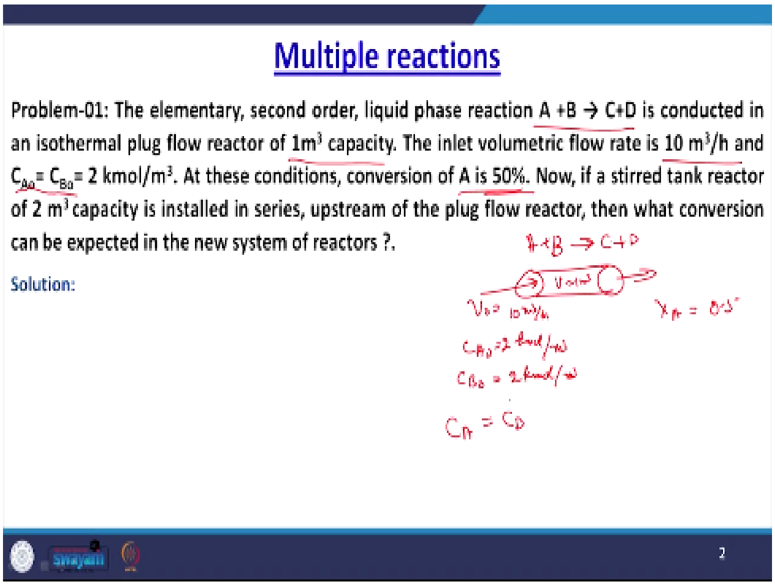
Polymer Reaction Engineering
Prof. Shishir Sinha
Department of Chemical Engineering
Indian Institute of Technology Roorkee

Lecture – 27
Problem Solving - III

Welcome to the problem-solving session of the polymer reaction engineering. Now, here we will discuss about the various problems related to this reaction engineering concept.

(Refer Slide Time: 00:33)



Multiple reactions

Problem-01: The elementary, second order, liquid phase reaction A +B → C+D is conducted in an isothermal plug flow reactor of 1m³ capacity. The inlet volumetric flow rate is 10 m³/h and $C_{A0} = C_{B0} = 2$ kmol/m³. At these conditions, conversion of A is 50%. Now, if a stirred tank reactor of 2 m³ capacity is installed in series, upstream of the plug flow reactor, then what conversion can be expected in the new system of reactors ?.

Solution:

$A+B \rightarrow C+D$

$V = 1m^3$

$V_0 = 10 m^3/h$

$X_A = 0.5$

$C_{A0} = 2$ kmol/m³

$C_{B0} = 2$ kmol/m³

$C_A = C_B$

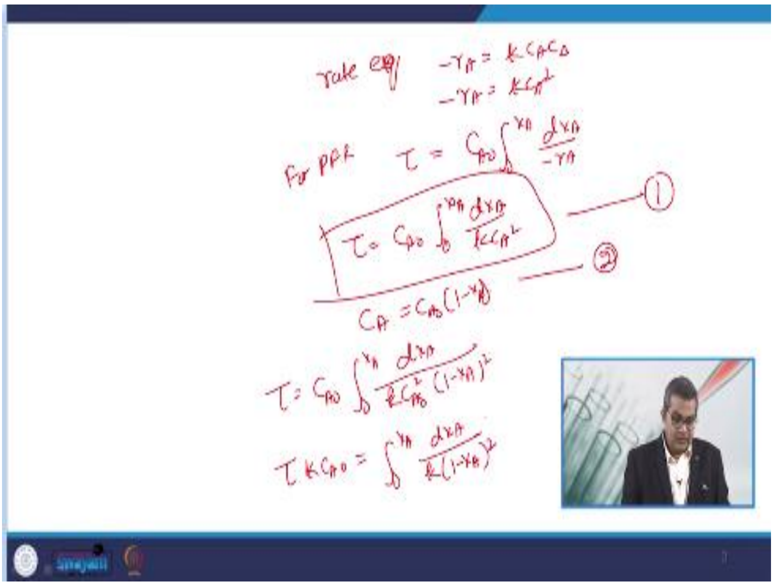
Here, this particular lecture, we are attributing ourselves with the multiple reactions. So, let us have the first problem into cognition. Now, the elementary second order reaction, we are dealing with, I mean the liquid phase reaction with A + B is equal to C + D. This is usually conducted in an isothermal plug flow reactor of 1 metre cube capacity. The inlet volumetric flow rate is 10 metre cube per hour.

And here the C_{A0} is equal to C_{B0} and this is equal to 2 kilo mole per metre cube. So, under these conditions, the conversion of A is 50%. So, now, if a stirred tank reactor of 2 metre cube capacities installed in series upstream of the plug flow reactor, then you need to find out the conversion what type, what conversion can be expected in the new system of reactor.

So, first, let us have a look at what is provided. So, it is given that this is the plug flow reactor. Here, the volume is 1 metre cube and V_0 is equal to, that is volumetric flow rate is equal to 10 metre cube per hour. C_{A0} is equal to 2 kilo mole per metre cube, then C_{B0} is equal to 2 kilo mole per metre cube. Obviously, because the C_0 is equal to C_{B0}. This is given and the reaction is A + B is converting into C + D.

And X_A is because the conversion is 50%, so, X_A is 0.5. So, based on the equalistic stoichiometric of the reaction, this is C_A is equal to C_B.

(Refer Slide Time: 02:34)



rate eq $-r_A = k C_A C_B$

$-r_A = k C_A^2$

For PFR $\tau = C_{A0} \int^{X_A} \frac{dX_A}{-r_A}$

$$\boxed{\tau = C_{A0} \int_0^{X_A} \frac{dX_A}{k C_A^2}} \text{ — ①}$$

$$C_A = C_{A0}(1-X_A) \text{ — ②}$$

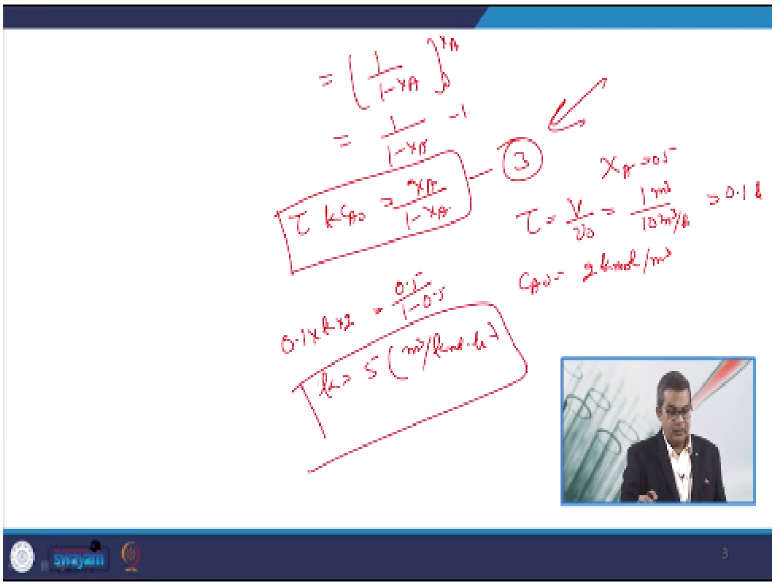
$$\tau = C_{A0} \int_0^{X_A} \frac{dX_A}{k C_{A0}^2 (1-X_A)^2}$$

$$\tau k C_{A0} = \int_0^{X_A} \frac{dX_A}{k(1-X_A)^2}$$

So far, the second order reaction, the rate equation can be given as $-r_A$ is equal to k C_A C_B or this because C_A is equal to C_B. So, r_A is equal to k C_A squared. Now, for PFR the performance equation can be written as tau is equal to C_{A0}, 0 to X_A, dX_A upon $-r_A$ or tau is equal to C_{A0}, 0 to X_A, dX_A upon k C_A square. So, this is my question number 1.

Now, as it is given that C_A is equal to C_{A0} 1 – X_A that is my question number 2. So, from equation 1 and equation 2, we have tau is equal to C_{A0}, 0 to X_A, dX_A upon k C_{A0} squared 1 – X_A squared and it can be represented or rearranged as the tau k C_{A0} is equal to 0 to X_A, dX_A upon k 1 – X_A squared.

