$$\Rightarrow k_o = e^{33.3} \text{ kmol/m}^3\text{.min}$$

Performance equation for PFR can be written as;

$$\tau = \frac{V}{v_o} = C_{A_o}\int_0^{X_A} \frac{dX_A}{-r_A}$$

$$V = v_o C_{A_o}\int_0^{X_A} \frac{dX_A}{k_o e^{-\frac{E}{RT}}}$$

$$V = \frac{v_o C_{A_o} X_A}{k_o e^{-\frac{E}{RT}}}$$

$$V = \frac{1 \times 5 \times 0.5}{e^{33.3}.\, e^{-\frac{83.1\times10^3}{8.31\times320}}}$$

$$V = 0.249 \text{ m}^3 \text{ (answer)}$$

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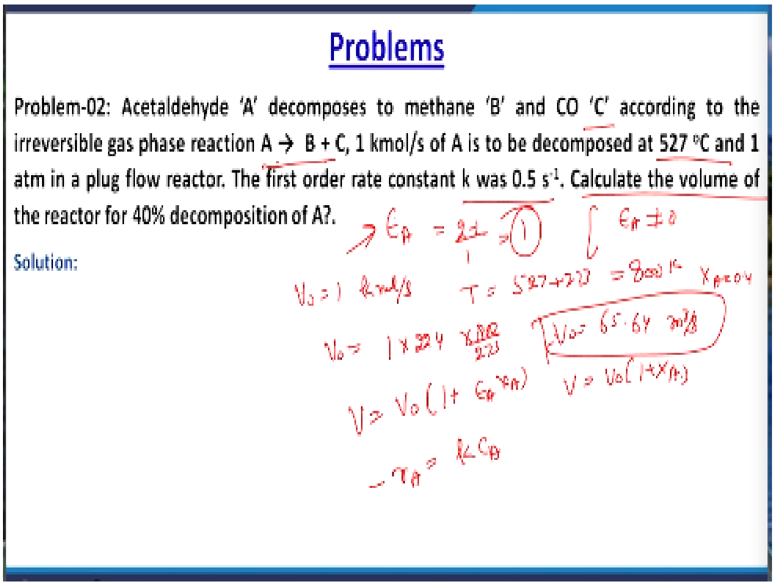

Problems

Problem-02: Acetaldehyde 'A' decomposes to methane 'B' and CO 'C' according to the irreversible gas phase reaction A → B + C, 1 kmol/s of A is to be decomposed at 527 °C and 1 atm in a plug flow reactor. The first order rate constant k was 0.5 s^{-1}. Calculate the volume of the reactor for 40% decomposition of A?.

Solution:

$\varepsilon_A = \frac{2-1}{1} = \boxed{1}$ $\varepsilon_A \neq 0$

$V_0 = 1$ kmol/s $T = 527+273 = 800$ K $X_A = 0.4$

$V_0 = 1 \times 22.4 \times \frac{800}{273}$ $\boxed{V_0 = 65.64\ m^3/s}$

$V = V_0(1+\varepsilon_A X_A)$ $V = V_0(1+X_A)$

$-r_A = kC_A$

Now, let us take another problem that is acetaldehyde A decomposes to the methane B and carbon monoxide C according to the irreversible gas phase reaction A is converting into B and C. Now, 1 kilo mole of A is to be decomposed at 527 degrees Celsius and 1 atmosphere especially in PFR you must say that this is the first order. So, the first order rate constant case given 0.5 second inverse.

Now, you need to calculate the volume of the reactor for 40% decomposition of A. So, we are we are provided with the reaction now, this is the irreversible gas phase reaction. So, the expansion factor or epsilon A that is given by 2 – 1 upon 1 that is equal to 1 that is epsilon A is not equal to 0. So, the varying volume system now, since this is equal to comes out to be 1. So, this is not equal to 1. So, you may say that this is the varying volume system.

Now, it is given that we are dealing with the first order reaction with the k is equal to 0.5 per second. So, V_0 is equal to 1 kilo mole per second and T is equal to 527 degrees Celsius + 273 that is 800 Kelvin and X_A is equal to 0.4 that is, you need to calculate the volume. Now, in that case, V_0 is equal to 1 into 22.4 into 800 upon 273 or V_0 is equal to 65.64 metre cube per second.

Now, if we talk about the varying volume system in that case V is equal to V_0 1 + epsilon A X_A or V is equal to V_0 1 + X_A that is because, we have already found out the value of epsilon as one. So, the rate for decomposition of reactant A can be written as – r_A is equal to k C_A.

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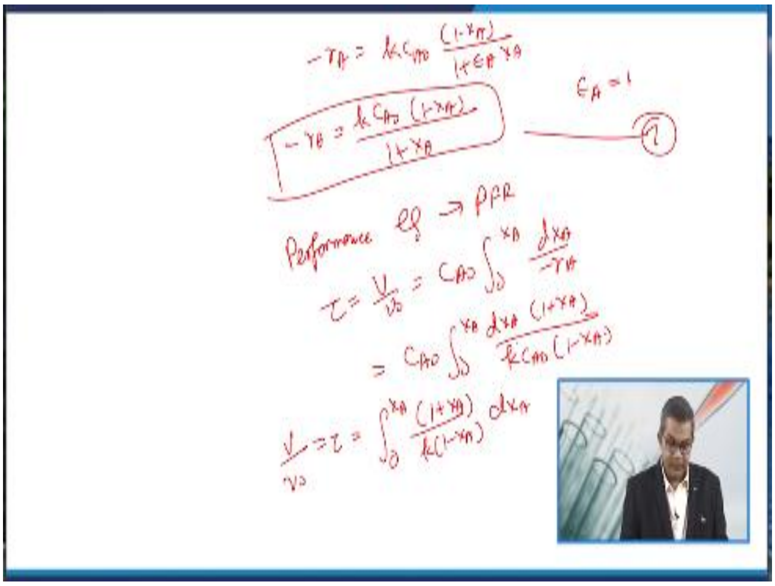

$-r_A = kC_{A0}\frac{(1-X_A)}{1+\epsilon_A X_A}$

$\epsilon_A = 1$

$\boxed{-r_A = \frac{kC_{A0}(1-X_A)}{1+X_A}}$ ——— ②

Performance eq → PFR

$\tau = \frac{V}{v_0} = C_{A0}\int_0^{X_A}\frac{dX_A}{-r_A}$

$= C_{A0}\int_0^{X_A}\frac{dX_A(1+X_A)}{kC_{A0}(1-X_A)}$

$\frac{V}{v_0} = \tau = \int_0^{X_A}\frac{(1+X_A)}{k(1-X_A)}dX_A$

Now, $-r_A$ is equal to k C_{A0} (1 – X_A) upon 1 + epsilon A X_A. So, $-r_A$ is equal to k C_{A0} (1 – X_A) upon 1+ X_A that is for epsilon A is equal to 1 this can be my question number. So, when we talk about the performance equation. So, Performance Equation for PFR can be written as tau is equal to V upon V_0 is equal to C_{A0}, 0 to X_A dX_A upon $-r_A$ and that is equal to C_{A0},0 to X_A dX_A (1 + X_A) upon k C_{A0} (1 – X_A).

So, V upon V_0 that is equal to tau that is equal to 0 to X_A into 1+ X_A upon k into 1 – X_A dX_A.

