Polymer Reaction Engineering
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Lecture - 25
Problem Solving - I

Welcome to the problem-solving session number 1 of the polymer reaction engineering. Now, previously, we have studied about the quantitative analysis of series reactions in plug flow reactor and a batch reactor.

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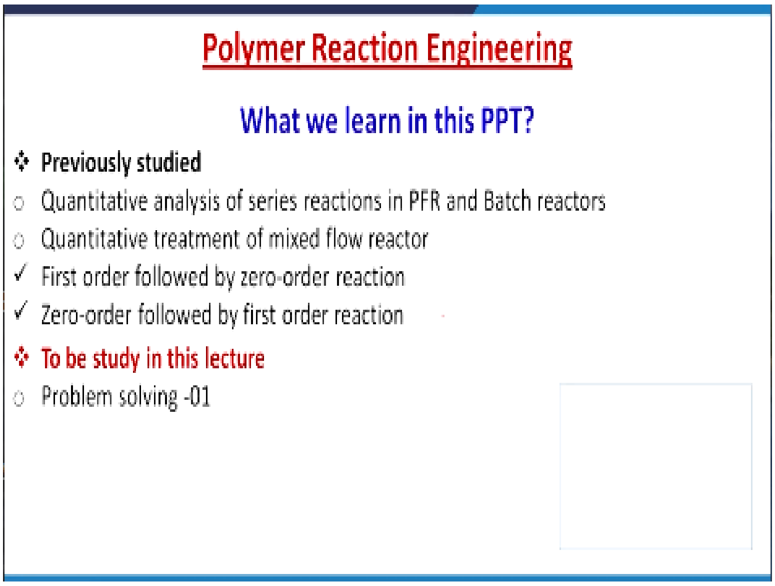

Polymer Reaction Engineering

What we learn in this PPT?

❖ Previously studied
- ○ Quantitative analysis of series reactions in PFR and Batch reactors
- ○ Quantitative treatment of mixed flow reactor
- ✓ First order followed by zero-order reaction
- ✓ Zero-order followed by first order reaction

❖ To be study in this lecture
- ○ Problem solving -01

We discussed about the quantitative treatment of mixed flow reactor, first order followed by the zeroth order reactor and zeroth order followed by the first order reaction. Now, here in this particular lecture, we are going to solve some typical numerical problems. So, let us start with the first problem here a liquid A decomposes by a second order kinetics and in a batch reactor, 50% of A is converted in 5 minutes.

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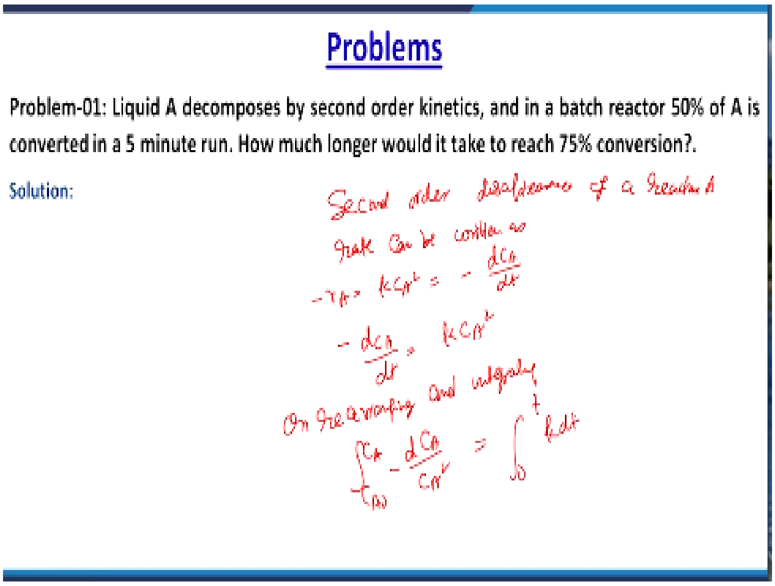

Problems

Problem-01: Liquid A decomposes by second order kinetics, and in a batch reactor 50% of A is converted in a 5 minute run. How much longer would it take to reach 75% conversion?.

Solution:

Second order disappearance of a reactant A

rate can be written as

$-r_A = kC_A^2 = -\frac{dC_A}{dt}$

$-\frac{dC_A}{dt} = kC_A^2$

On rearranging and integrating

$\int_{C_{A0}}^{C_A} -\frac{dC_A}{C_A^2} = \int_0^t kdt$

So, the thing is that, how much longer would it take to reach 75% conversion. Now, for the second order disappearance, let us start with the second order disappearance of a reactant A. Now, rate can be written as $-r_A$ is equal to kC_A square that is equal to the dC_A upon dt or $- dC_A$ upon dt is equal to kC_A square. Now, on rearranging and integrating, we have C_{A0} C_A dC_A upon C_A squared is equal to 0 to t kdt.

For second order disappearance of reactant 'A' rate equation can be written as;

$$-r_A = -\frac{dC_A}{dt} = kC^2{}_A$$

On rearranging and integrating with the initial condition for concentration C_{Ao} to C_A form time t=0 to t.

$$-\int_{C_{A_o}}^{C_A} \frac{dC_A}{C^2{}_A} = \int_0^t kdt$$

On integrating we have

$$\Rightarrow \left[\frac{1}{C_A} - \frac{1}{C_{A_o}}\right] = kt$$

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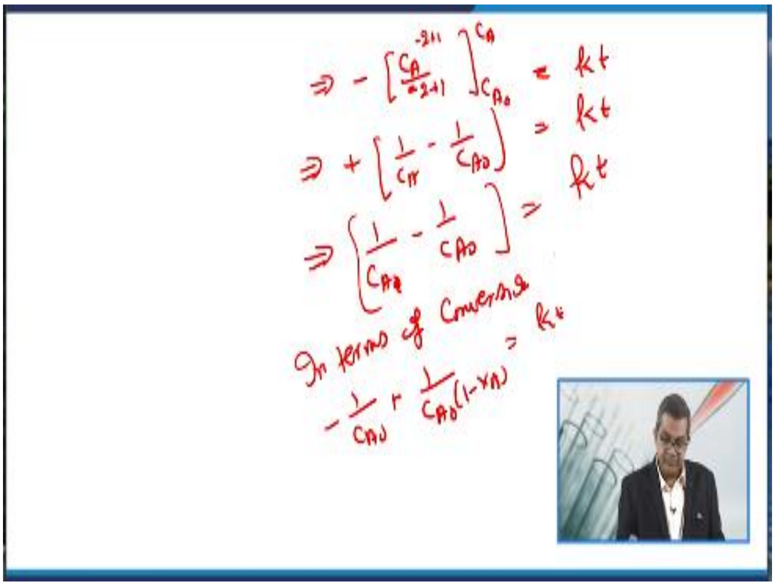

$$\Rightarrow -\left[\frac{C_A^{-2+1}}{-2+1}\right]_{C_{A0}}^{C_A} = kt$$

$$\Rightarrow +\left[\frac{1}{C_A} - \frac{1}{C_{A0}}\right] = kt$$

$$\Rightarrow \left[\frac{1}{C_A} - \frac{1}{C_{A0}}\right] = kt$$

In terms of Conversion

$$-\frac{1}{C_{A0}} + \frac{1}{C_{A0}(1-X_A)} = kt$$

This can be written as, –C_A upon –2 + 1 –2 + 1 C_{A0} C_A, this is equal to k t. This can implies to, 1 upon C_A – 1 upon C_{A0} this is equal to k t or 1 upon C_A - 1 upon C_{A0}, this is equal to k t. So, in terms of conversion – 1 upon C_{A0} + 1 upon C_{A0} 1 – x_A, this is equal to k t.