(Refer Slide Time: 03:58)



$$= \left(\frac{1}{1-X_A}\right)_0^{X_A}$$

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

$$\boxed{\tau k C_{A0} = \frac{X_A}{1-X_A}} \quad ③$$

$X_A = 0.5$

$$\tau = \frac{V}{v_0} = \frac{1\,m^3}{10\,m^3/h} = 0.1\,h$$

$C_{A0} = 2\,kmol/m^3$

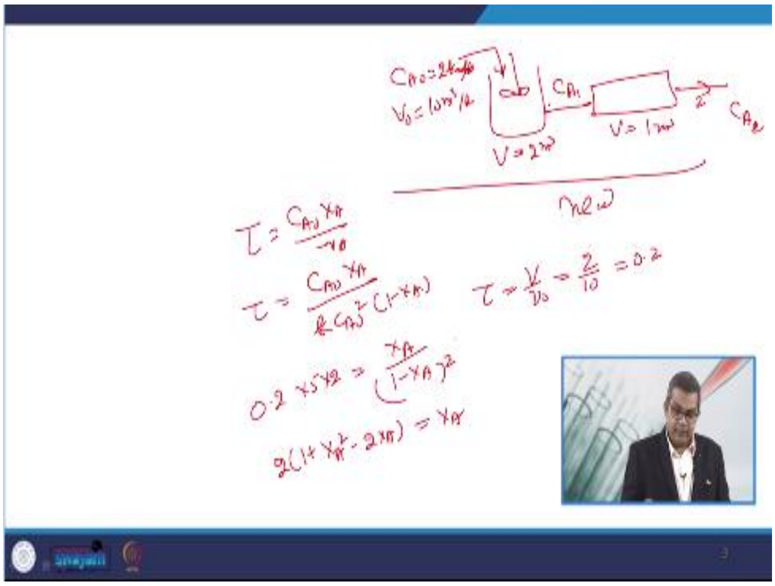
$$0.1 \times k \times 2 = \frac{0.5}{1-0.5}$$

$$\boxed{k = 5\ (m^3/kmol \cdot h)}$$

Now, this is comes out to be 1 upon 1 – X_A, 0 to X_A and this is 1 upon 1 – X_A – 1 or it can be represented as tau k C_{A0} is equal to X_A – 1 – X_A that is my equation number 3. Now, if given X_A is equal to 0.5, the tau is equal to V upon V_0 V divided by a volumetric flow rate at the start 1 metre cube upon 10 metre cube per hour that comes out to be 0.1 hour and C_{A0} is equal to 2 kilo mole per metre cube which is already given.

So, if you substitute all these values in this particular equation, we will have 0.1 into k into 2 that is equal to 0.5, 1 – 0.5 and k is equal to 5 metre cube per kilo mole hour.

(Refer Slide Time: 05:14)



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

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

$$\tau = \frac{V}{v_0} = \frac{2}{10} = 0.2$$

$$0.2 \times 5 \times 2 = \frac{X_A}{(1-X_A)^2}$$

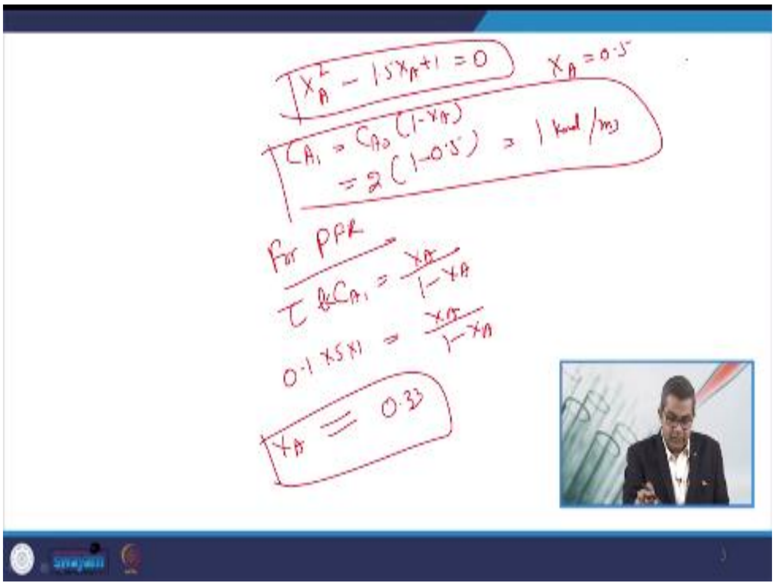
$$2(1 + X_A^2 - 2X_A) = X_A$$

Now, if as per the problem, if a new MFR is attached before the plug flow reactor in series, then we may have this type of reaction stream. Now, this is C_{A2}, this is the second phase V is given 1 metre cube and here this V is given us 2 metre cube, this is the C_{A1} and these are having the initial conditions which is given the problem V_0 volumetric flow rate is 10 metre cube per hour.

So, performance, this is my new scheme. So, the performance equation for the CSTR is, as we know that tau is equal to C_{A0} X_A upon minus r_A and we can write this tau is equal to C_{A0} X_A upon k C_{A0} 1 – X_A. Now, if we substitute all the values to this particular equation keeping the mu that for CSTR or MFR, V upon, tau is equal to V upon volumetric flow rate that is start that is given us 2 by 10 that is 0.2.

So, if we substitute all the values, then it becomes 0.2 into 5 into 2 that is equal to X_A upon 1 – X_A square and that comes out to be 2 into 1 + X_A square 2 X_A is equal to X_A.

(Refer Slide Time: 07:04)



$$\boxed{X_A^2 - 1.5X_A + 1 = 0} \quad X_A = 0.5$$

$$\boxed{\begin{aligned} C_{A_1} &= C_{A_0}(1-X_A) \\ &= 2(1-0.5) = 1 \text{ kmol/m3} \end{aligned}}$$

For PFR

$$\tau k C_{A_1} = \frac{X_A}{1-X_A}$$

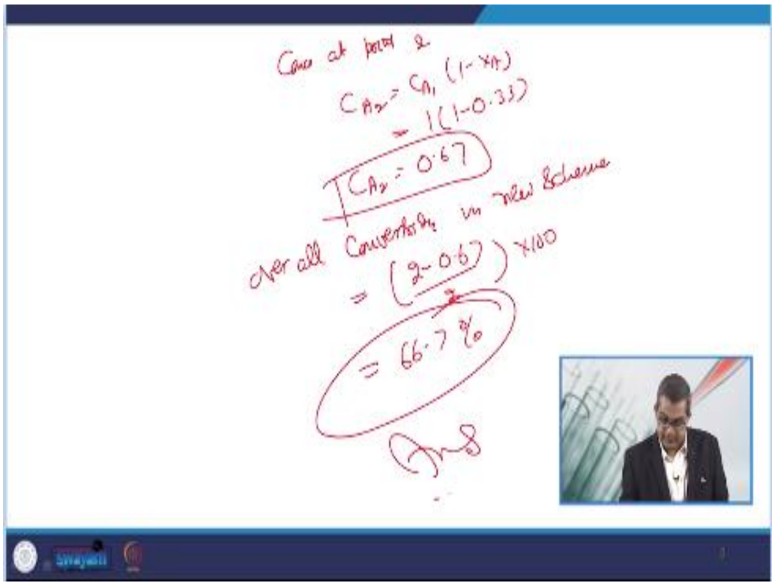
$$0.1 \times 5 \times 1 = \frac{X_A}{1-X_A}$$

$$\boxed{X_A = 0.33}$$

And we have this equation upon rearrangement X_A square 1 point, X_A squared – 1.5 into X_A + 1 that is equal to 0. So, if we solve this, then we have that X_A is equal to 0.5. Now, the concentration at point 1 in the previous equation that is 0.1, this can be given as C_{A1} is equal to C_{A0} 1 – X_A and if we substitute all the values, this is given is equal to 2 into 1 – 0.5 and that is 1 kilo mole per metre cube.

So, now, for PFR, the tau k C_{A1} is equal to X_A upon 1 – X_A or 0.1 into 5 into 1 that is X_A upon 1 – X_A and X_A in this condition is given as 0.33. We have find it out. So, now, we need to find out that concentration at this particular point, this particular point, so, how we can calculate? That we will deal in this point that the concentration at point 2.

(Refer Slide Time: 08:36)



Conc at point 2

$C_{A_2} = C_{A_1}(1-X_A)$

$= 1(1-0.33)$

$\boxed{C_{A_2} = 0.67}$

Over all Conversion in new Scheme

$= \left(\frac{2-0.67}{2}\right)\times 100$

$\boxed{= 66.7\,\%}$

Ans

So, C_{A2} is equal to C_{A1} $1 - X_A$ and that is 1 into 1 – 0.33 and that C_{A2} is equal to 0.67. So, the overall conversion in the new scheme can be given by the overall conversion in new scheme that is equal to 2 – 0.67 upon 2 into 100 and that is 66.7% that is my answer.