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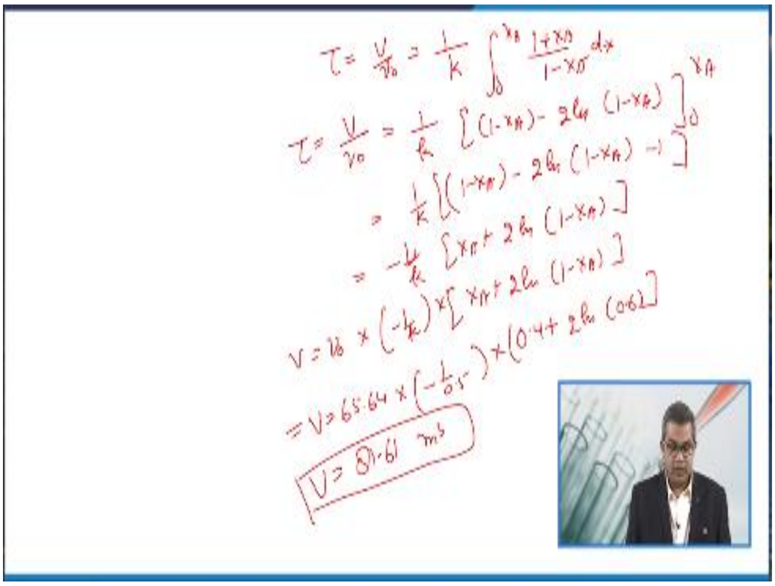

$\tau = \frac{V}{v_0} = \frac{1}{k}\int_0^{X_A}\frac{1+X_A}{1-X_A}dx$

$\tau = \frac{V}{v_0} = \frac{1}{k}\left[(1-X_A) - 2\ln(1-X_A)\right]_0^{X_A}$

$= \frac{1}{k}\left[(1-X_A) - 2\ln(1-X_A) - 1\right]$

$= -\frac{1}{k}\left[X_A + 2\ln(1-X_A)\right]$

$V = v_0 \times \left(-\frac{1}{k}\right) \times \left[X_A + 2\ln(1-X_A)\right]$

$= V = 65.64 \times \left(-\frac{1}{0.5}\right) \times (0.4 + 2\ln(0.6))$

$\boxed{V = 81.61\ m^3}$

So, tau is equal to V upon V_0 that is equal to 1 upon k, 0 to X_A (1 + X_A) upon 1 – X_A) dX_A. So, if we integrate the things, then we may have, tau is equal to V upon V_0 that is 1 upon K 1 – X_A – 2ln 1 – X_{A0} to X_A. And that is equal to 1 upon k 1 – X_A – 2ln 1 – X_A – 1 and that is equal to 1 upon k X_A + 2ln 1 – X_A or V is equal to V_0 into – 1 upon k into X_A + 2ln 1 – X_A.

So, if we substitute all the values, then V is equal to 65.64 into 1 upon 0.5 – into 0.4 + 2ln 0.6. Now, V will become at 81.61 metre cube. Now, this is my answer. And this is the required volume for plug flow reactor for 40% conversion.

Solution

$$\varepsilon_A = 2 - 1 = 1$$

i.e., variable density system

Given

T = 527 +273 = 800 K

$X_A = 0.4$

$$v_0 = 1 \times 22.4 \times \frac{800}{273} = 65.64\, m^3/s$$

$$-\mathrm{r_A} = C_A\mathrm{k} = \frac{C_{A_o}(1 - X_A)}{1 + \varepsilon_A X_A}$$

$$\Rightarrow -\mathrm{r_A} = C_A\mathrm{k} = \frac{C_{A_o}(1 - X_A)}{(1 + X_A)}$$

Performance equation for PFR

$$\tau = \frac{\mathrm{V}}{\mathrm{v_o}} = \mathrm{C_{A_o}} \int_0^{\mathrm{X_A}} \frac{\mathrm{dX_A}}{-\mathrm{r_A}}$$

$$\tau = \frac{\mathrm{V}}{\mathrm{v_o}} = \frac{1}{k} \int_0^{\mathrm{X_A}} \frac{(1 + X_A)\mathrm{dX_A}}{(1 - X_A)}$$

On integration we have

$$\tau = \frac{\mathrm{V}}{\mathrm{v_o}} = \frac{1}{k}[(1 - X_A) - 2\ln(1 - X_A)]_0^{X_A}$$

$$\Rightarrow \tau = \frac{\mathrm{V}}{\mathrm{v_o}} = \frac{1}{k}[(1 - X_A) - 2\ln(1 - X_A) - 1]$$

$$\Rightarrow \mathrm{V} = -\frac{\mathrm{v_o}}{k}[X_A + 2\ln(1 - X_A)]$$

$$\Rightarrow \mathrm{V} = 65.64 \times (-\frac{1}{0.5})[0.4 + 2\ln(0.6)]$$

$$\Rightarrow \mathrm{V} = 81.61\, m^3$$

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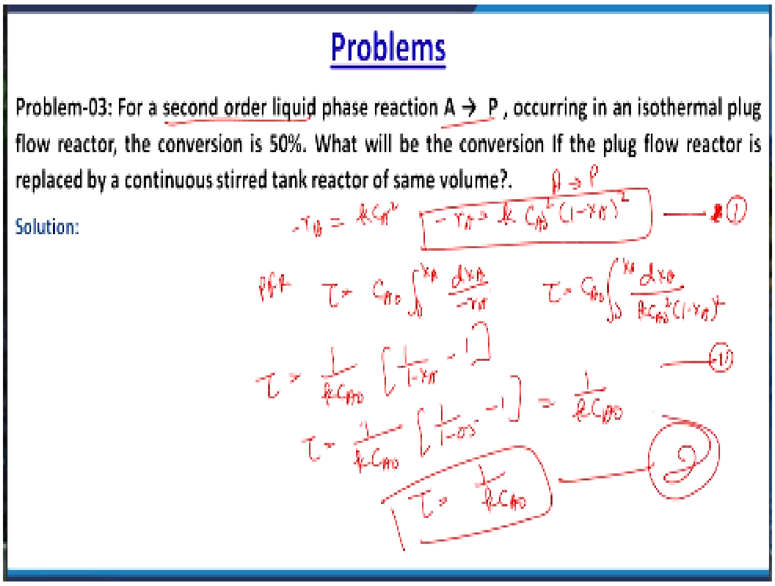

Problems

Problem-03: For a second order liquid phase reaction A → P, occurring in an isothermal plug flow reactor, the conversion is 50%. What will be the conversion If the plug flow reactor is replaced by a continuous stirred tank reactor of same volume?.

Solution:

$A \rightarrow P$

$-r_A = kC_A^2 \quad \boxed{-r_A = kC_{A0}^2(1-X_A)^2} \longrightarrow ①$

PFR $\tau = C_{A0}\int_0^{X_A}\frac{dX_A}{-r_A} \quad \tau = C_{A0}\int_0^{X_A}\frac{dX_A}{kC_{A0}^2(1-X_A)^2}$

$\tau = \frac{1}{kC_{A0}}\left[\frac{1}{1-X_A}-1\right] \longrightarrow ①$

$\tau = \frac{1}{kC_{A0}}\left[\frac{1}{1-0.5}-1\right] = \frac{1}{kC_{A0}}$

$\boxed{\tau = \frac{1}{kC_{A0}}} \longrightarrow ②$

Now, let us take another problem that is for a second order liquid phase reaction A is converting to P. Now, occurring this particular this thing in an isothermal plug flow reactor, the conversion is 50%. Now, you need to find out that what will be the conversion if the plug flow reactor is replaced by CSTR in the same volume. So, let us take the cognizance of this particular reaction A is converting into P.

So, the rate equation for the second order because it is given that second order, so, the rate equation for the second order can be given as – r_A is equal to k C_A square and that is – r_A is equal to k C_{A0} squared 1 – X_A square. So, this is my equation number 1. So, when we write the performance equation for PFR then tau is equal to C_{A0}, 0 to X_A dX_A upon – r_A and tau is equal to C_{A0}, 0 to X_A dX_A upon k C_{A0} squared 1 – X_A squared that is from the equation number 1.

So, if we integrate this particular equation, then we may have tau is equal to 1 upon k C_{A0} 1 upon 1 – X_A – 1 and tau is equal to 1 upon k C_{A0} 1 upon 1 – 0.5 – 1 that is equal to 1 upon k C_{A0} and tau is equal to 1 upon k C_{A0} that is my equation number 2.