In terms of conversion, we can write this equation as

$$\Rightarrow \left[\frac{1}{C_{A_o}(1-X_A)} - \frac{1}{C_{A_o}}\right] = \mathrm{kt}$$

$$\Rightarrow \left[\frac{1}{(1-X_A)} - 1\right] = C_{A_o}\mathrm{kt}$$

$$\Rightarrow \left[\frac{X_A}{(1-X_A)}\right] = C_{A_o}\mathrm{kt}$$

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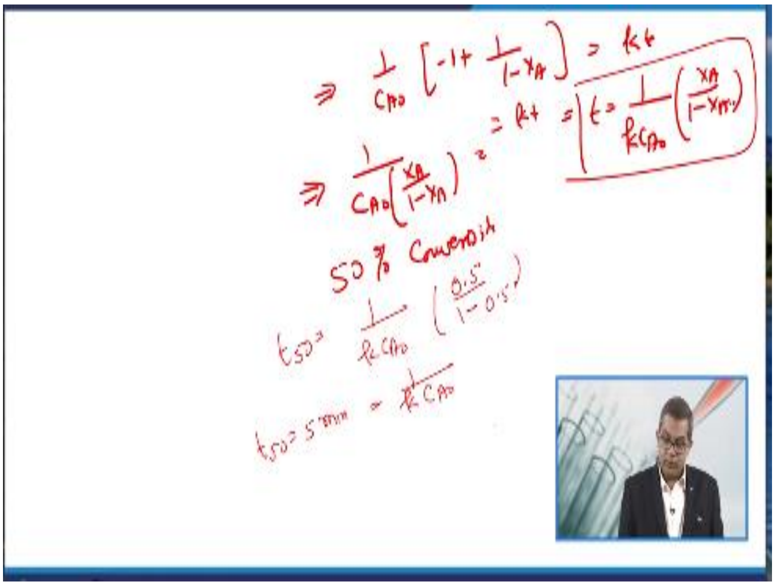

$$\Rightarrow \frac{1}{C_{A0}}\left[-1 + \frac{1}{1-X_A}\right] = kt$$

$$\Rightarrow \frac{1}{C_{A0}}\left(\frac{X_A}{1-X_A}\right) = kt \Rightarrow \boxed{t = \frac{1}{kC_{A0}}\left(\frac{X_A}{1-X_A}\right)}$$

50% Conversion

$$t_{50} = \frac{1}{kC_{A0}}\left(\frac{0.5}{1-0.5}\right)$$

$$t_{50} = 5\ \text{min} = \frac{1}{kC_{A0}}$$

And this is equal to 1 upon C_{A0} into – 1 + 1 upon 1 – X_A, this is equal to k t. And 1 upon C_{A0} into X_A upon 1 – X_A, this is equal to k t or t is equal to 1 upon k C_{A0} X_A upon 1 – X_A. So, now for 50% conversion, so, for 50% conversion t_{50} is equal to 1 upon k C_{A0} 0.5 upon 1 – 0.5 and t_{50} is equal to 5 minute that is equal to 1 upon k C_{A0}.

$$\Rightarrow \left[\frac{X_A}{(1-X_A)}\right] = C_{A_o}\mathrm{kt}$$

$$\Rightarrow \frac{1}{C_{A_o}\mathrm{k}}\left[\frac{X_A}{(1-X_A)}\right] = \mathrm{t}$$

For 50% conversion of reactant A

$$\Rightarrow \frac{1}{C_{A_o}\mathrm{k}}\left[\frac{0.5}{(1-0.5)}\right] = t_{50}$$

$$\Rightarrow \frac{1}{C_{A_o}\mathrm{k}} = t_{50} = 5\, minutes$$

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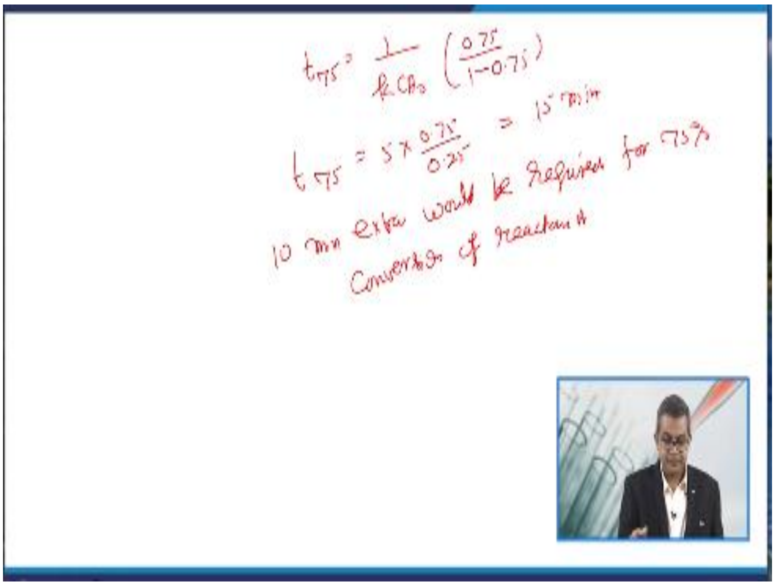

$$t_{75} = \frac{1}{k C_{A_0}}\left(\frac{0.75}{1-0.75}\right)$$

$$t_{75} = 5 \times \frac{0.75}{0.25} = 15 \text{ min}$$

10 min extra would be required for 75% conversion of reactant A

So, when we thought about the time required for 75%, so, it can be represented as t_{75} is equal to 1 upon k C_{A0} 0.75 upon 1 – 0.75 and t_{75} is equal to 5 into 0.75 upon 0.25 that is equal to 15 minutes. So, here 10 minutes extra, you see that here 10 minutes extra would be required for 75% conversion of reactant A. So, this is an answer.

For 75% conversion of reactant A

$$\Rightarrow \frac{1}{C_{A_o}\mathrm{k}}\left[\frac{0.75}{(1-0.75)}\right] = t_{75}$$

$$\Rightarrow 5\left[\frac{0.75}{(0.25)}\right] = t_{75}$$

$$\Rightarrow t_{75} = 15\, minutes$$

i.e., 10 minutes extra required for 75% conversion of reactant A than 50% conversion.