(Refer Slide Time: 09:26)

Solution;

Given

$v_0 = 10\ m^3/h$

$C_{A0} = C_{B0} = 2\ kmol/m^3$

$X_A = 0.5$

$C_A = C_B$

Rate equation

$-r_A = kC_AC_B$

For PFR

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

$$C_A = C_{A_o}(1 - X_A) \quad (2)$$

$$\tau = \frac{V}{v_o} = C_{A_o}\int_0^{X_A}\frac{dX_A}{kC_{A_0}{}^2(1+X_A)^2}$$

$$\tau C_{A_o}k = \int_0^{X_A}\frac{dX_A}{(1+X_A)^2}$$

$$\tau C_{A_o}k = [\frac{1}{(1+X_A)}]_0^{X_A}$$

on solving it we have

$$\tau C_{A_o} k = \frac{X_A}{(1+X_A)} \quad (3)$$

$$X_A = 0.5$$

$$\tau = \frac{V}{v_0} = \frac{1}{10} = 0.1\ h$$

$$C_{A_o} = 2\ \text{kmol/m}^3$$

$$0.1 \times 2 \times k = \frac{0.5}{(1+0.5)}$$

$$k = 5\ \text{m}^3/\text{kmol.h}$$

If two reactors are connected in series

For first one MFR

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

$$\tau = \frac{V}{v_o} = \frac{2}{10} = 0.2$$

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

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

$$0.2 \times 5 \times 2 = \frac{X_A}{(1-X_A)^2}$$

$$\Rightarrow X_A{}^2 - 1.5X_A + 1 = 0$$

On solving we have

$$X_A = 0.5$$

$$C_{A1} = C_{A_o}(1-X_A)$$

$$C_{A1} = 2(1-0.5)$$

$$C_{A1} = 1\ \text{kmol/m}^3$$

For PFR

From equation (3), on putting the value of variables we have

$$0.1 \times 5 \times 1 = \frac{X_A}{(1+X_A)}$$

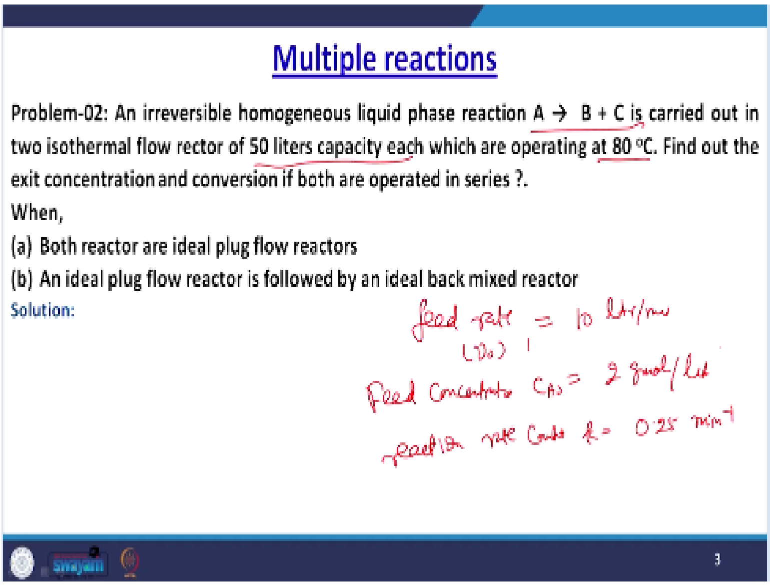
$$\Rightarrow X_A = 0.33$$

$$C_{A_2} = C_{A_1}(1-X_A)$$

$$\Rightarrow C_{A_2} = 0.67$$

Overall conversion in new scheme is

$$= \frac{2-0.67}{2} \times 100 = 66.7\% \text{ (answer)}$$



Multiple reactions

Problem-02: An irreversible homogeneous liquid phase reaction A → B + C is carried out in two isothermal flow rector of 50 liters capacity each which are operating at 80 °C. Find out the exit concentration and conversion if both are operated in series ?.

When,

(a) Both reactor are ideal plug flow reactors

(b) An ideal plug flow reactor is followed by an ideal back mixed reactor

Solution:

feed rate (v_0) = 10 ltr/min

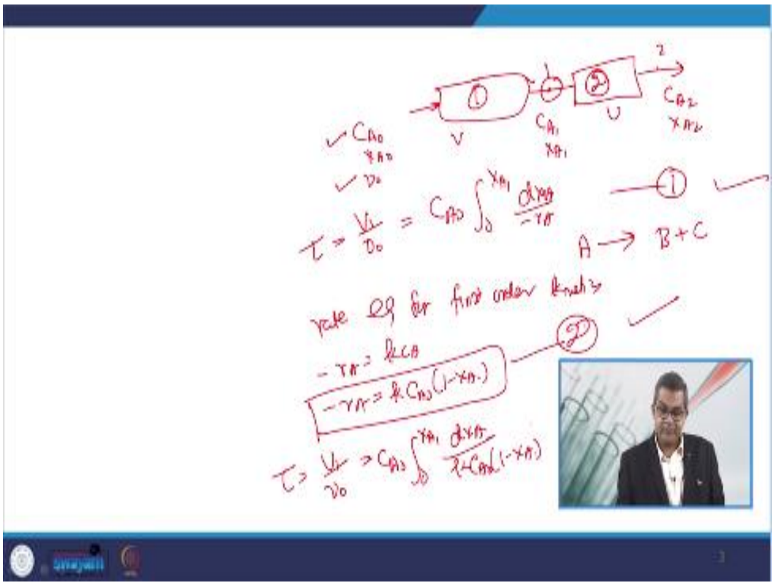
Feed Concentration C_{A0} = 2 gmol/ltr

reaction rate Const $k = 0.25\ \text{min}^{-1}$

Now, let us take another problem. Here, an irreversible homogeneous liquid phase reaction is carried out with this scheme that A is decomposes or A is converted into B and C. The reactors are 2 isothermal flow reactors with a capacity of 50 litre each and these reactors are operating at a condition of 80 degrees Celsius. You need to find out the exit concentration and conversion if both are operated in series.

Now, there are 2 conditions are given. Both reactors are ideal plug flow reactor and second condition is given that an ideal plug flow reactor is followed by an ideal back mixed reactor. Now, data is given. The supporting data is given that is the feed rate is 10 that is v, small v 0 that is 10 litre per minute. Now, feed concentration that is C_{A0} is 2-gram mole per litre and reaction rate constant that is k is equal to 0.25-minute inverse.

(Refer Slide Time: 10:52)



$$\tau = \frac{V_1}{v_0} = C_{A0}\int_0^{X_{A1}} \frac{dX_A}{-r_A} \text{ ——— } ①$$

$$A \rightarrow B + C$$

rate eq for first order kinetics

$$-r_A = kC_A$$

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

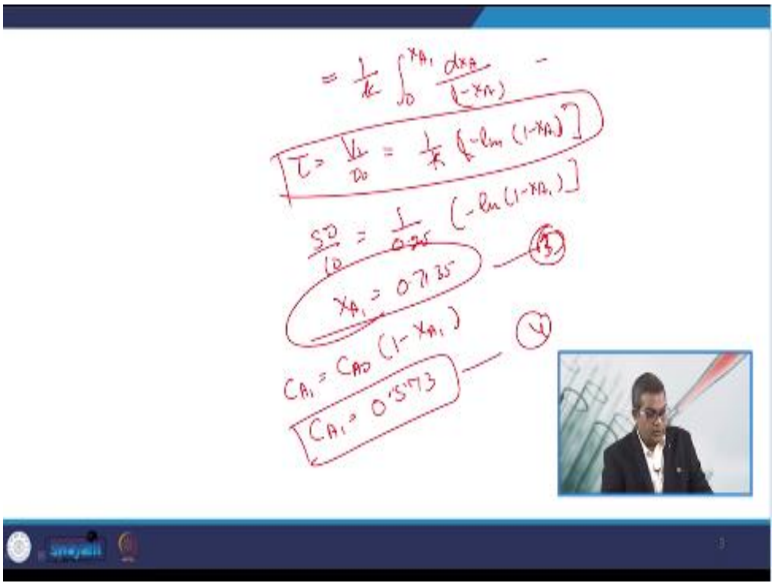
$$\tau = \frac{V_1}{v_0} = C_{A0}\int_0^{X_{A1}} \frac{dX_A}{kC_{A0}(1-X_A)}$$

So, let us have that how we can solve if both reactors are ideal because the conditions are given that both reactors are ideal plug flow reactor. Now, in that case, we can have this reactor like this 1 and 2. Now, here C_{A2} X_{A2}, V, V and here the C_{A1} and X_{A1} and here the C_{A0} X_{A0} and V_0. So, both plug flow reactors are connected in the series. They are having the same volume of 50 litre.

Now, if initially feeds charging to the first reactor having the concentration of reactant C_{A0} and the feed rate v small v 0 with no conversion that is X_A is equal to 0. Now, for the conversion at point 1, they are at the exit of the first reactor the performance equation for the first plug flow reactor can be written as tau is equal to V_1 upon v_0 is equal to C_{A0} X_{A1} dX_A upon – r_A that is equation number 1.