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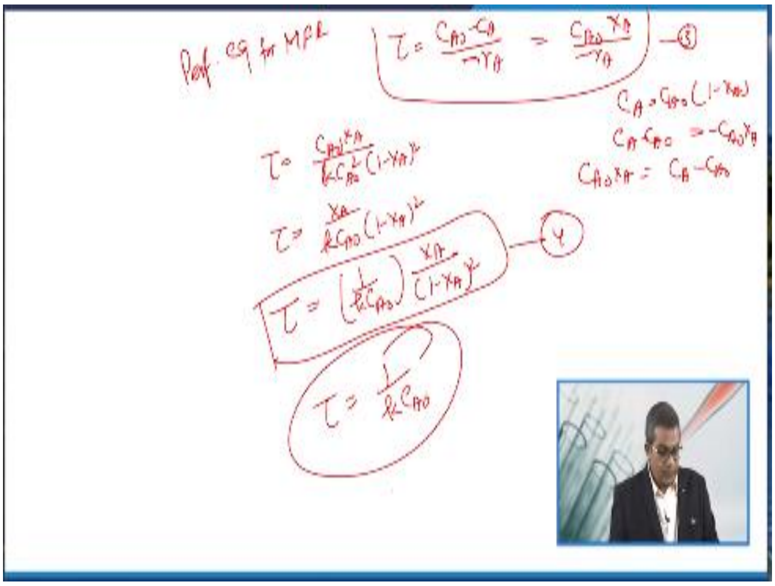

Perf. eq for MFR

$$\tau = \frac{C_{A0} - C_A}{-r_A} = \frac{C_{A0} X_A}{-r_A} \quad \text{—③}$$

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

$$C_A - C_{A0} = -C_{A0} X_A$$

$$C_{A0} X_A = C_A - C_{A0}$$

$$\tau = \frac{C_{A0} X_A}{k C_{A0}^2 (1 - X_A)^2}$$

$$\tau = \frac{X_A}{k C_{A0} (1 - X_A)^2}$$

$$\tau = \left(\frac{1}{k C_{A0}}\right) \frac{X_A}{(1 - X_A)^2} \quad \text{—④}$$

$$\tau = \frac{1}{k C_{A0}}$$

So, similarly, the performance equations for the equation for MFR that is tau is equal to performance equation for MFR, tau is equal to $C_{A0} – C_A$ upon $– r_A$ and this particular equation, we can say that this is equal to C_{A0} X_A upon $– r_A$ that is my equation number 3. Now, how it can achieve that is C_A is equal to C_{A0} into $1 – X_A$ that comes out to be $C_A – C_{A0}$ is equal to $– C_{A0}$ X_A and C_{A0} X_A is equal to $C_A – C_{A0}$.

So, from equation 3 and 1, we may have tau is equal to C_{A0} X_A upon k C_{A0} $1 – X_A$ squared and tau is equal to X_A upon k C_{A0} $1 – X_A$ square. So, this equation if we take all the things into co-ordination, then we may write X_A upon $1 – X_A$ squared that is my equation number 4. So, for same value of the mixed flow reactor, the tau will become 1 upon k C_{A0} that is from the equation number 2.

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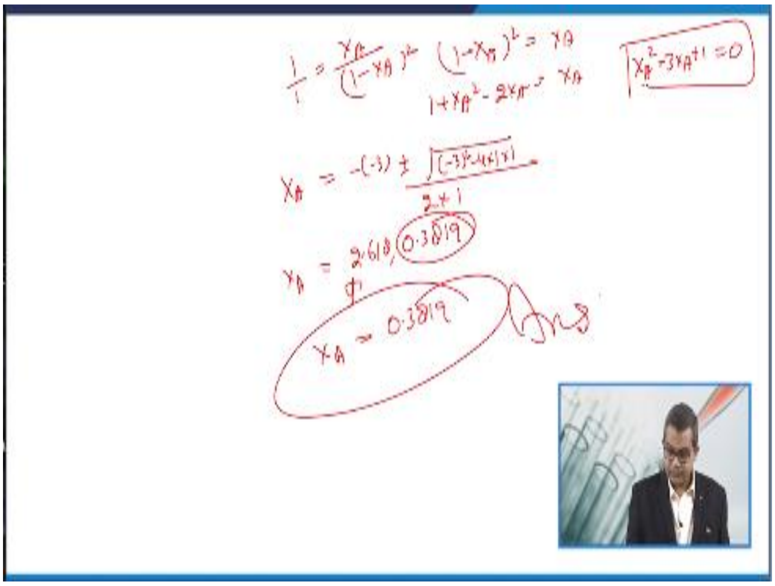

$$\frac{1}{1} = \frac{X_A}{(1 - X_A)^2} \qquad (1 - X_A)^2 = X_A$$

$$1 + X_A^2 - 2X_A = X_A$$

$$\boxed{X_A^2 - 3X_A + 1 = 0}$$

$$X_A = \frac{-(-3) \pm \sqrt{(-3)^2 - 4 \times 1 \times 1}}{2 \times 1}$$

$$X_A = 2.618, \; 0.3819$$

$$X_A = 0.3819 \quad \text{Ans}$$

So, if we take the equation number 4, this one and equation number 2, then we may have 1 upon 1 is equal to X_A upon 1 – X_A is square or 1 – X_A squared is equal to X_A or this may become 1 + X_A squared – 2 X_A is equal to X_A or X_A squared 3 X_A+ 1 is equal to 0. So, X_A, this is the cubic root equation. So, X_A is equal to – 3 + –, – 3 square – 4 into 1 into 1 upon 2 into 1. And if we calculate the final value of X_A that is comes out to be 2.618, 0.3819.

Now, in this the most feasible because this one is more than 1. So, this one is most feasible. So, X_A is equal to 0.3819 and that is my answer. Now, we have nullified this, this route just because it is more than 1.

Solution;

Given that

A→P (second order liquid phase reaction)

$$-r_A = kC_A{}^2$$

$$-r_A = kC_{A_o}^2(1 - X_A)^2$$

Performance equation for PFR

$$\tau = \frac{V}{v_o} = C_{A_o}\int_0^{X_A}\frac{dX_A}{-r_A}$$

$$\tau = \frac{V}{v_o} = C_{A_o}\int_0^{X_A}\frac{dX_A}{kC_{A_o}^2(1 - X_A)^2}$$

on integration we have

$$\tau = \frac{V}{v_o} = \frac{1}{kC_{A_o}}[\frac{1}{1 - X_A} - 1]$$

$$\tau = \frac{1}{kC_{A_o}}[\frac{1}{1 - 0.5} - 1]$$

$$\Rightarrow \tau = \frac{1}{kC_{A_o}} \qquad (1)$$

Performance equation for MFR

$$\tau = \frac{V}{v_o} = \frac{C_{A_o} - C_A}{-r_A} = \frac{C_{A_o}X_A}{-r_A}$$

$$\tau = \frac{X_A}{kC_{A_o}(1 - X_A)^2} \qquad (2)$$

now, form equation (1) and (2) we have

$$\frac{1}{kC_{A_o}} = \frac{X_A}{kC_{A_o}(1 - X_A)^2}$$

On rearranging we have

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

$$\Rightarrow X_A = (1 - X_A)^2$$

$$\Rightarrow {X_A}^3 - 3X_A + 1 = 0$$

On solving we have

$X_A = 2.618\ or\ 0.3819$

As conversion can’t exceed to 1 so, 2.618 is not a valid option.

$X_A = 0.3819$ (answer)

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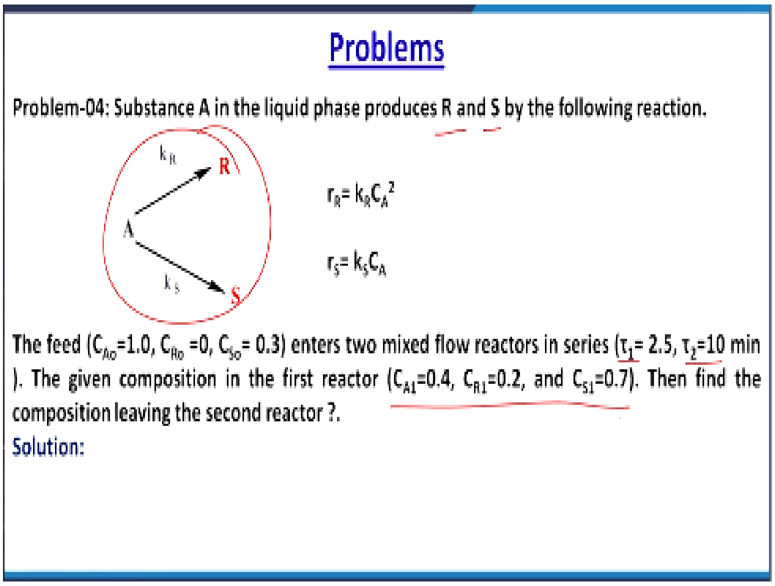

Problems

Problem-04: Substance A in the liquid phase produces R and S by the following reaction.

$r_R = k_R C_A^2$

$r_S = k_S C_A$

The feed (C_{Ao}=1.0, C_{Ro} =0, C_{So}= 0.3) enters two mixed flow reactors in series (τ_1= 2.5, τ_2=10 min). The given composition in the first reactor (C_{A1}=0.4, C_{R1}=0.2, and C_{S1}=0.7). Then find the composition leaving the second reactor ?.