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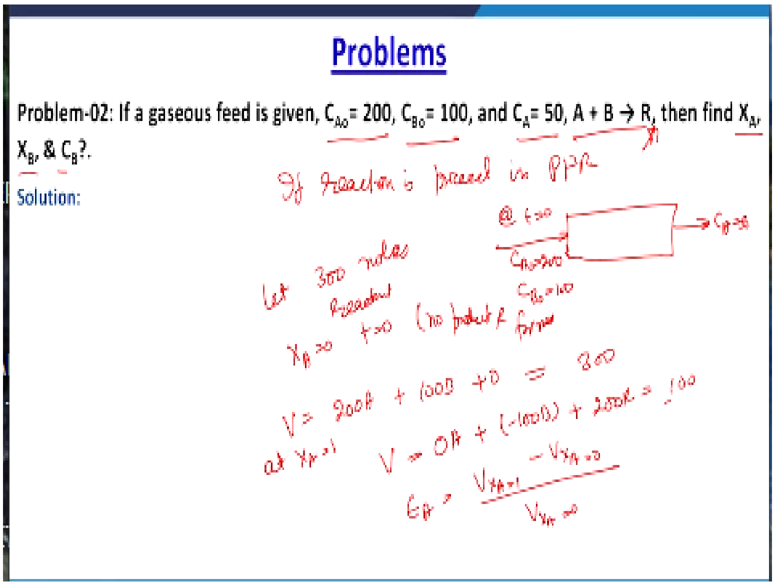

Problems

Problem-02: If a gaseous feed is given, $C_{A0} = 200$, $C_{B0} = 100$, and $C_A = 50$, $A + B \rightarrow R$, then find X_A, X_B, & C_B?.

Solution:

If reaction is proceed in PFR

@ t=0

$C_{A0}=200$

$C_{B0}=100$

$\rightarrow C_A=50$

Let 300 moles Reactant

$X_A=0$ t=0 (no product R form)

$V = 200A + 100B + 0 = 300$

at $X_A=1$ $V = 0A + (-100B) + 200R = 100$

$$\varepsilon_A = \frac{V_{X_A=1} - V_{X_A=0}}{V_{X_A=0}}$$

Now, let us take the second problem. Now, this problem says that if a gaseous feed is given, these are the following co-ordinates like C_{A0} is equal to 200, C_{B0} is equal to 100 and C_A is equal to 50 for the reaction A + B is equal to R, then you need to find out the values of X_A, X_B and C_B. So, you see that we are having this particular reaction, in an isothermal single phase flow reactor.

Let us assume that this is an isothermal single phase flow reactor that is operating under the constant pressure. So, if reaction is proceed in PFR, so, in that case, you are having this symbolic representation. So, at t is equal to 0, C_{A0} is equal to 200, C_{B0} is equal to 100 and C_A is equal to 50, so, let initially 300 moles of reactant that is feed gas to the reactor, then X_A is equal to 0, t is equal to 0 that is no product are being formed.

So, V is equal to 200 A + 100 B + 0 that is equal to 300. Now, at X_A is equal to 1, so, you can represent V is equal to 0 A + B + 200 R and that is equal 100. So, epsilon A can be written as V X_A is that 1 – V X_A equal to 0 upon V X_A equal to 0.

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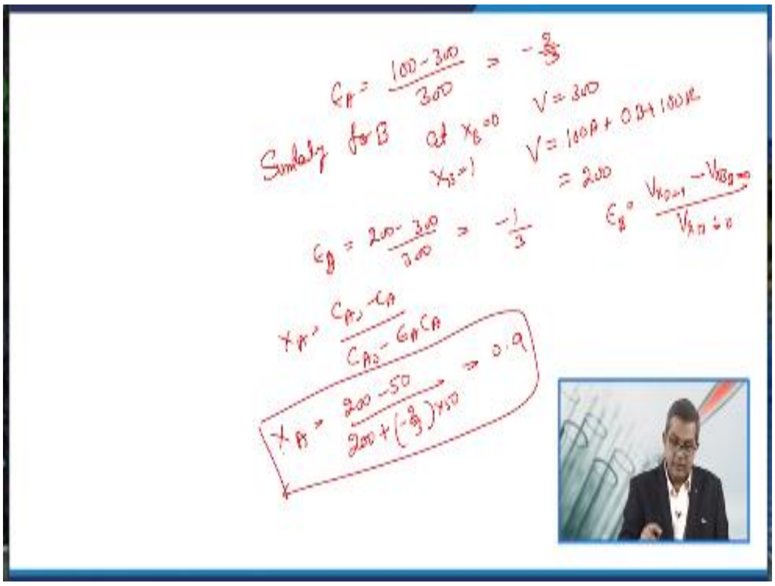

$\varepsilon_A = \frac{100-300}{300} = -\frac{2}{3}$

Similarly for B at $X_B = 0$ $V = 300$

$X_B = 1$ $V = 100A + 0B + 100R$

$= 200$

$\varepsilon_B = \frac{200-300}{300} = -\frac{1}{3}$

$\varepsilon_B = \frac{V_{X_B=1} - V_{X_B=0}}{V_{X_B=0}}$

$X_A = \frac{C_{A0} - C_A}{C_{A0} - \varepsilon_A C_A}$

$\boxed{X_A = \frac{200-50}{200+\left(-\frac{2}{3}\right)\times 50} = 0.9}$

So, in that case, epsilon A that is equal to 100 – 300 upon 300 that is equal to – 2 upon 3. Now, similarly, for B now, at X_B is equal to 0, V is equal to 300. Now, X_B is equal to 1, V is equal to 100 A + 0 B + 100 R and that is 200. So, when we write about the epsilon B that is 200 – 300 upon 300 that is equal to – 1 upon 3. Now, here we need not, needless not to mention that V X_B is equal to 1 – V B at 0 point then V X_B at 0.

So, X_A is equal to C_{A0} – C_A upon C_{A0} – epsilon A C_A or we can write X_A is equal to 200 – 50 upon 200 + minus 2 upon 3 into 50 and that comes out to be 0.9.

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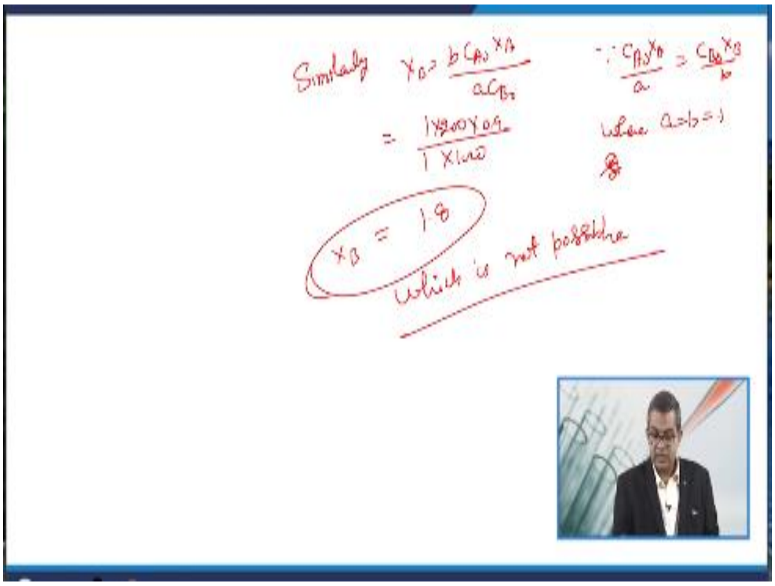

Similarly $X_B = \frac{b C_{A0} X_A}{a C_{B0}}$

$= \frac{1\times 200\times 0.9}{1\times 100}$

$\because \frac{C_{A0} X_A}{a} = \frac{C_{B0} X_B}{b}$

where $a = b = 1$

$\boxed{X_B = 1.8}$

which is not possible

Similarly, X_B is equal to b C_{A0} X_A upon a C_{B0} and that is 1 into 200 into 0.9 upon 1 into 100, that is C_{A0} X_A upon a is equal to CB0 X_B upon b where a is equal to b is equal to 1, as the stoichiometric co-efficient of a and b are 1. So, in that case X_B is equal to 1.8 and which is not at all possible. So, this is the answer to this one.