Now, if A is having converting into B + C, so, the rate equation for first order kinetics can be written as – r_A is equal to k C_A or – r_A is equal to k C_{A0} 1 – X_A. This is my equation number 2. Now, so, from equation 1 and equation 2, we have tau is equal to V_1 upon v_0 that is equal to C_{A0}, 0 to X_{A1} dX_A upon k C_{A0} 1 – X_A.

(Refer Slide Time: 13:06)



$$= \frac{1}{k}\int_0^{X_{A_1}} \frac{dX_A}{(1-X_A)}$$

$$\boxed{\tau = \frac{V_1}{v_0} = \frac{1}{k}\left[-\ln(1-X_{A_1})\right]}$$

$$\frac{50}{10} = \frac{1}{0.25}\left(-\ln(1-X_{A_1})\right] \quad ③$$

$$\boxed{X_{A_1} = 0.7135}$$

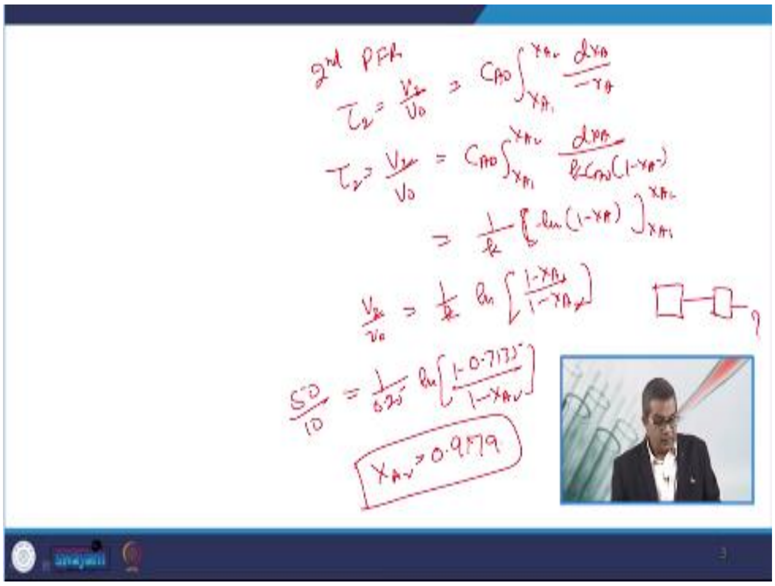
$$C_{A_1} = C_{A0}(1-X_{A_1}) \quad ④$$

$$\boxed{C_{A_1} = 0.573}$$

Or upon rearranging, we can write this as X_A 1 dX_A upon 1 – X_A which is comes out to be, upon integration which comes out to be tau is equal to V_1 upon v_0 is equal to 1 upon k – ln 1 – X_{A1}. So, if we substitute the values which is given in the problem that is 50 upon 10 is equal to 1 upon 0.25 into ln 1 – X_{A1}. Now, X_{A1} is equal to 0.7135.

Now, the concentration at point 1 that is the outlet of first reactor that can be find it out by C_{A1} is equal to C_{A0} 1 – X_{A1} which we have already determined, C_0 is given to 2. So, C_{A1} is equal to 0.573. Now, this, let us termed that the equation number 3 and this is termed as 4. So, if similarly, we can find out for plug flow reactor number 2.

(Refer Slide Time: 14:35)



2nd PFR

$$\tau_2 = \frac{V_2}{v_0} = C_{A0}\int_{X_{A_1}}^{X_{A_2}} \frac{dX_A}{-r_A}$$

$$\tau_2 = \frac{V_2}{v_0} = C_{A0}\int_{X_{A_1}}^{X_{A_2}} \frac{dX_A}{kC_{A0}(1-X_A)}$$

$$= \frac{1}{k}\left[-\ln(1-X_A)\right]_{X_{A_1}}^{X_{A_2}}$$

$$\frac{V_2}{v_0} = \frac{1}{k}\ln\left[\frac{1-X_{A_1}}{1-X_{A_2}}\right]$$

$$\frac{50}{10} = \frac{1}{0.25}\ln\left[\frac{1-0.7135}{1-X_{A_2}}\right]$$

$$\boxed{X_{A_2} = 0.9779}$$

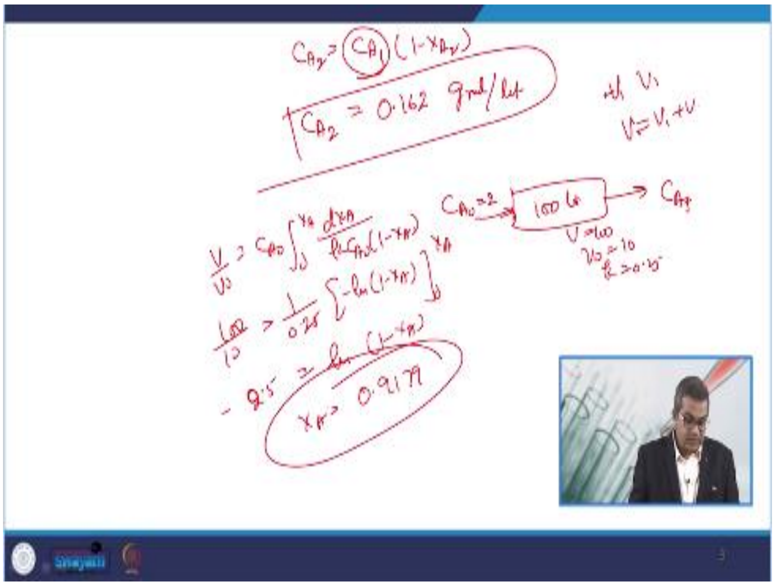
Now, the exit is streamed from the first reactor become the feed stream to the second reactor with the concentration C_{A1}. So, the initial conversion is X_{A1} and the final conversion is X_{A2}.

So, both of things we have already find out that is C_{A1} already find it out and initial concentration X_{A1}, we have already find out. So, the performance equation for the second plug flow reactor, this can be tau 2 is equal to V_2 upon v_0 that is equal to C_{A0} X_{A1} X_{A2} dX_A upon $-r_A$.

And if we try to solve it, tau 2 is equal to V_2 upon v_0 that is C_{A0} X_{A1} X_{A2} dX_A upon k C_{A0} 1 – X_A or this comes out to be 1 upon k – ln 1 – X_A X_{A2} X_{A1} and V_2 upon v_0 is equal to 1 upon k ln 1 – X_{A1} upon 1 – X_{A2}. So, if we substitute the values this to this particular equation that is given that 50 upon 10 which is already given in the problem and k is given as 0.25 ln 1 – 0.7135 upon 1 – X_{A2}.

So, the X_{A2} comes out to be 0.9179. So, now, let us talk about the concentration at point 2 that is at the exit of the second reactor.

(Refer Slide Time: 16:38)



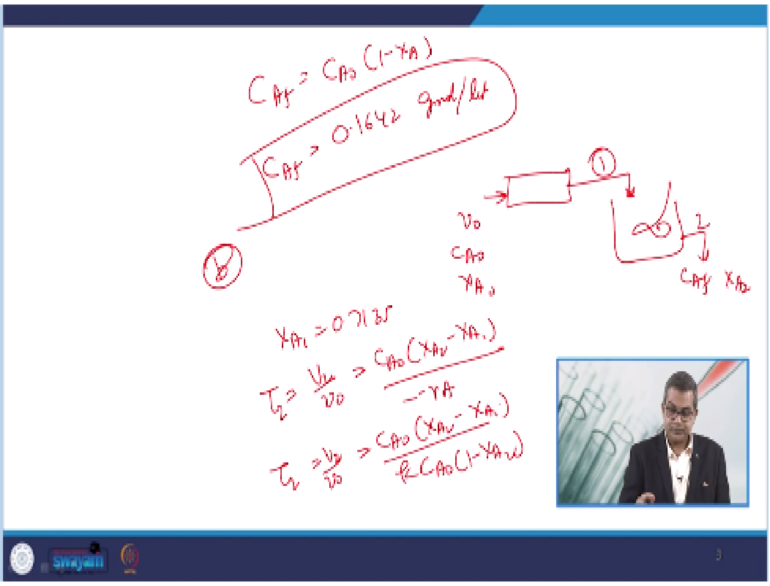
So, this C_{A2} is equal to C_{A1} into 1 – X_2. Remember here, this is the initial concentration of for reactor number 2. So, if we put all the values, then we will find that C_{A2} is comes out to be 0.162 gram mole per litre, because every other things are given in this (( )) (17:04). So far, to plug flow reactor in series the volume V_1, V_2, a single plug flow reactor of volume V is equal to $V_1 + V_2$.

So, gives us the same conversion at the exit of as 2 given is combined. So, if both are having the individual volume V_1 and V_2 and if they are having a single plug flow reactor, then V is equal to $V_1 + V_2$. So, both are giving the same conversion. Now, to prove this, we have taken a single reactor of volume 100 litre and check whether the final conversion and concentration.