Solution:

Now, let us take another example. Now, here, the substance A in the liquid phase produces R and S by this following reaction. Now, the feed having C_{A0} is equal to 1 and C_{R0} is equal to 0 and C_{S0} is equal to 2.3. Now, this interest into 2 mixed flow reactors in series, the values of tau 1 and tau 2, they are given that is 2.5 and 10 minutes.

The given composition the first reactor is given like this that is C_{A1} is equal to 0.4 and C_{R2} is, C_{R1} is equal to 0.2 and C_{S1} 0.7. Then you need to find the composition leaving the second reactor.

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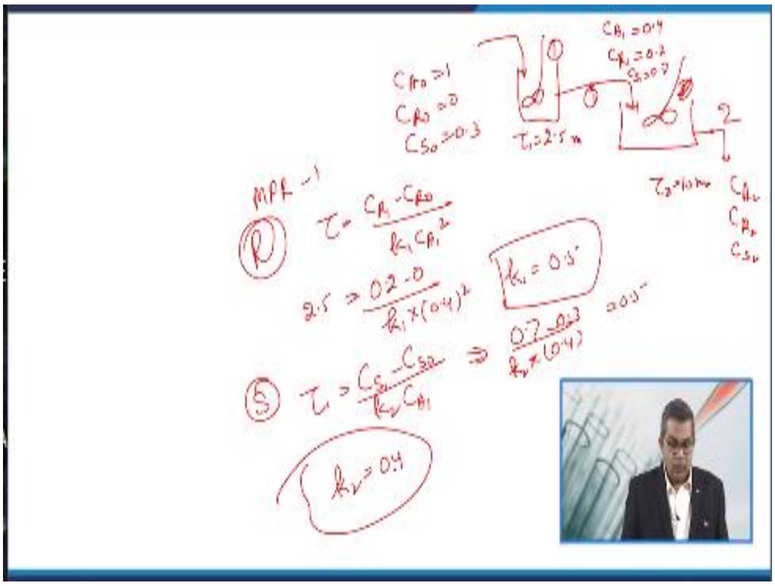

$C_{A0} = 1$, $C_{R0} = 0$, $C_{S0} = 0.3$

$\tau_1 = 2.5$ m

$C_{A1} = 0.4$, $C_{R1} = 0.2$, $C_{S1} = 0.7$

$\tau_2 = 10$ min

C_{A2}, C_{R2}, C_{S2}

MFR-1

Ⓡ $\tau = \frac{C_{R1} - C_{R0}}{k_1 C_{A1}^2}$

$2.5 = \frac{0.2 - 0}{k_1 \times (0.4)^2}$

$\boxed{k_1 = 0.5}$

Ⓢ $\tau_1 = \frac{C_{S1} - C_{S0}}{k_2 C_{A1}} \Rightarrow \frac{0.7 - 0.3}{k_2 \times (0.4)} = 0.5$

$\boxed{k_2 = 0.4}$

Now, it is given that we are having the 2 MFR in series. So, let us first the advisable to have a pictorial representation, these are my 2 MFR. Now, here, the tau is given 2.5 minute and then C_{A1} this is 0.4, C_{R1}, it is equal to 0.2 and C_{S1} that is 0.7, this is my 2 and 1. And here, the C_{A0} is equal to 1, C_{R0} is equal to 0 and C_{S0} is equal to 0.3. So, you need to find out C_{A2}, C_{R2} and C_{S2}.

So, for MFR 1, this is first my first reactor and this is my second reactor. The performance equation for MFR 1, the performance equation tau is equal to $C_{R1} – C_{R0}$ upon k 1 C_{A1}. Now, this can be 2.5 equal to 0.2 – 0 upon k 1 into 0.4 and that k 1 comes out to be 0.5. This is for R. Now, for S, the tau 1 that is $C_{S1} – C_{S0}$ upon k 2 C_{A1}. Now, if we substitute the value 0.7 – 0.3 upon k_2 into 0.4. This is coming out to be 0.5. So, k_2 is equal to 0.4.

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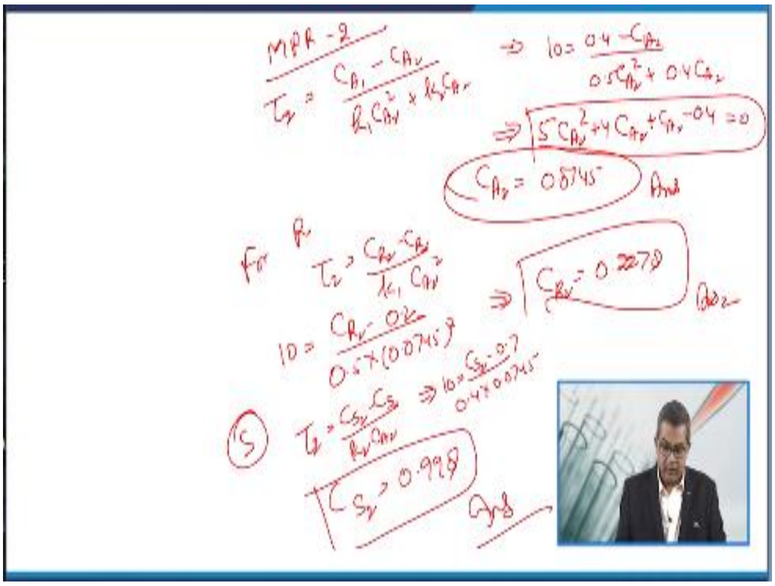

MFR-2

$\tau_2 = \frac{C_{A1} - C_{A2}}{k_1 C_{A2}^2 + k_2 C_{A2}} \Rightarrow 10 = \frac{0.4 - C_{A2}}{0.5 C_{A2}^2 + 0.4 C_{A2}}$

$\Rightarrow \boxed{5C_{A2}^2 + 4C_{A2} + C_{A2} - 0.4 = 0}$

$\boxed{C_{A2} = 0.0745}$ Ans

For R

$\tau_2 = \frac{C_{R2} - C_{R1}}{k_1 C_{A2}^2}$

$10 = \frac{C_{R2} - 0.2}{0.5 \times (0.0745)^2} \Rightarrow \boxed{C_{R2} = 0.2278}$ Ans

Ⓢ $\tau_2 = \frac{C_{S2} - C_{S1}}{k_2 C_{A2}} \Rightarrow 10 = \frac{C_{S2} - 0.7}{0.4 \times 0.0745}$

$\boxed{C_{S2} = 0.998}$ Ans

Now, for the second MFR the steam exit from the first MFR is the feed stream for the second 1. So, tau 2 is equal to C_{A1} – C_{A2} upon k_1 C_{A2} square + k_2 C_{A2}. Now, let us put all the values 10 is equal to 0.4 – C_{A2} upon 0.5 C_{A2} + 0.4 C_{A2}. Now, if we substitute all the values and rearrange all those things, then we find that it is 5 C_{A2} square + 4 C_{A2} + C_{A2} – 0.4. This comes out to be 0.

Now, if we solve this particular equation, we have C_{A2} is equal to 0.0745 and that is my answer, first answer. Now, for R, we are having tau 2 is equal to C_{R2} – C_{R1} upon k_1 C_{A2}. And if we substitute the value 10 is equal to C_{R2} – 0.2 upon 0.5 into 0.0745 and that is C_{R2} is equal to 0.2278 that is my answer number 2. Now, similarly, if we talk about for S, then tau 2 is equal to C_{S2} – C_{S1} upon k_2 C_{A2}.

And if we substitute all the values, then it comes out to be 10 is equal to C_{S2} – 0.7 upon 0.4 into 0.0745, which we already determined, then C_{S2} would be 0.998 that is my answer. So, by this way, we solved all these things which are needed.