Solution:

If the reaction is proceeds in PFR

Let 300 moles of reactant are presents at initial t=0 then $X_A=0$

V = 200A+100B+0R= 300

At $X_A = 1$

V = 0A+(-100B) + 200 R = 100

$$\varepsilon_A = \frac{V_{X_{A=1}} - V_{X_{A=0}}}{V_{X_{A=0}}}$$

$$\varepsilon_A = \frac{100 - 300}{300} = -\frac{2}{3}$$

Similarly for B

At $X_B=0$, V=300

$X_B=1$, V=100A +0B +100R

X_B =200

$$\varepsilon_A = \frac{V_{X_{B=1}} - V_{X_{B=0}}}{V_{X_{B=0}}}$$

$$\varepsilon_A = \frac{200 - 300}{300} = -\frac{1}{3}$$

$$X_A = \frac{C_{A_o} - C_A}{C_{A_o} - \varepsilon_A C_{A_o}}$$

$$X_A = \frac{200 - 50}{200 - \frac{2}{3} \times 50} = 0.9$$

Similarly, for X_B

$$X_B = \frac{bC_{A_o}X_A}{aC_{B_o}}$$

$$\therefore \frac{C_{A_o}X_A}{a} = \frac{C_{B_o}X_B}{b}$$

Where, a=b=1

$$X_B = \frac{1 \times 200 \times 0.9}{1 \times 100}$$

$X_B = 1.8$, which is not possible, i.e., conversion reached over 1.

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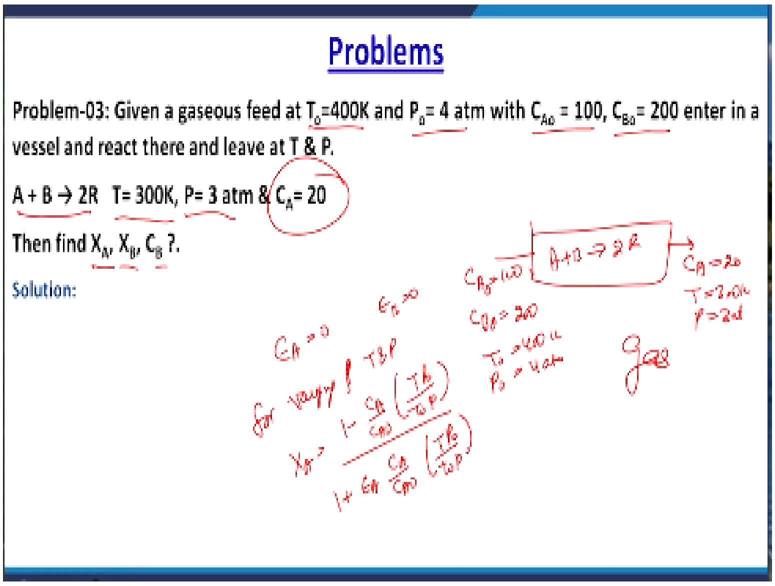

Problems

Problem-03: Given a gaseous feed at T_0=400K and P_0= 4 atm with C_{A0} = 100, C_{B0}= 200 enter in a vessel and react there and leave at T & P.

A + B → 2R T= 300K, P= 3 atm & C_A= 20

Then find X_A, X_B, C_B ?.

Solution:

$C_{A0}=100$, $C_{B0}=200$, $T_0=400K$, $P_0=4atm$ → A+B → 2R → $C_A=20$, $T=300K$, $P=3atm$

gas

$\varepsilon_A=0$, $\varepsilon_B=0$

for varying T&P

$$X_A = \frac{1-\frac{C_A}{C_{A0}}\left(\frac{TP_0}{T_0P}\right)}{1+\varepsilon_A\frac{C_A}{C_{A0}}\left(\frac{TP_0}{T_0P}\right)}$$

Now, let us take the problem number 3. Here, we have given a gaseous feed which is maintained at T 0 is equal to 400 and initial pressure is 4 atmosphere and initial concentration of A is 100 and the initial concentration of B is 200. They enter into the vessel and you need to find out the temperature and the pressure. Now, here, the reaction is given as A + B is equal to 2 R and temperature is 300 Kelvin and final pressure is 3 atmosphere and C is 20 then you need to find out the X_A, X_B and C_B.

So, again we see that this is my reactor, we are performing A + B 2R. Now, the initial condition that is maintained at C_{A0} is equal to 100, C_{B0} is equal to 200, T 0 is equal to 400 Kelvin and p 0 is that is pressure initial pressure is 4 atmosphere. Now, the final thing that is C_A is equal to 20, T is 300 Kelvin and B is 3 atmosphere. Since, the above system is a gas and change in moles are negligible. Therefore, epsilon A is equal to 0 and epsilon B also be 0.

So, for varying temperature and pressure for varying density, we know that X_A is equal to 1 – C_A upon C_{A0} T P_0 upon T_0 P divided by 1 + epsilon A C_A upon C_{A0} T P_0 T_0 P.

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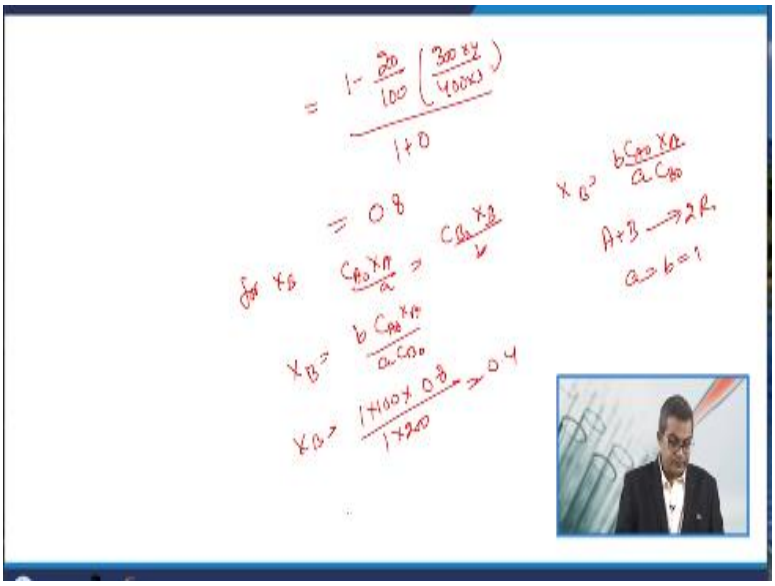

$$= \frac{1 - \frac{20}{100}\left(\frac{300\times4}{400\times3}\right)}{1+0}$$

$$= 0.8$$

for X_B $\frac{C_{A0}X_A}{a} = \frac{C_{B0}X_B}{b}$

$$X_B = \frac{b\,C_{A0}X_A}{a\,C_{B0}}$$

$$X_B = \frac{1\times100\times0.8}{1\times200} = 0.4$$

$$X_B = \frac{b\,C_{A0}X_A}{a\,C_{B0}}$$

$A+B \longrightarrow 2R$

$a = b = 1$

Now, this comes out to be 1 – 20 upon 100 into 300 into 4 upon 400 into 3 divided by 1 + 0 and that is 0.8. Now, for X_B, we know C_{A0} X_A upon a is equal to C_{B0} X_B upon b, X_B is equal to b C_{A0} X_A upon a C_{B0}. Where a and b both are the stoichiometric co-efficient, that is a small a and small b, they are the stoichiometric co-efficient of the reactant and again the reference reaction is A + B is 2 R.