So, if we take the single reactor of volume 100 litre, now, here this is 100 litres. Now, this C_{Af} and this one is C_{A0} that is equal to 2. Now, V is equal to 100, V_0 is equal to 210, k is equal to 0.25. I am not putting the units of this one because it is quite evident and given the problem. Now, if we write V upon v_0 is equal to C_{A0}, 0 to X_A dX_A upon k C_{A0} $1 – X_A$ or 100 upon 10 is equal to 1 upon 0.25 – ln $1 – X_A$, 0 to X_A.

And if we substitute the values that – 2.5 is equal to ln $1 – X_A$, then X_A find out to be 0.9179. This is the value of X_A at the exit.

(Refer Slide Time: 18:58)



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

$C_{Af} = 0.1642$ gmol/lit

$X_{A1} = 0.7135$

$\tau_2 = \frac{V_2}{v_0} = \frac{C_{A0}(X_{A2}-X_{A1})}{-r_A}$

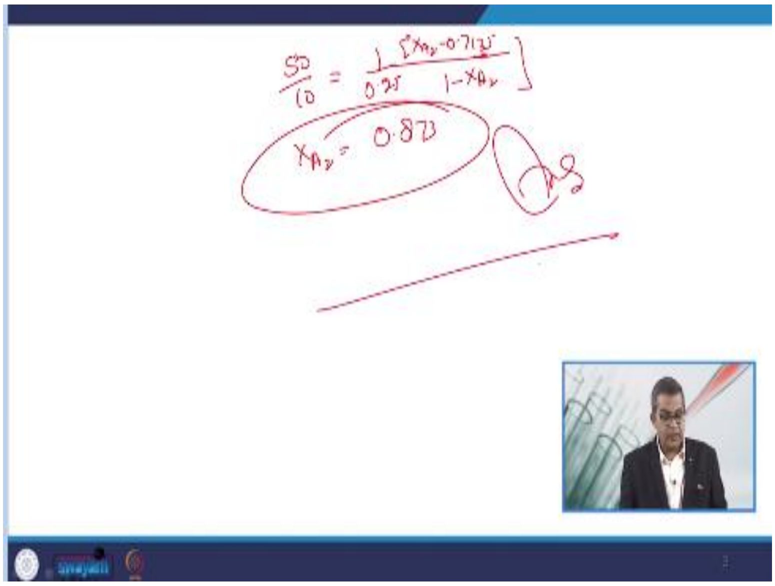
$\tau_2 = \frac{V_2}{v_0} = \frac{C_{A0}(X_{A2}-X_{A1})}{kC_{A0}(1-X_{A2})}$

Now, the concentration at the exit of the PFR reactor, which is having the volume of 100, then C_{Af} is equal to C_{A0} $1 – X_A$, we have find out the value of X_A. We are having the value of C_{A0} equal to 2. So, C_{Af} is 0.1642-gram moles per litre. So, therefore, single plug flow reactor of total volume that is equal to 100 litre gives the same conversion as the 2-plug flow reactor of the volume having V 1 is equal to 50 and V 2 is equal to 50.

Now, let us move to the part B of this particular problem. Here, the ideal plug flow reactor followed by the mixed flow reactor. So, here, this is my plug flow reactor and this is my mixed flow reactor. Now, here, we are having C_{Af} that is point 2 and point 1 and X_{A2} and here, C these are the coordinates and the values are given as. Now, the first plug flow reactor, the value V the conversion which we have already found out that is X_{A1} is equal to 0.7135.

Now, let X_{A2} be the conversion at the exit of the mixed flow reactor at point 2. So, the performance equation, which we can write V_2 upon v_0 is equal to C_{A0} $X_{A2} – X_{A1}$ upon $– r_A$ and tau, this is tau 2, tau 2 is equal to V_2 upon v_0 that is equal to C_{A0} $X_{A2} – X_{A1}$ upon k C_{A0} $1 – X_{A2}$.

(Refer Slide Time: 21:00)



$$\frac{50}{10} = \frac{1}{0.25}\left[\frac{X_{A_2}-0.7135}{1-X_{A_2}}\right]$$

$$\boxed{X_{A_2} = 0.873}$$

$\boxed{\text{Ans}}$

Now, if we substitute all the values, then it becomes the 50 upon 10 is equal to 1 upon 0.25 into X_{A2} – 0.7135, already find out this one, – 1 upon X_{A2}. Now, if we solve this X_{A2}, it is coming out to be 0.873. So, this is my answer to this particular problem.

(Refer Slide Time: 21:34)

Solution;

Given

Feed rate (v_0) = 10 litre/min

Feed concentration (C_{A0}) = 2 mol/litre

Reaction rate constant (k) = 0.25 min^{-1}

(i) If both PFR of capacity 50 L connected in series

$$\tau = \frac{V_1}{v_o} = C_{A_o}\int_0^{X_A} \frac{dX_A}{-r_A}$$

Rate equation for first order reaction

$$-r_A = kC_A$$

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

$$\tau = \frac{V_1}{v_o} = C_{A_o}\int_0^{X_{A1}} \frac{dX_A}{kC_{A_o}(1 - X_A)}$$

$$\tau = \frac{V_1}{v_o} = -\frac{1}{k}\ln(1 - X_A)$$

on putting value of V_1 v_0 and X_A in the above equation we have

$$X_{A1} = 0.7135$$

$$C_{A_1} = C_{A_o}(1 - X_{A_1})$$

$$C_{A_1} = 0.573$$

In second PFR

$$\tau_2 = \frac{V_2}{v_o} = C_{A_o}\int_{X_{A_1}}^{X_{A_2}} \frac{dX_A}{-r_A}$$

$$\tau_2 = C_{A_o}\int_{X_{A_1}}^{X_{A_2}} \frac{dX_A}{kC_{A_o}(1 - X_A)}$$

$$\tau_2 = C_{A_o}\int_{X_{A_1}}^{X_{A_2}} \frac{dX_A}{kC_{A_o}(1 - X_A)}$$

$$\tau_2 = -\frac{1}{k}[\ln(1 - X_A)]_{X_{A_1}}^{X_{A_2}}$$

$$\Rightarrow \tau_2 = \frac{1}{k}\ln\left[\frac{(1 - X_{A_1})}{1 - X_{A_2}}\right.$$

$$\Rightarrow \tau_2 = \frac{50}{10} = \frac{1}{0.25}\ln\left[\frac{(1 - 0.7135)}{(1 - X_{A_2})}\right]$$

$$X_{A_2} = 0.9179$$

$$C_{A_2} = C_{A_1}(1 - X_{A_2})$$

$$\Rightarrow C_{A_2} = 0.162$$

If single reactor of 100 litre is used instead of two 50 litre volume reactors in series, then we have

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

$$\tau_2 = \frac{100}{10} = -\frac{1}{0.25}[\ln(1 - X_A)]_0^{X_A}$$

$$-0.25 = \ln(1 - X_A)$$

$$X_A = 0.9179$$

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

$$C_{A_S} = 0.162 \text{ gmol/litre}$$

i.e., two PFR in series gives same conversion if a single reactor of same volume is operated.

If PFR followed by MFR

$$X_{A1} = 0.7135$$

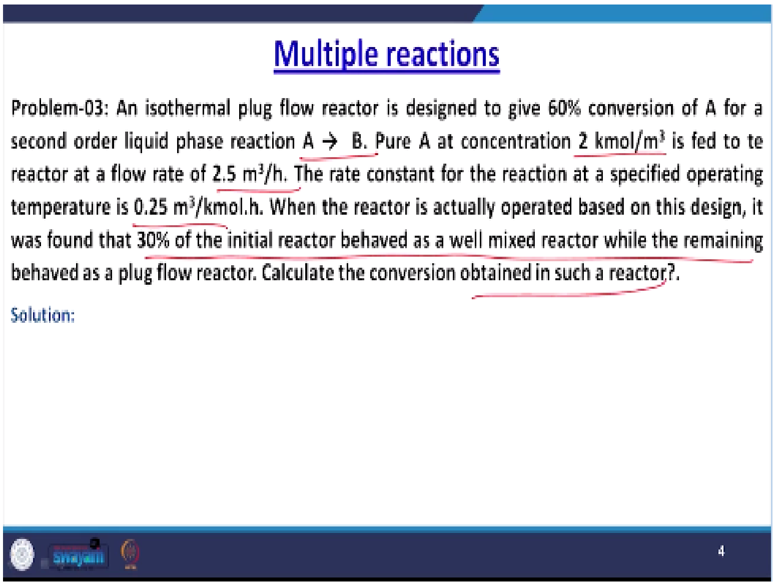
$$\tau_2 = \frac{V_2}{v_o} = \frac{C_{A_o}(X_{A_2} - X_{A_1})}{-r_A}$$