Solution;

At the entrance of first reactor

C_{Ao}=1

C_{Ro} = 0

C_{So} = 0.3

At the entrance of the second reactor

C_{A1}=0.4

C_{R1} = 0.2

C_{S1} = 0.7

For reactor 1, formation of desired product R can be calculated as

$$\tau_1 = \frac{C_{R1} - C_{R0}}{k_1 {C_{R1}}^2}$$

$$2.5 = \frac{0.2 - 0}{k_1 \times (0.4)^2}$$

$$k_1 = 0.5$$

Similarly for undesired product ‘S’

$$\tau_1 = \frac{C_{S1} - C_{S0}}{k_2 C_{S1}}$$

$$2.5 = \frac{0.7 - 0.3}{k_2 \times (0.4)}$$

$$k_2 = 0.4$$

In MFR 2

$$\tau_2 = \frac{C_{A1} - C_{A2}}{k_1 {C_{A2}}^2 + k_2 C_{A2}}$$

$$10 = \frac{0.4 - C_{A2}}{0.5 {C_{A2}}^2 + 0.4 C_{A2}}$$

$$5{C_{A2}}^2 + 4C_{A2} + C_{A2} - 0.4 = 0$$

On solving it we have

$$C_{A2} = 0.8345 \text{ (answer)}$$

For formation of desired product R

$$\tau_2 = \frac{C_{R2} - C_{R1}}{k_1 {C_{A2}}^2}$$

$$10 = \frac{C_{R2} - 0.2}{0.5 \times 0.0745^2}$$

$$C_{R2} = 0.2278 \text{ (answer)}$$

For formation of desired product ‘S’

$$\tau_2 = \frac{C_{S2} - C_{S1}}{k_2 C_{A2}}$$

$$10 = \frac{C_{S2} - 0.7}{0.4 \times 0.0745}$$

$$C_{S2} = 0.998 \text{ (answer)}$$

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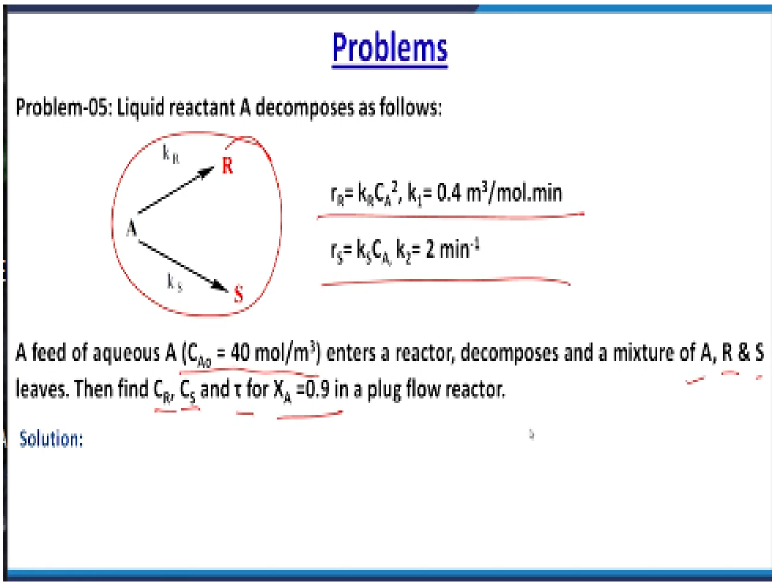

Problems

Problem-05: Liquid reactant A decomposes as follows:

$r_R = k_R C_A^2$, $k_1 = 0.4$ m^3/mol.min

$r_S = k_S C_A$, $k_2 = 2$ min^{-1}

A feed of aqueous A (C_{A0} = 40 mol/m^3) enters a reactor, decomposes and a mixture of A, R & S leaves. Then find C_R, C_S and τ for X_A =0.9 in a plug flow reactor.

Solution:

Now, let us take another problem that is problem number 5. Here, the liquid reactants reactant A is decomposing as per this following scheme. And the rate is given like this, a feed of aqueous A that is initial gradients are given that C_{A0} is equal to 40 moles per metre cube. This enters into a reactor, decompose it, it is and the mixture of A, R and S are coming out. Then you need to find out the C_R, C_S and tau for X_A is equal to 0.9 in the plug flow reactor.

So, let us solve and it is advisable that every time when you need to solve this thing, then you draw a rough figure.

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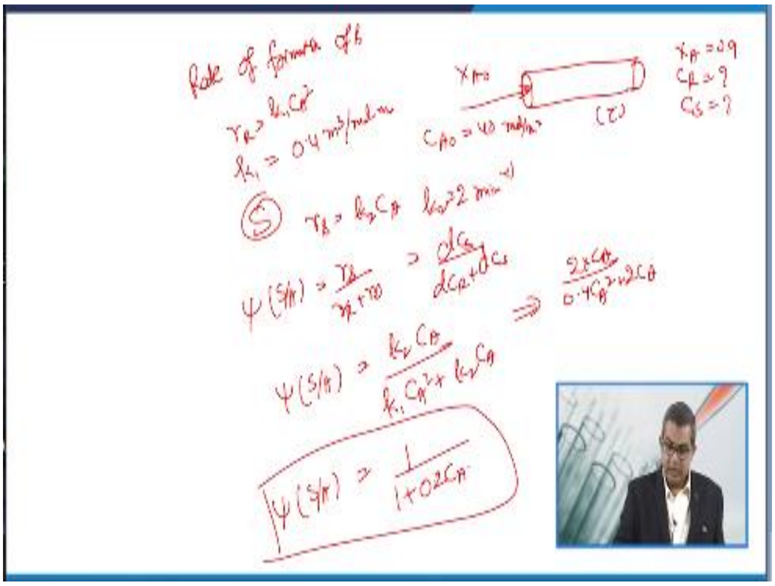

Rate of formation of R

$r_R = k_1 C_A^2$

$k_1 = 0.4\ m^3/mol\ min$

X_{A0}

$C_{A0} = 40\ mol/m^3$

(τ)

$X_A = 0.9$

$C_R = ?$

$C_S = ?$

Ⓢ $r_S = k_2 C_A \quad k_2 = 2\ min^{-1}$

$\psi(S/A) = \frac{r_S}{r_R + r_S} = \frac{dC_S}{dC_R + dC_S}$

$\psi(S/A) = \frac{k_2 C_A}{k_1 C_A^2 + k_2 C_A} \Rightarrow \frac{2 \times C_A}{0.4 C_A^2 + 2 C_A}$

$$\boxed{\psi(S/A) = \frac{1}{1 + 0.2 C_A}}$$

So, let us draw the rough figure of my plug flow reactor that is X_A is equal to 0.9, C_R you need to find out, C_S you need to find out. Here, the X_{A0} and C_{A0} is given 40 moles per metre cube. So, the rate of formation of R that is r_R is equal to k_1 C_A and k_1 is equal to 0.4 metre cube per mole minute. So, rate of formation of S, r_S is equal to k_2 C_A and k_2 is equal to 2-minute inverse.

Now, for desired product S the instantaneous fractional yield we discuss this, this one though. So, instantaneous fractional yield chi is given as r_S upon r_R + r_S and that is dC_S upon dC_R + dC_S. Now, chi S upon A that is equal to k 2 C_A upon k_1 C_A square + k_2 C_A. Now, it comes out to be 2 into C_A upon 0.4 C_A + 2 C_A or chi S upon A that is equal to 1 + 0.2 C_A.

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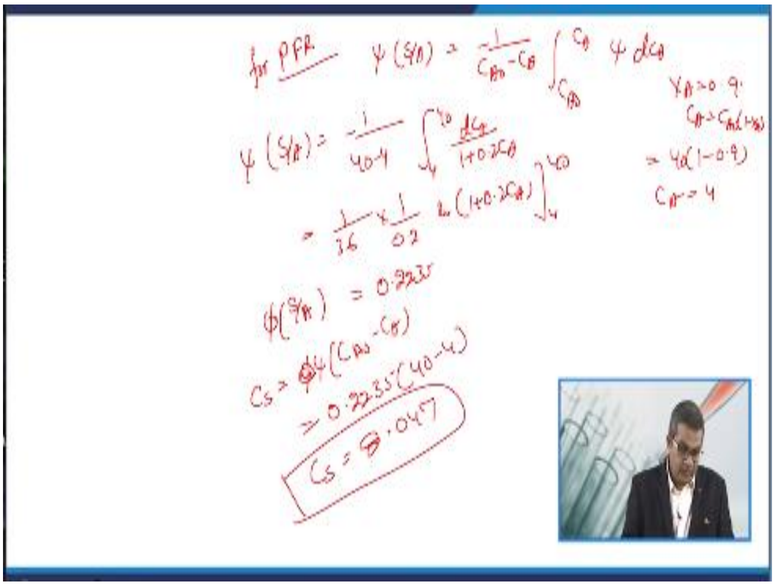

for PFR $\psi(S/A) = \frac{-1}{C_{A0}-C_A}\int_{C_{A0}}^{C_A}\psi \, dC_A$

$X_A = 0.9$

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

$= 40(1-0.9)$

$C_A = 4$

$\psi(S/A) = \frac{-1}{40-4}\int_{4}^{40}\frac{dC_A}{1+0.2C_A}$

$= \frac{1}{36}\times\frac{1}{0.2}\ln(1+0.2C_A)\Big]_4^{40}$

$\phi(S/A) = 0.2235$

$C_S = \psi(C_{A0}-C_A)$

$= 0.2235(40-4)$

$\boxed{C_S = 8.047}$

Now, for PFR that is chi S upon A is equal to – 1 upon C_{A0} – C_A that is C_{A0} to C_A chi dC_A. Now, here we are having X_A is equal to 0.9 and C_A is equal to C_{A0} 1 – X_A that is 40 into 1 – 0.9 and C_A is comes out to be 4. So, chi S upon A that is equal to – 1 upon 40 – 4, 4 to 40 dC_A upon 1 + 0.2 C_A. And if we substitute all the values upon integration, so, this is 1 upon 36 into 0.2 ln 1 + 0.2 C_A 4 to 40 or phi, this comes out to be chi S upon A comes out to be 0.2235.