So, a is equal to b is equal to 1, that is the stoichiometric number. So, if we substitute the things and this particular equation C_{A0} X_A upon a C_{B0}, then X_B will become 1 into 100 into 0.8 upon 1 into 200 that is equal to 0.4.

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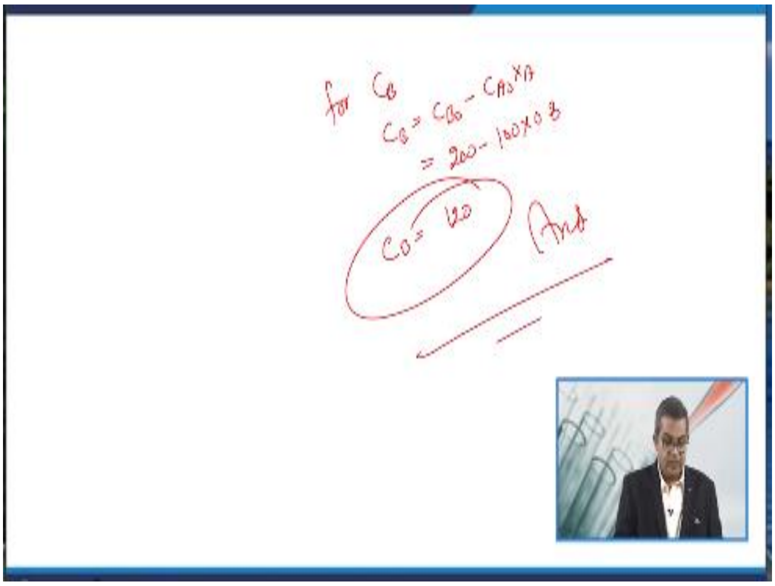

for C_B

$$C_B = C_{B0} - C_{A0}X_A$$

$$= 200 - 100\times0.8$$

$$\boxed{C_B = 120}$$ Ans

So, if for C_B, we can write C_B is equal to C_{B0} – C_{A0} X_A and this is 200 – 100 into 0.8 and C_B comes out to be 120 that is my desired answer.

Solution:

For varying T & P, conversion term can be written as;

$$X_A = \frac{1 - {C_A}/{C_{A_o}} \left(\frac{TP_o}{T_oP}\right)}{1 + \varepsilon_A \, {C_A}/{C_{A_o}} \left(\frac{TP_o}{T_oP}\right)}$$

$$X_A = \frac{1 - {20}/{100} \left(\frac{300 \times 4}{400 \times 3}\right)}{1 + 0}$$

$$X_A = 0.8$$

For X_B

$$\therefore \frac{C_{A_o} X_A}{a} = \frac{C_{B_o} X_B}{b}$$

$$X_B = \frac{b C_{A_o} X_A}{a C_{B_o}}$$

$$X_B = \frac{1 \times 100 \times 0.8}{1 \times 200} = 0.4$$

For C_B

$$C_B = C_{Bo} - C_{Ao}X_A$$

$$=200-100 \times 0.8$$

$$C_B = 120 \text{ (answer)}$$

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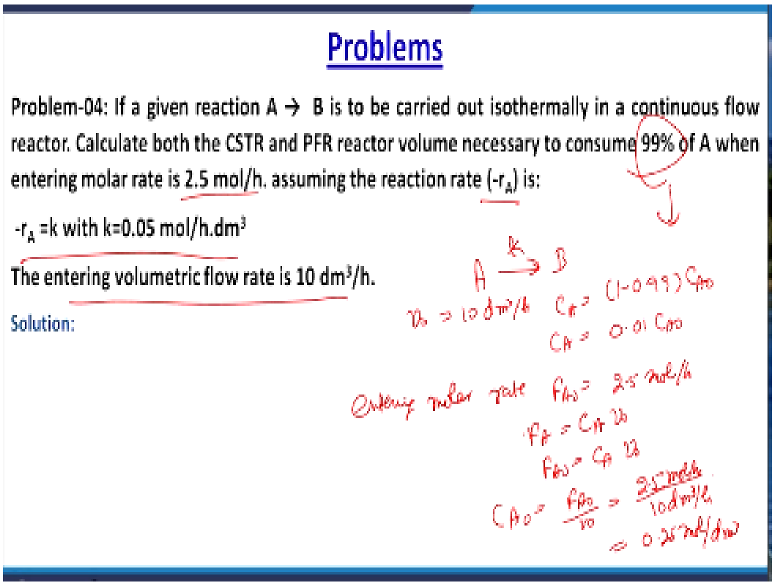

Problems

Problem-04: If a given reaction A → B is to be carried out isothermally in a continuous flow reactor. Calculate both the CSTR and PFR reactor volume necessary to consume 99% of A when entering molar rate is 2.5 mol/h. assuming the reaction rate ($-r_A$) is:

$-r_A = k$ with $k=0.05$ mol/h.dm^3

The entering volumetric flow rate is 10 dm^3/h.

Solution:

$$A \xrightarrow{k} B$$

$$v_o = 10\ dm^3/h \qquad C_A = (1-0.99) C_{Ao}$$

$$C_A = 0.01\, C_{Ao}$$

Entering molar rate $F_{Ao} = 2.5$ mol/h

$$F_A = C_A v_o$$

$$F_{Ao} = C_A v_o$$

$$C_{Ao} = \frac{F_{Ao}}{v_o} = \frac{2.5\ mol/h}{10\ dm^3/h}$$

$$= 0.25\ mol/dm^3$$

So, let us take another example that is problem number 4. Now, here if a given reaction that is the reaction is given to you that is A is converting into B. Now, this particular reaction is to be carried out isothermally in a continuous flow reactor, you need to calculate both the CSTR and PFR reactor volume necessary to consume 99% of A when entering molar rate is 2.5 moles per hour. You may assume that the reaction rate – r_A is given with this one.

And the entering volumetric flow rate is 10 decimeter cubed per hour. Now, here, we have given A is converted into B. Now, initial things are 10 volumetric flow rate is 10 decimetre cube per hour, C_A is equal to 1 – 0.9 and because this is the 99% conversion C_{A0} and C_A is equal to 0.01 C_{A0}. So, entering molar rate F_{A0} that is equal to 2.5 moles per hour.