$$\Rightarrow \tau_2 = \frac{V_2}{v_o} = \frac{(X_{A_2} - X_{A_1})}{k(1 - X_{A_2})}$$

$$\Rightarrow \frac{50}{10} = \frac{(X_{A_2} - 0.7135)}{0.25(1 - X_{A_2})}$$

On solving we have

$$X_{A_2} = 0.823 \text{ (answer)}$$



Multiple reactions

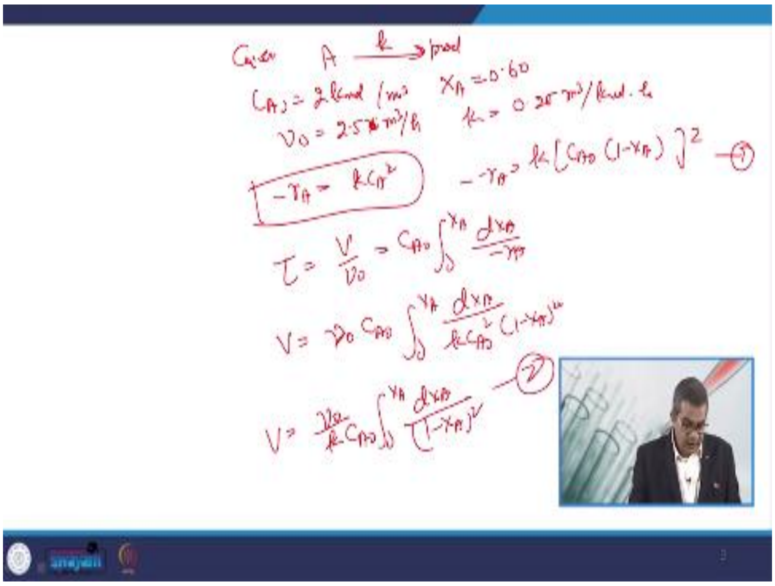
Problem-03: An isothermal plug flow reactor is designed to give 60% conversion of A for a second order liquid phase reaction A → B. Pure A at concentration 2 kmol/m³ is fed to te reactor at a flow rate of 2.5 m³/h. The rate constant for the reaction at a specified operating temperature is 0.25 m³/kmol.h. When the reactor is actually operated based on this design, it was found that 30% of the initial reactor behaved as a well mixed reactor while the remaining behaved as a plug flow reactor. Calculate the conversion obtained in such a reactor?.

Solution:

Let us take another problem that is in isothermal plug flow reactor is designed to give the 60% conversion of A for a second order liquid phase reaction that is given as A is converting into B. Now, pure A at a concentration of 2 kilo mole per metre cube is fed to be the reactor at a flow rate of 2.5 metre cube per hour. The rate constant for the reaction at a specified operating temperature is given as 0.25 metre cube upon kilo mole per hour.

Now, when that reactor is actually operated based on this design, it was found that 30% of initial reactor behaved as a well-mixed reactor while that remaining behaved as a plug flow reactor. So, you need to calculate the conversion and obtained in such type of reactor. So, it is, you can say, a mix type of a problem. So, let us have a look of this particular problem in a different mode.

(Refer Slide Time: 22:41)



Given $A \xrightarrow{k} \text{prod}$

$C_{A0} = 2\ \text{kmol/m}^3$ $X_A = 0.60$

$v_0 = 2.5\ \text{m}^3/\text{h}$ $k = 0.25\ \text{m}^3/\text{kmol}\cdot\text{h}$

$\boxed{-r_A = kC_A^2}$ $-r_A = k[C_{A0}(1-X_A)]^2$ —①

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

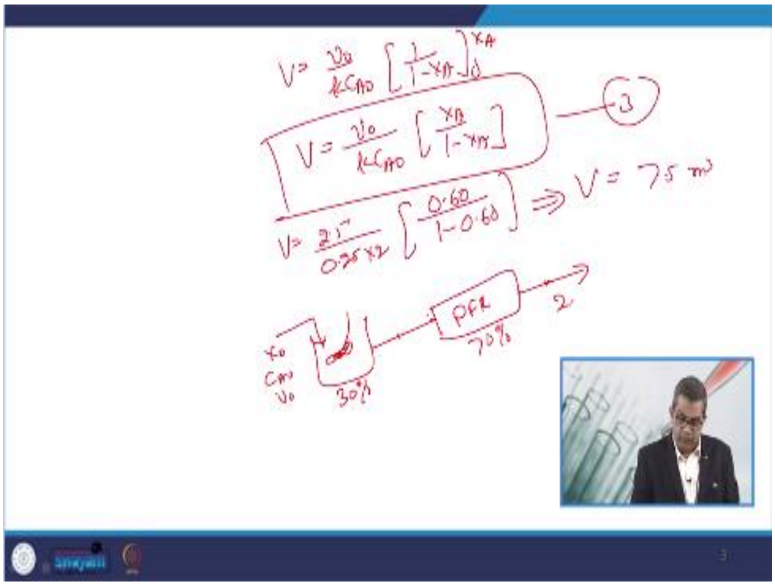
$V = v_0 C_{A0}\int_0^{X_A}\frac{dX_A}{kC_{A0}^2(1-X_A)^2}$

$V = \frac{v_0}{kC_{A0}}\int_0^{X_A}\frac{dX_A}{(1-X_A)^2}$ —②

Now, it is given that A is converted into product and C_{A0} is equal to 2 kilo mole per metre cube, where you see that X_A is given that 60% of the conversion that means X_A is 0.60. Initial flow rate is given 2.5 into metre cube per hour. Now, k is given to 0.255 metre cube per kilo mole per hour. Now, decomposition of reactant A in the second order, so, we require, we equate the second order decomposition of the reactant A. So, this is equal to – r_A k C_A square.

Now, in terms of a conversion – r_A is equal to k C_{A0} 1 – X_A. This is my first equation. So, when we talk about the performance equation for plug flow reactor that is tau is equal to V upon v_0 C_{A0}, 0 to X_A dX_A upon – r_A or V is equal to v_0 C_{A0}, 0 to X_A dX_A upon k C_{A0} 1 – X_A square or V is equal to V_0 k upon C_{A0}, 0 to X_A dX_A upon 1 – X_A square that is equation number 2.

(Refer Slide Time: 24:28)



$V = \frac{v_0}{kC_{A0}}\left[\frac{1}{1-X_A}\right]_0^{X_A}$

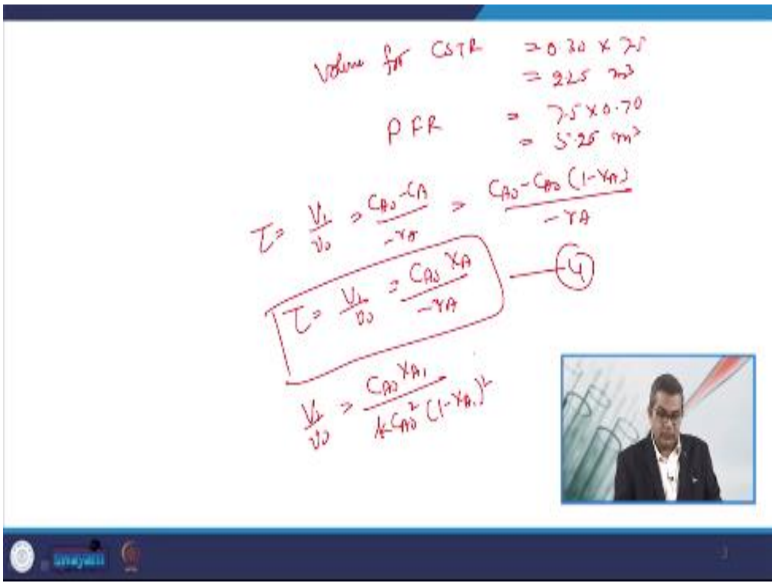
$\boxed{V = \frac{v_0}{kC_{A0}}\left[\frac{X_A}{1-X_A}\right]}$ —③

$V = \frac{2.5}{0.25\times 2}\left[\frac{0.60}{1-0.60}\right] \Rightarrow V = 7.5\ \text{m}^3$

So, if we integrate this equation number 2, then we find that V is equal to v_0 k C_{A0} 1 upon 1 – X_A that is this one and upon rearranging all these things, we find that V is equal to v_0 upon k C_{A0} X_A upon 1 – X_A. That is my equation number 3. So, if we substitute the given value whatever given in the question in this equation, we may find that V is equal to 2.5 upon 0.25 into 2 into 0.60 upon 1 – 0.60 that is V is equal to 7.5 metre cube.

Now, it is given that when reactor operated based on this design then 30% of initial reactor behaved as a mixed flow reactor and remaining as a plug flow reactor. So, let us redesign the things here, this is your MFR 30%. Now, it is my PFR which handles with 70%. So, initially, we have X_0, C_{A0}, V_0.