So far final concentration of desired product would be C_S is equal to phi sorry, chi this is chi C_{A0} – C_A and that is 0.2235 into 40 – 4 and this C_S comes out to be 8.047.

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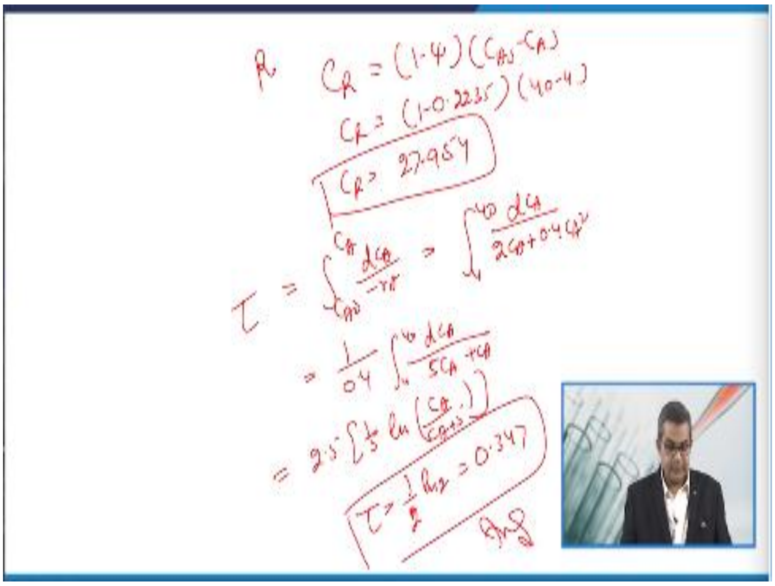

R $C_R = (1-\psi)(C_{A0}-C_A)$

$C_R = (1-0.2235)(40-4)$

$\boxed{C_R = 27.954}$

$\tau = \int_{C_{A0}}^{C_A}\frac{dC_A}{-r_A} = \int_4^{40}\frac{dC_A}{2C_A+0.4C_A^2}$

$= \frac{1}{0.4}\int_4^{40}\frac{dC_A}{5C_A+C_A^2}$

$= 2.5\left[\frac{1}{5}\ln\left(\frac{C_A}{C_A+5}\right)\right]$

$\boxed{\tau = \frac{1}{2}\ln 2 = 0.347}$

Ans

Now, if we say for the other before R, then C_R is equal to 1 – chi into C_{A0} – C_A and this C_R is equal to 1 – 0.2235 into 40 – 4 and C_R comes out to be 27.954 and if we need to find out the tau, tau is equal to C_{A0} C_A dC_A – r_A that is 4 to 40 dC_A upon 2 C_A + 0.4 C_A. Now, this is 0.4, 4 to 40 dC_A upon 5 C_A + C_A square. Now, if we substitute all the values, then it comes out to be 2.5 into 1 upon 5 ln C_A upon C_A + 5 and tau is equal to 1 half ln 2, this is 0.347. This is my answer.

Solution;

Rate of formation of R

$r_R = k_1 C_A^2$

$k_1 = 0.4\ m^3/mol.min$

Rate of formation of S

$r_S = k_2 C_A$

$k_2 = 2\ min^{-1}$

$$\varphi\left(\frac{S}{A}\right) = \frac{r_s}{r_s + r_A} = \frac{dC_s}{dC_s + dC_A}$$

$$\varphi\left(\frac{S}{A}\right) = \frac{r_s}{r_s + r_A} = \frac{k_2 C_A}{k_1 {C_A}^2 + k_2 C_A}$$

$$\Rightarrow \varphi\left(\frac{S}{A}\right) = \frac{2C_A}{0.4{C_A}^2 + 2C_A}$$

$$\Rightarrow \varphi\left(\frac{S}{A}\right) = \frac{1}{1 + 0.2C_A}$$

For PFR

$$\Rightarrow \varphi\left(\frac{S}{A}\right) = \frac{1}{C_{A_0} - C_A}\int_{C_A}^{C_{A_0}} \varphi dC_A$$

As we know the relation of C_{A0} and C_A in terms of conversion i.e.,

$$C_A = C_{A_0}(1 - X_A)$$

$$C_A = 40(1 - 0.9) = 4$$

$$\Rightarrow \varphi\left(\frac{S}{A}\right) = \frac{1}{(40 - 4)}\int_4^{40} \frac{dC_A}{1 + 0.2C_A}$$

$$\Rightarrow \varphi\left(\frac{S}{A}\right) = -\frac{1}{(36)} \times \frac{1}{0.2} \times \ln\,(1 + 0.2C_A)_4^{40}$$

$$\Rightarrow \varphi\left(\frac{S}{A}\right) = 0.2235$$

$$C_S = \varphi(C_{A_0} - C_A)$$

$$C_S = 0.2235(40 - 4)$$

$$C_S = 8.047$$

For R

$$C_R = (1 - \varphi)(C_{A_0} - C_A)$$

$$C_R = (1 - 0.2235)(40 - 4)$$

$$C_R = 27.954$$

Now

$$\tau = \int_{C_{A_0}}^{C_A} \frac{dC_A}{-r_A} = \int_{4}^{40} \frac{dC_A}{2C_A + 0.4\ \times {C_A}^2}$$

$$\tau = \frac{1}{0.4}\int_{4}^{40} \frac{dC_A}{5C_A + {C_A}^2}$$

$$\tau = \frac{1}{0.4}\int_{4}^{40} \frac{dC_A}{(5 + C_A)C_A}$$

$$\tau = \frac{1}{0.4} \times \frac{1}{5} \ln \left(\frac{C_A}{5 + C_A}\right)_4^{40}$$

$$\tau = \frac{1}{2}\ln 2$$

$$\tau = 0.347 \text{ min (answer)}$$

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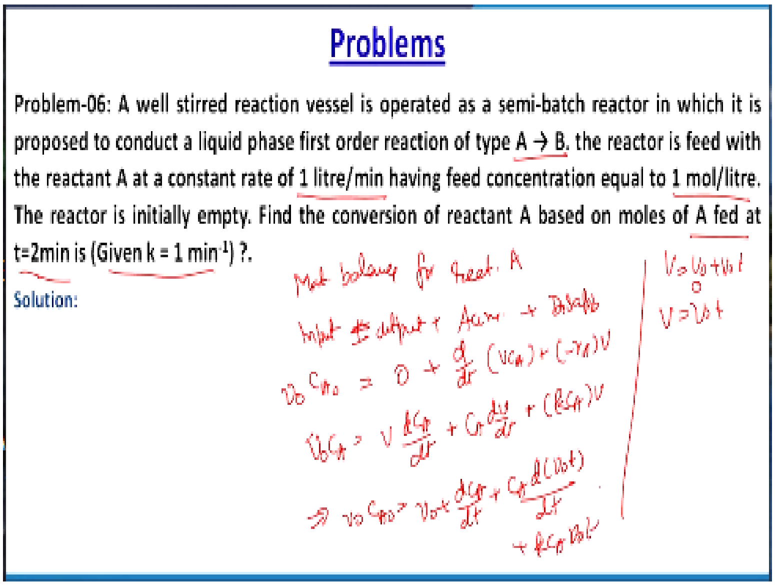

Problems

Problem-06: A well stirred reaction vessel is operated as a semi-batch reactor in which it is proposed to conduct a liquid phase first order reaction of type A → B. the reactor is feed with the reactant A at a constant rate of 1 litre/min having feed concentration equal to 1 mol/litre. The reactor is initially empty. Find the conversion of reactant A based on moles of A fed at t=2min is (Given k = 1 min^{-1}) ?.