Now, F_A is equal to C_A υ_0 and F_{A0} is equal to C_A υ_0. And we can write C_{A0} is equal to F_{A0} /υ_0 that is equal to 2.5 mole per hour divided by 10 hour and that comes out to be 0.25 moles per decimetre cube.

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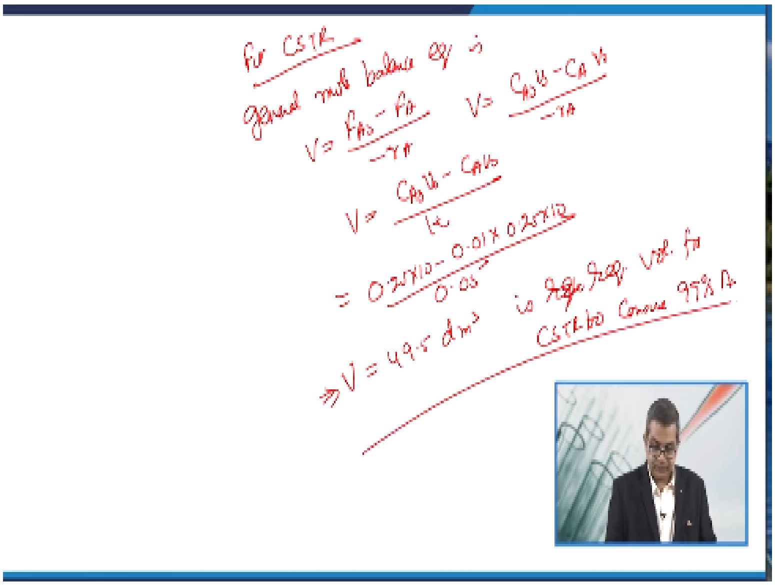

For CSTR

general mole balance eq is

$$V = \frac{F_{A0} - F_A}{-r_A} \qquad V = \frac{C_{A0}\upsilon_0 - C_A\upsilon_0}{-r_A}$$

$$V = \frac{C_{A0}\upsilon_0 - C_{A}\upsilon_0}{k}$$

$$= \frac{0.25\times10 - 0.01\times0.25\times10}{0.05}$$

$\Rightarrow V = 49.5\ dm^3$ is req. vol. for CSTR to consume 99% A.

Now, let us take the gradual example like for CSTR, the general mole balance equation is V is equal to F_{A0} – F_A upon – r_A or V is equal to C_{A0} υ_0 – C_A υ_0 upon – r_A or it can be represented as V is equal to C_{A0} υ_0 – C_A υ_0 upon k and that is 0.25 into 10 – 0.01 into 0.25 into 10 upon 0.5. So, this V comes out to be 49.5 decimetre cube. Now, this is the required volume for CSTR to consume 99% of A.

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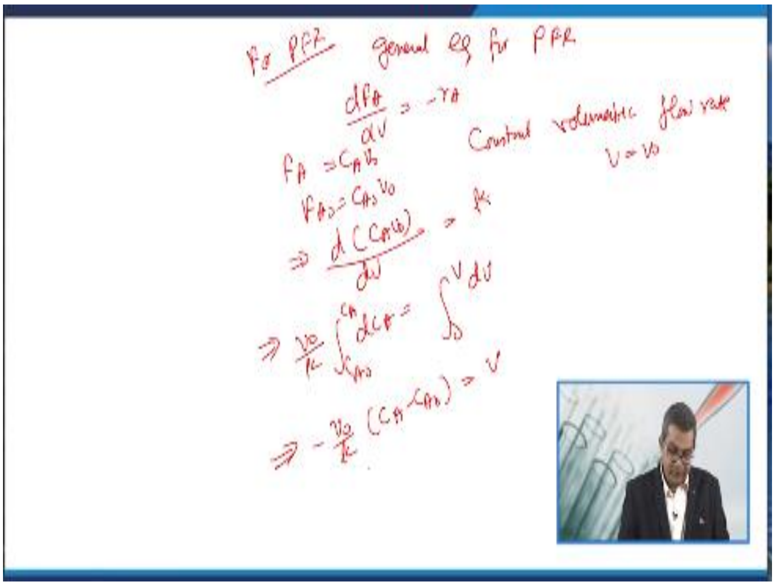

For PFR   general eq for PFR

$\frac{dF_A}{dV} = -r_A$

Constant volumetric flow rate

$v = v_0$

$F_A = C_A v_0$

$F_{A0} = C_{A0} v_0$

$\Rightarrow \frac{d(C_A v_0)}{dV} = k$

$\Rightarrow \frac{v_0}{k}\int_{C_{A0}}^{C_A} dC_A = \int_0^V dV$

$\Rightarrow -\frac{v_0}{k}(C_A - C_{A0}) = V$

Now, if we talk about the PFR, for PFR that general equation for PFR that is the dF A upon dV is equal to – r_A. Now, if we can write F_A is equal to C_A υ_0 or F_{A0} is equal to C_{A0} υ_0. That is the constant volumetric flow rate V is equal to υ_0. Now, here dC_A υ_0 upon dV that is equal to k. Now, if we integrate both the side, we may have υ_0 upon k C_{A0} to C_A dC_A that is equal to 0 to V dV. And that comes out to be υ_0 over k C_A– C_{A0} and that is equal to V.

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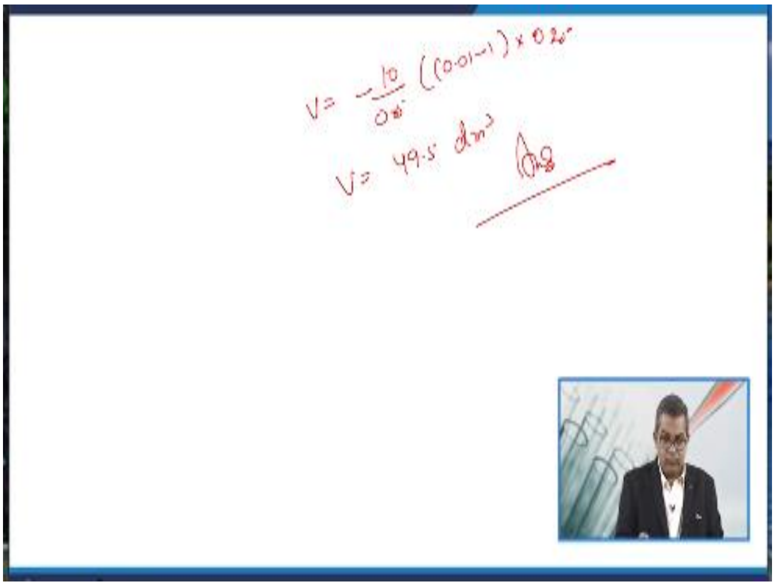

$V = -\frac{10}{0.05}((0.01-1)\times 0.25$

$V = 49.5\ dm^3$

Ans

So, V is equal to – 10 upon 0.05 into 0.01 – 1 into 0.25 and V comes out to be 49.5 decimetre cube. So, the volume required for CSTR and PFR is same due to the rate constant k is independent of the concentration term. So, by this way, you can evaluate both the things.