(Refer Slide Time: 26:04)



Volume for CSTR $= 0.30 \times 7.5$

$= 2.25\ m^3$

PFR $= 7.5 \times 0.70$

$= 5.25\ m^3$

$$\tau = \frac{V_1}{v_0} = \frac{C_{A0} - C_A}{-r_A} = \frac{C_{A0} - C_{A0}(1 - X_A)}{-r_A}$$

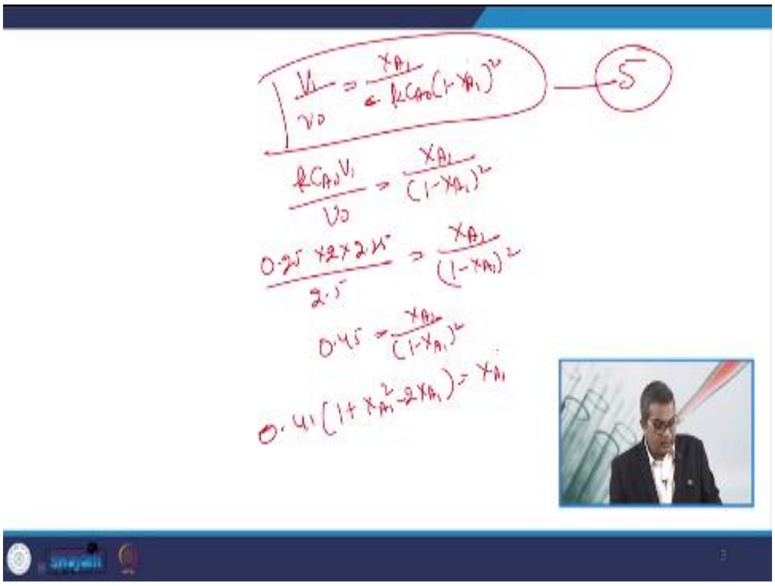
$$\boxed{\tau = \frac{V_1}{v_0} = \frac{C_{A0} X_A}{-r_A}} \quad ④$$

$$\frac{V_1}{v_0} = \frac{C_{A0} X_{A1}}{k C_{A0}^2 (1 - X_{A1})^2}$$

Now, the volume for CSTR would be 0.30 into 7.5 and that is 2.25 metre cube and for PFR that is 7.5 into 0.70 and that is comes out to be 5.25 metre cube. Now, the conversion X 1 add the exit of the CSTR in the previous problem, the performance equation can be written as V_1 upon v_0 that is equal to C_{A0} – C_A upon – r_A and that is C_{A0} – C_{A0} into 1 – X_A upon – r_A and tau is equal to V_1 upon v_0 that is equal to C_{A0} X_A upon – r_A that is my equation number 4.

So, from equation 1 and 4, we may have this V_1 upon 0 is equal to C_{A0} X_{A1} upon k C_{A0} square, 1 – X_{A1} square.

(Refer Slide Time: 27:18)



$$\boxed{\frac{V_1}{v_0} = \frac{X_{A1}}{kC_{A0}(1-X_{A1})^2}} \longrightarrow ⑤$$

$$\frac{kC_{A0}V_1}{v_0} = \frac{X_{A1}}{(1-X_{A1})^2}$$

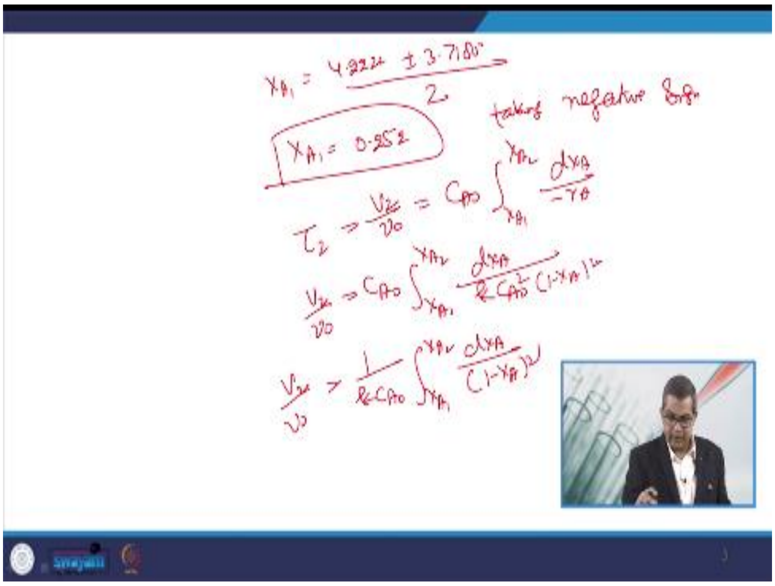
$$\frac{0.25 \times 2 \times 2.25}{2.5} = \frac{X_{A1}}{(1-X_{A1})^2}$$

$$0.45 = \frac{X_{A1}}{(1-X_{A1})^2}$$

$$0.41(1+X_{A1}^2-2X_{A1}) = X_{A1}$$

So, V_1 upon v_0 is equal to X_{A1} – upon k C_{A0}, 1 – X_{A1} squared that is my equation number 5. So, if we go ahead with this thing, then k C_{A0} V_1 upon v_0 is equal to X_{A1} into 1 – X_{A1} square. So, on putting the values for known parameter, we may have 0.25 into 2 into 2.25 upon 2.5, this is equal to X_{A1} upon 1 – X_{A1} squared or 0.45 equal to X_{A1} upon 1 – X_{A1} squared or 0.41 into 1 + X_{A1} squared – 2 X_{A1} is equal to X_{A1}.

(Refer Slide Time: 28:34)



$$X_{A1} = \frac{4.2222 \pm 3.7185}{2}$$

$$\boxed{X_{A1} = 0.252}$$

taking negative sign

$$\tau_2 = \frac{V_2}{v_0} = C_{A0}\int_{X_{A1}}^{X_{A2}} \frac{dX_A}{-r_A}$$

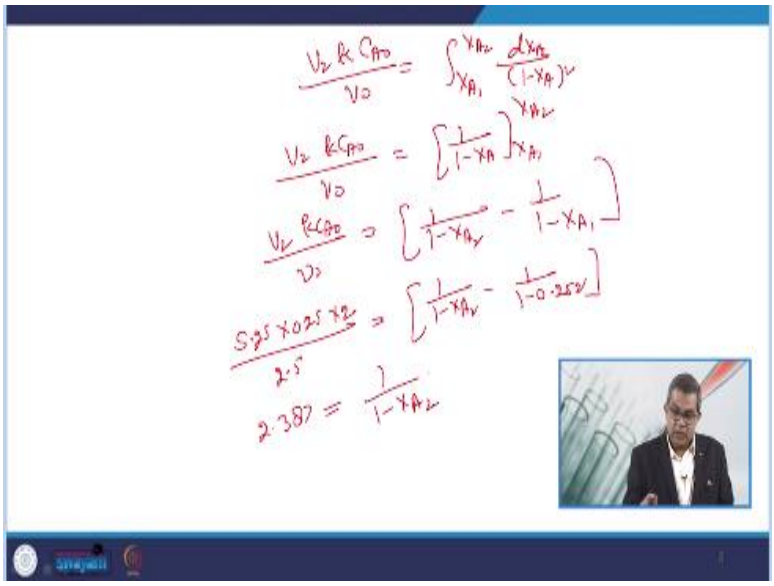
$$\frac{V_2}{v_0} = C_{A0}\int_{X_{A1}}^{X_{A2}} \frac{dX_A}{kC_{A0}^2(1-X_A)^2}$$

$$\frac{V_2}{v_0} = \frac{1}{kC_{A0}}\int_{X_{A1}}^{X_{A2}} \frac{dX_A}{(1-X_A)^2}$$

And if we calculate this thing, this X A 1, we find that it is exit A 1 is equal to 4.2222 plus minus 3.7185 upon 2 and X A 1 comes out to be 0.2252 that is taking the negative sign because it cannot go beyond 1 so, taking negative sign. Now, for conversion at exit of PFR that is give the performance equation, you can write that tau 2 is equal to V_2 upon v_0 that is equal to C_{A0} X_{A1} X_{A2} dX_A upon – r_A.

Or V_2 is equal to, V_2 upon v_0 is equal to C_{A0} X_{A1} X_{A2} dX_A upon k C_{A0} into 1 – X_A square or V_2 upon v_0 is equal to 1 upon k C_{A0} X_{A1} X_{A2} dX_A upon 1 – X_A square.