Solution:

Mat balance for react. A

Input = output + Accum + Disapp

$v_0 C_{A0} = 0 + \frac{d}{dt}(VC_A) + (-r_A)V$

$v_0 C_A = V\frac{dC_A}{dt} + C_A\frac{dV}{dt} + (kC_A)V$

$\Rightarrow v_0 C_{A0} = v_0 t\frac{dC_A}{dt} + C_A\frac{d(v_0 t)}{dt} + kC_A v_0 t$

$V = V_0 + v_0 t$

$V = v_0 t$

Now, let us take the last example of this particular lecture. Here, well stirred reaction vessel is operated as a semi batch reactor in which it is proposed to conduct a liquid phase first order reaction of type A is converting into B. Now, the reactor is fed with the reactant A at a constant rate which is given to be 1 litre per minute having the feed concentration equal to 1 mole per litre.

Now, the reactor is initially empty. So, you need to find out the conversion of reactant A based on moles of A fed at the time ‘t’ is equal to 2 minutes. Now, the k is given as 1 metre inverse. So, first here, we need to find out, we need to write the material balance for reactant A. So, material balance for reactant A that is input + output sorry, input is equal to output + accumulation + disappearance.

So, if we try to write the mathematically, v_0 C_{A0} is equal to 0 + d upon dt V C_A + – r_A V and v_0 C_{A0} this is equal to V dC_A upon dt + C_A dV dt + k C_A V. Now, this is because V is equal to v_0 + v_0 t and this V is equal to v_0 t, if we put this equal to 0. So, we can write this as nu 0, v_0 C_{A0} is equal to v_0 + dC_A dt + C_A d dt + k C_A t.

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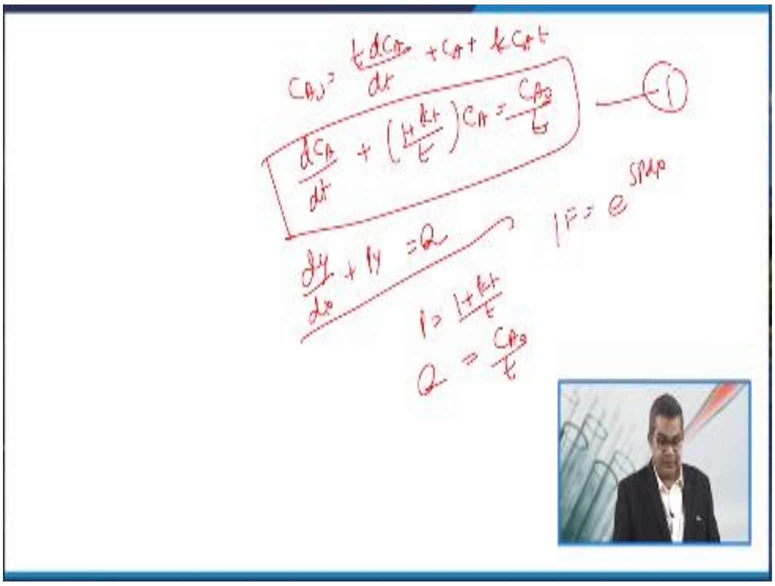

$$C_{A0} = \frac{t\,dC_A}{dt} + C_A + k C_A t$$

$$\boxed{\frac{dC_A}{dt} + \left(\frac{1+kt}{t}\right) C_A = \frac{C_{A0}}{t}} \text{ --- } ①$$

$$\frac{dy}{dx} + Py = Q \quad IF = e^{\int P dx}$$

$$P = \frac{1+kt}{t}$$

$$Q = \frac{C_{A0}}{t}$$

So, finally, the we can write that C_{A0} is equal to t dC_A upon dt + C_A + k C_A t or dC_A dt + 1 + k t upon t C_A is equal to C_{A0} upon t that is my equation number 1. So, this equation is the form of you can say, dy over dx + P y equal to Q. So, we can write IF is equal to P dx, now, P is equal to 1+ k t upon t and this is equal to C_{A0} upon t.

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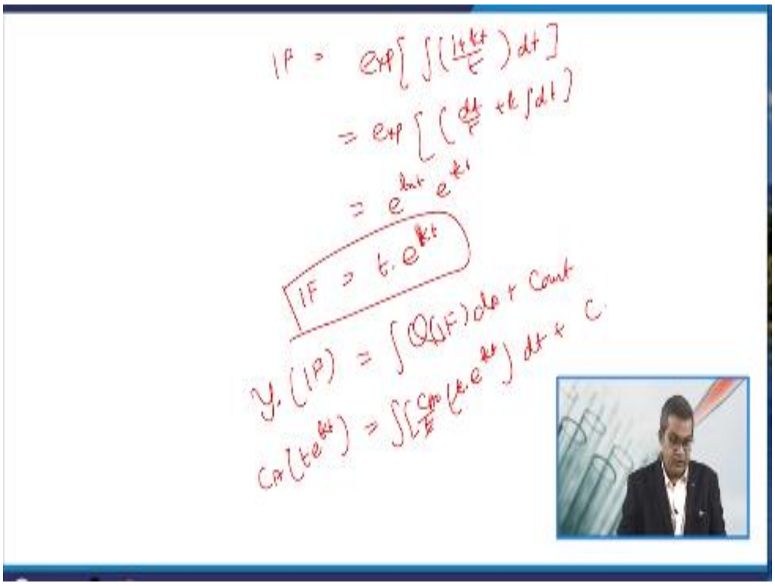

$$IF = \exp\left[\int\left(\frac{1+kt}{t}\right)dt\right]$$

$$= \exp\left[\left(\int\frac{dt}{t} + k\int dt\right)\right]$$

$$= e^{\ln t}\, e^{kt}$$

$$\boxed{IF = t.e^{kt}}$$

$$y.(IF) = \int Q(IF)\,dx + Const$$

$$C_A(te^{kt}) = \int\left[\frac{C_{A0}}{t}(t.e^{kt})\right]dt + C$$

So, when we talk about the integration factor, this IF can be represented as exponential of 1 + k t upon t dt. Now, this is equal to dt over t + k dt and this can be written as e to the power ln t e k t. So, integration factor that is equal to t into e to the power k t. Now, if we talk about the solution of equation number 1 which we developed previously, so, y 0 into integration factor is equal to integration factor dx plus constant.

So, this can be C_A into t e to the power k t is equal to C_{A0} t t e to the power k t dt plus integration constant C.

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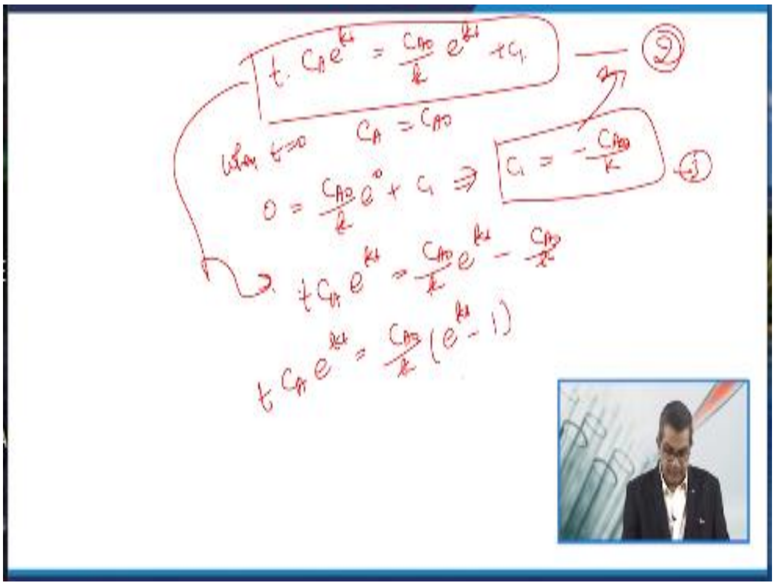

$$\boxed{t.C_A e^{kt} = \frac{C_{A0}}{k}e^{kt} + C_1} \text{ ——— } ②$$

when $t = 0$ $\quad C_A = C_{A0}$

$$0 = \frac{C_{A0}}{k}e^{0} + C_1 \Rightarrow \boxed{C_1 = -\frac{C_{A0}}{k}} \text{ — } ③$$

$$\Rightarrow t C_A e^{kt} = \frac{C_{A0}}{k}e^{kt} - \frac{C_{A0}}{k}$$

$$t C_A e^{kt} = \frac{C_{A0}}{k}(e^{kt} - 1)$$

And this can be written more precise manner, t C_{A0} e to the power k t C_{A0} upon k e to the power k t + C_1. This is my equation number 2. So, when t is equal to 0, C_A is equal to C_{A0}. So, from equation to this from this equation, we can write 0 is equal to C_{A0} upon k e to the power 0 + C_1, C_1 is equal to k. This is my equation number 3.