Solution;

Given

A→B

$\upsilon_o = 10\ dm^3/h$

$C_A = (1-0.99)C_{Ao}$

$C_A = 0.01C_{Ao}$

$F_{Ao} = 2.5$ mol/h

$F_A = C_A\ \upsilon_o$

$F_{Ao} = C_{Ao}\ \upsilon_o$

$C_{Ao} = F_{Ao}/\ \upsilon_o = (2.5\ mol/h)/(10\ dm^3/h)$

$C_{Ao} = 0.25\ mol/dm^3$

For CSTR:

General mole balance equation is

$$V = \frac{F_{A_o} - F_A}{-r_A} = \frac{C_{A_o}\nu_0 - C_A\nu_0}{-r_A}$$

For Zero order reaction system

$-r_A = k$

$-r_A = 0.05$

$$\Rightarrow V = \frac{0.2 \times 10 - 0.01 \times 0.25 \times 10}{0.05}$$

$\Rightarrow V = 49.5\ dm^3$ is required volume of a CSTR for 99% conversion of reactant A.

For PFR:

General equation for PFR

$$\frac{dF_A}{dV} = -r_A$$

$F_A = C_A\nu_0$ i.e., constant volumetric flow rate

$$\nu_0 = \nu$$

$$F_{A_o} = C_{A_o}\nu_0$$

$$\Rightarrow \frac{d(C_A\nu_{0)}}{dV} = k$$

$$\Rightarrow \frac{V_o}{k}\int_{C_{A_o}}^{C_A} dC_A = \int_0^V dV$$

$$\Rightarrow -\frac{V_o}{k}(C_{A_o} - C_A) = V$$

$$\Rightarrow V = -\frac{10 \times 0.25}{0.05}(0.01 - 1)$$

$$\Rightarrow V = 49.5\ dm^3$$

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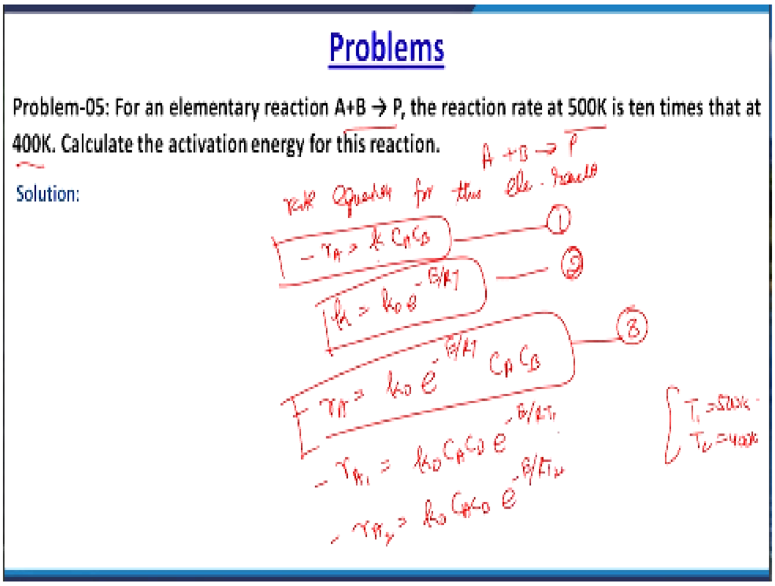

Problems

Problem-05: For an elementary reaction A+B → P, the reaction rate at 500K is ten times that at 400K. Calculate the activation energy for this reaction.

Solution:

$A + B \rightarrow P$

rate equation for the ele. reaction

$-r_A = k C_A C_B$ ①

$k = k_0 e^{-E/RT}$ ②

$-r_A = k_0 e^{-E/RT} C_A C_B$ ③

$-r_{A_1} = k_0 C_A C_B e^{-E/RT_1}$

$-r_{A_2} = k_0 C_A C_B e^{-E/RT_2}$

$T_1 = 500K$

$T_2 = 400K$

Now, let us, take another problem that is for an elementary reaction A + B equals to P. The reaction rate is given at 500 Kelvin is 10 times that at 400 Kelvin. So, you need to calculate the activation energy for this particular reaction. So, here you can have A + B, we can utilise this reaction A + B to P. So, the rate equation for this elementary reaction can be $-r_A$ is equal to k C_A C_B that is equation number 1.

Now, here k is the rate constant. Now, if we write in terms of the (( )) (20:01) law, then it can be represented k is equal to k 0 e to the power – E upon R T, because it is the need of the question problem. Now, from equation 1 and 2, we can write $-r_A$ is equal to k_0 e to the power – E upon R T C_A C_B that is the equation number 3. Now, according to the question if the reaction rate at 500 Kelvin is 10 times that for 400 Kelvin.

So, $-r_{A1}$ is equal to k_0 C_A C_B e to the power – E upon R T_1. Now, let T_1 is equal to 500 Kelvin and T_2 is equal to 400 Kelvin and $-r_{A2}$ is equal to k_0 C_A C_B e to the power – E upon R T_2.

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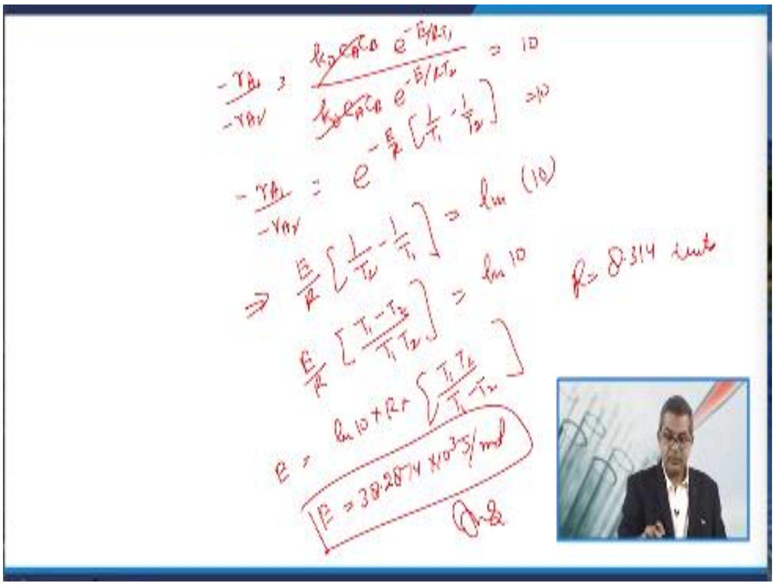

$$\frac{-r_{A_1}}{-r_{A_2}} = \frac{\cancel{k_0 C_A C_B}\, e^{-E/RT_1}}{\cancel{k_0 C_A C_B}\, e^{-E/RT_2}} = 10$$

$$\frac{-r_{A_1}}{-r_{A_2}} = e^{-\frac{E}{R}\left[\frac{1}{T_1}-\frac{1}{T_2}\right]} = 10$$

$$\Rightarrow \frac{E}{R}\left[\frac{1}{T_2}-\frac{1}{T_1}\right] = \ln(10)$$

$$\frac{E}{R}\left[\frac{T_1-T_2}{T_1T_2}\right] = \ln 10$$

$$E = \ln 10 \times R \times \left[\frac{T_1T_2}{T_1-T_2}\right]$$

$$\boxed{E = 38.2874 \times 10^3\ J/mol}$$

$R = 8.314$ unit

Q-2

So, if we write this – r_{A1} upon – r_{A2} that is k_0 C_A C_B e to the power – E upon R T_1 upon k_0 C_A C_B e to the power – E upon R T_2 is equal to 10. This is given. So, – r_{A1} upon – r_{A2} that is equal to e to the power – E upon R into 1 upon T_1 – 1 upon T_2 that is equal to 10. And that is why E upon R into 1 upon T_2 – 1 upon T_1 that is ln 10 or E upon R into T_1 – T_2 upon T_1 T_2 that is ln 10.