(Refer Slide Time: 30:00)



$$\frac{V_2 k C_{A0}}{v_0} = \int_{X_{A1}}^{X_{A2}} \frac{dX_A}{(1-X_A)^2}$$

$$\frac{V_2 k C_{A0}}{v_0} = \left[\frac{1}{1-X_A}\right]_{X_{A1}}^{X_{A2}}$$

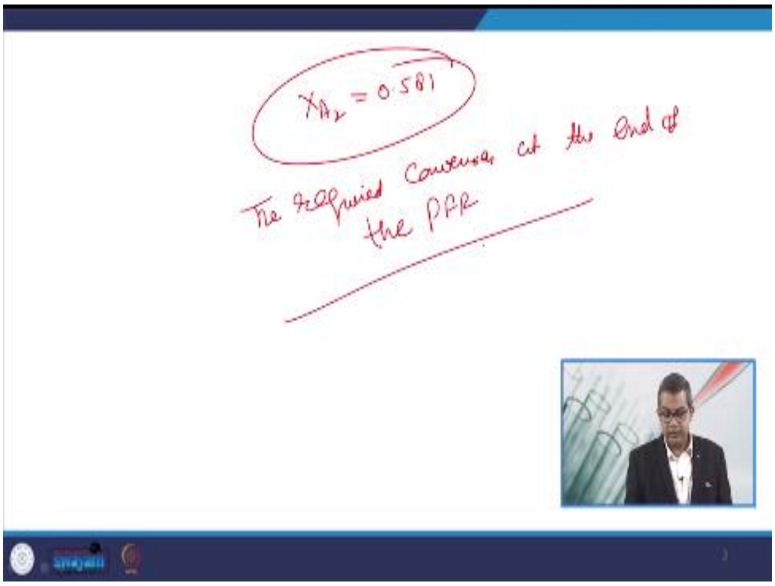
$$\frac{V_2 k C_{A0}}{v_0} = \left[\frac{1}{1-X_{A2}} - \frac{1}{1-X_{A1}}\right]$$

$$\frac{5.25 \times 0.25 \times 2}{2.5} = \left[\frac{1}{1-X_{A2}} - \frac{1}{1-0.252}\right]$$

$$2.387 = \frac{1}{1-X_{A2}}$$

So, if we go on further rearrangement, then it comes out to be V 2 k C_{A0} upon v_0 that is equal to X_{A1} X_{A2} dX_A upon the 1 – X_A square. So, upon integrating, we have V 2 k C_{A0} upon V_0 is equal to 1 upon 1 – X_A X_{A1} X_{A2}. So, V 2 k C_{A0} upon v_0 is equal to 1 upon 1 – X_{A2} – 1 upon 1 – X_{A1}. So, if we put all the known values of the parameter and solve, then we have 5.25 into 0.25 into 2 upon 2.5 that is equal to 1 upon 1 – X_{A2} – 1 upon 1 – 0.252, which we have already determined and that is 2.387 is equal to 1 upon 1 – X_{A2}.

(Refer Slide Time: 31:24)



$$\boxed{X_{A2} = 0.581}$$

The required conversion at the end of the PFR

And finally, the X_{A2} comes out to be 0.581. Now, this is the required conversion at the end of the PFR. So, by this way, we find it out for the entire segment.

(Refer Slide Time: 31:55)

Solution;

Given

For second order liquid phase reaction

$X_A = 0.6$

$C_{A0} = 2$ kmol/m^3

$v_0 = 2.5$ m^3/h

K = 0.25 m^3/kmol.h

$$-\mathrm{r_A} = C_A{}^2\mathrm{k}$$

$$-\mathrm{r_A} = \mathrm{k}C_{A_o}{}^2(1 - X_A)^2 \quad (1)$$

For PFR, the performance equation can be written as;

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

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

$$\mathrm{V} = \frac{\mathrm{v_o}}{\mathrm{kC_{A_o}}}\left[\frac{1}{1 - X_A}\right]_0^{X_A}$$

$$\mathrm{V} = \frac{\mathrm{v_o}}{\mathrm{kC_{A_o}}}\frac{X_A}{(1 - X_A)}$$

$$\mathrm{V} = \frac{2.5}{0.25 \times 2}\frac{0.6}{(1 - 0.6)}$$

$$\mathrm{V} = 75\ \mathrm{m^3}$$

Now based on question, when actually operated based on this design it was found that 30% of reactor act as MFR and rest of which act as PFR then the final conversion of such types of design is?

Volume of CSTR = 0.3x75 = 22.5 m^3

Volume of PFR = 75x0.7 = 52.5 m^3

Conversion for first CSTR

$$\tau = \frac{\mathrm{V_1}}{\mathrm{v_o}} = \frac{\mathrm{C_{A_o}} - \mathrm{C_A}}{-\mathrm{r_A}} = \frac{\mathrm{C_{A_o}X_A}}{-\mathrm{r_A}} = \frac{\mathrm{C_{A_o}X_{A1}}}{\mathrm{kC_{A_0}^2}(1 - \mathrm{X_{A1}})^2}$$

$$\Rightarrow \frac{\mathrm{V_1kC_{A_o}}}{\mathrm{v_o}} = \frac{\mathrm{X_{A1}}}{(1 - \mathrm{X_{A1}})^2}$$

$$\Rightarrow \frac{0.25 \times 2 \times 22.5}{2.5} = \frac{X_{A1}}{(1 - X_{A1})^2}$$

$$\Rightarrow 4.5(1 - X_{A1})^2 = X_{A1}$$

$$\Rightarrow 4.5{X_{A1}}^2 - 10X_{A1} + 4.5 = 0$$

$$\Rightarrow {X_{A1}}^2 - 2.22X_{A1} + 1 = 0$$

On solving above quadratic equation we have

$$X_{A1} = 0.628$$

For second operating PFR in series

$$\tau_2 = \frac{V_2}{v_o} = C_{A_o} \int_{X_{A1}}^{X_{A2}} \frac{dX_A}{-r_A}$$

$$\tau_2 = \frac{V_2}{v_o} = C_{A_o} \int_{X_{A1}}^{X_{A2}} \frac{dX_A}{kC_{A_0}^{\;2}(1 - X_{A0})^2}$$

$$\tau_2 = \frac{V_2}{v_o} = \frac{1}{kC_{A_o}} \int_{X_{A1}}^{X_{A2}} \frac{dX_A}{(1 - X_{A0})^2}$$

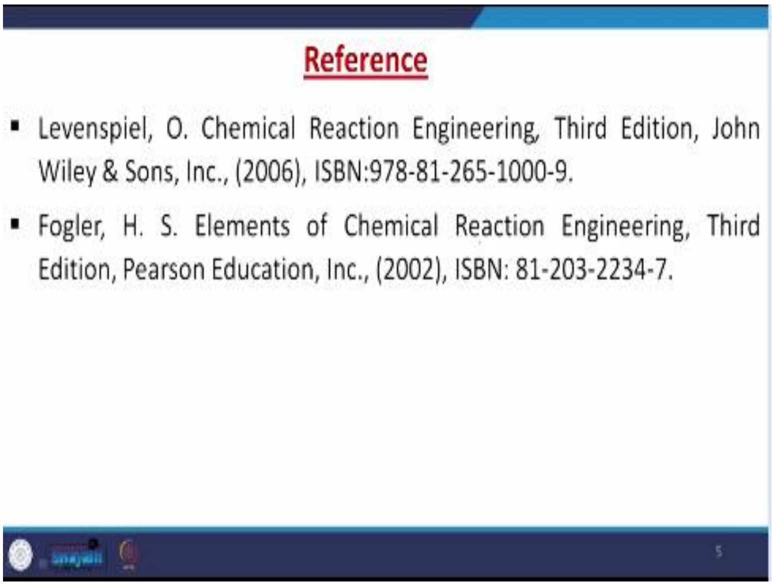
$$\tau_2 = \frac{V_2}{v_o} = \frac{1}{kC_{A_o}} [\frac{1}{1 - X_{A0}}]_{X_{A1}}^{X_{A2}}$$

$$\frac{kC_{A_o}V_2}{v_o} = [\frac{1}{1 - X_{A2}} - \frac{1}{1 - X_{A2}}]$$

On putting the value of know variables in the above equation we have

$$\frac{52.5 \times 0.25 \times 2}{2.5} = [\frac{1}{1 - X_{A2}} - \frac{1}{1 - 0.628}]$$

$$X_{A2} = 0.9242 \text{ (answer)}$$



Reference

- Levenspiel, O. Chemical Reaction Engineering, Third Edition, John Wiley & Sons, Inc., (2006), ISBN:978-81-265-1000-9.
- Fogler, H. S. Elements of Chemical Reaction Engineering, Third Edition, Pearson Education, Inc., (2002), ISBN: 81-203-2234-7.

So, in this particular lecture, we deal with the various kind of multiple reactors and multiple reaction systems. And if you wish to have further more studies related to these problems, there are a couple of references in listed in this particular slide. You may seek the help of these references for further studies. Thank you very much.