So, again we take the help of this equation, then this is t C_A e to the power k t is equal to C_{A0} upon k e to the power k t – C_{A0} upon k. So, t C_A e to the power k t is equal to C_{A0} upon k e to the power k t – t.

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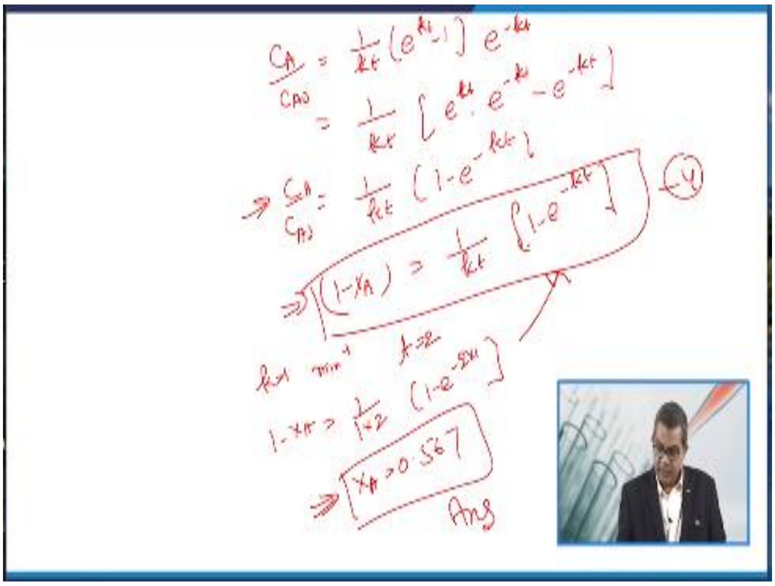

$$\frac{C_A}{C_{A0}} = \frac{1}{kt}(e^{kt}-1]\, e^{-kt}$$

$$= \frac{1}{kt}[e^{kt}\cdot e^{-kt} - e^{-kt}]$$

$$\Rightarrow \frac{C_A}{C_{A0}} = \frac{1}{kt}(1-e^{-kt}]$$

$$\Rightarrow \boxed{(1-X_A) = \frac{1}{kt}[1-e^{-kt}]} \quad -④$$

$k=1$ min^{-1} $t=2$

$$1-X_A = \frac{1}{1\times 2}(1-e^{-2\times 1}]$$

$$\Rightarrow \boxed{X_A = 0.567}$$

Ans

Now, further if we go on carrying out this particular rearrangement, then C_A upon C_{A0} is equal to 1 upon k t e to the power k t – 1 e to the power – k t and this is equal to 1 upon k t e k t e – k t or C upon C_{A0} is equal to 1 upon k t 1 – e to the power – k t. So, if we put the value of this C_{A0} over here and rearrange, then we find that this particular equation becomes 1 – X_A is equal to 1 upon k t 1 – e to the power – k t. So, this is my equation number 4.

So, now, here, we are given that k is equal to 1 minute per minute inverse, t is equal to 2. So, if we utilise this equation, we may have 1 – X_A is equal to 1 upon 1 into 2, 1 – e to the power – 2 into 1 and that comes out to be X_A is equal to 0.567 and that is my final answer.

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Solution;

Mole balance for reactant A

I/P = O/P + Accumulation + Disappearance

$v_0 C_{A0} = 0 + d(VC_A)/dt + (-r_A)V$

$$v_0 C_{A_0} = \frac{V dC_A}{dt} + \frac{C_A dV}{dt} + kC_A V$$

$$v_0 C_{A_0} = v_0 + \frac{dC_A}{dt} + \frac{C_A(dv_0 t)}{dt} + kC_A v_0 t$$

$$V = V_0 + v_0 t$$

As $V_0 = 0$ so,

$$V = v_0 t$$

$$C_{A_0} = \frac{tdC_A}{dt} + C_A + kC_A t$$

$$\frac{dC_A}{dt} + (\frac{1+kt}{t})C_A = \frac{C_{A_0}}{t} \quad (1)$$

The above equation is the form of differential equation which can be written as

$$\frac{dY}{dX} + PY = Q$$

Integration factor for the above equation can be written as

$$I.F = e^{\int PdX}$$

Here P = (1+kt)/t

Q = C_{A0}/t

For the above equation (1) the integration factor can be written as

$$\mathrm{I.F} \; = \; e^{\int \frac{1+kt}{t} dt}$$

On solving this we have

$$\mathrm{I.F} \; = \; te^{kt} \qquad (2)$$

The solution for the above differential equation can be written as

$$Y(I.F) = \int Q.IF.dX \; + C$$

$$C_A(t.e^{kt}) = \int \left[\frac{C_{A_0}}{t}(t.e^{kt})dt\right] + C$$

$$C_A(t.e^{kt}) = \frac{C_{A_0}}{k}(\, e^{kt}) + C \qquad (3)$$

When t=0 and $C_A = C_{A_0}$

$$0 = \frac{C_{A_0}}{k}(\, e^0) + C_1$$

$$C_1 = -\frac{C_{A_0}}{k}$$

On putting this value of integration constant in the above equation (3) we have

$$C_A(t.e^{kt}) = \frac{C_{A_0}}{k}(\, e^{kt}) + -\frac{C_{A_0}}{k}$$

$$\Rightarrow C_A(t.e^{kt}) = \frac{C_{A_0}}{k}(\, e^{kt} - 1)$$

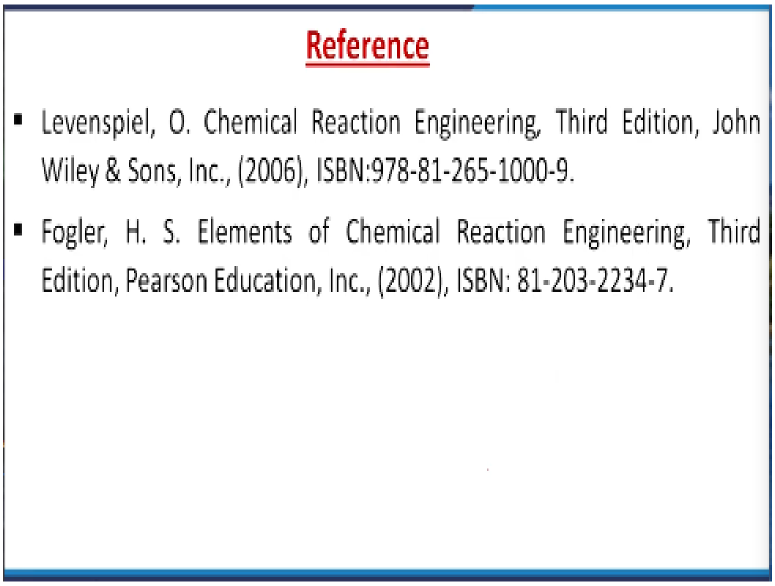
$$\Rightarrow \frac{C_A}{C_{A_0}} = \frac{1}{kt}\left(e^{kt} - 1\right)e^{-kt}$$

$$\Rightarrow (1 - X_A) = \frac{1}{kt}\left(1 - e^{-kt}\right) \qquad (4)$$

Here we have given k = 1 min^{-1} t = 2

$$\Rightarrow (1 - X_A) = \frac{1}{1 \times 2}\left(1 - e^{-2}\right)$$

$$X_A = 0.567 \quad \text{(answer)}$$



Reference

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Now, in this particular chapter, we discussed a variety of problems related to the space time etcetera. And we took the help of these 2 references which are listed over here. And thank you very much.