Now, E is equal to ln 10 into R into T_1 T_2 upon T_1 – T_2. Now, if we substitute all the values that T_1 is given, T_1 is 500 and T_2 is 400 and ln 10, then if we substitute the value of R is equal to 8.314 with the units, then E is comes out to be 38.2874 into 10 to the power 3 joules per mole that is my answer.

Solution;

$$A \xrightarrow{k} R$$

Rate equation

$$-r_A = kC_AC_B \qquad (1)$$

$$k = k_o e^{-E/RT} \qquad (2)$$

$$-r_A = k_o e^{-E/RT} C_AC_B \qquad (3)$$

$$-r_{A_1} = k_o e^{-E/RT_1} C_AC_B$$

$$-r_{A_2} = k_o e^{-E/RT_2} C_AC_B$$

If $T_1 = 500K$ and $T_2 = 400K$

$$\frac{-r_{A_1}}{-r_{A_2}} = \frac{k_o e^{-E/RT_1} C_AC_B}{k_o e^{-E/RT_2} C_AC_B} = 10$$

$$\frac{-r_{A_1}}{-r_{A_2}} = e^{-E/R\left(\frac{1}{T_1} - \frac{1}{T_2}\right)} = 10$$

$$E/_R\left(\frac{1}{T_1} - \frac{1}{T_2}\right) = \ln(10)$$

$$E = \ln(10) \times R \times \left[\frac{T_1 T_2}{T_1 - T_2}\right]$$

On solving the above equation with the different value of Temperature.

$$E = 38.2874 \text{x} 10^3 \text{ J/mol} \quad \text{(answer)}$$

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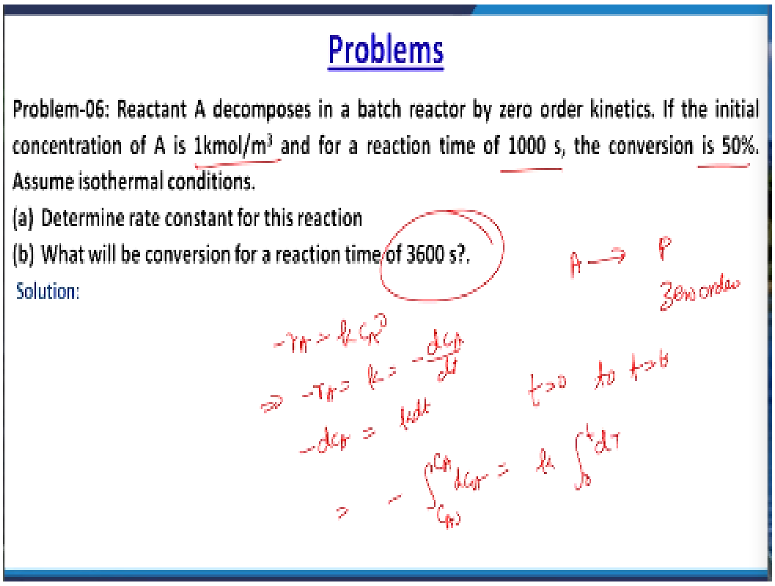

Problems

Problem-06: Reactant A decomposes in a batch reactor by zero order kinetics. If the initial concentration of A is 1kmol/m³ and for a reaction time of 1000 s, the conversion is 50%. Assume isothermal conditions.

(a) Determine rate constant for this reaction

(b) What will be conversion for a reaction time of 3600 s?.

Solution:

Now, let us take another example that is problem number 6 that reactant A decomposes in a batch reactor by zero order kinetics. If initial concentration of A is 1 kilo mole per metre cube and for a reaction time of say,1000 seconds the conversion is 50%. Now, you may assume the isothermal condition, then you need to find out the rate constant for this particular reaction which is given and what will be the conversion for a reaction time of 3600 seconds.

Now, see, as per the problem, the reactant A decomposes into the product by zero order kinetics. So, the rate equation can be given as with respect to the A – r_A is equal to k C_{A0} and that is equal to – r_A is equal to k – dC_A upon d t and – dC_A is equal to k dt. So, if we integrate both the side from time t is equal to 0 to time t is equal to t, then it can become – C_{A0} to C_A dC_A that is equal to k_0 to t dt.

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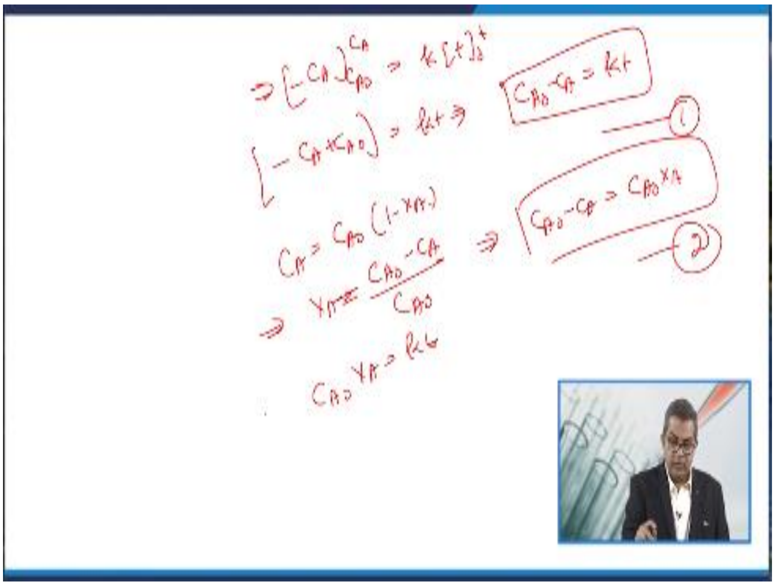

$\Rightarrow [-C_A]_{C_{A0}}^{C_A} = k[t]_0^t$

$[-C_A + C_{A0}] = kt \Rightarrow \boxed{C_{A0} - C_A = kt}$ ①

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

$\Rightarrow X_A = \frac{C_{A0} - C_A}{C_{A0}} \Rightarrow \boxed{C_{A0} - C_A = C_{A0} X_A}$ ②

$\Rightarrow C_{A0} X_A = kt$

Now, if we go ahead with this one then this may become – C_A C_{A0} C_A equal to k t 0 to t or – C_A + C_{A0}, this is equal to k t. And finally, we can write this C_{A0} – C_A is equal to k t that is my equation number 1 for this problem. Now, as we know that for conversion C_A is equal to C_{A0} (1 – X_A). Now, this can be X_A is equal to C_{A0} – C_A upon C_{A0} that is equal to C_{A0} – C_A that equal to C_{A0} X_A that is my equation number 2. Now, see from these 2 equations, we may have C_{A0} X_A is equal to k t.

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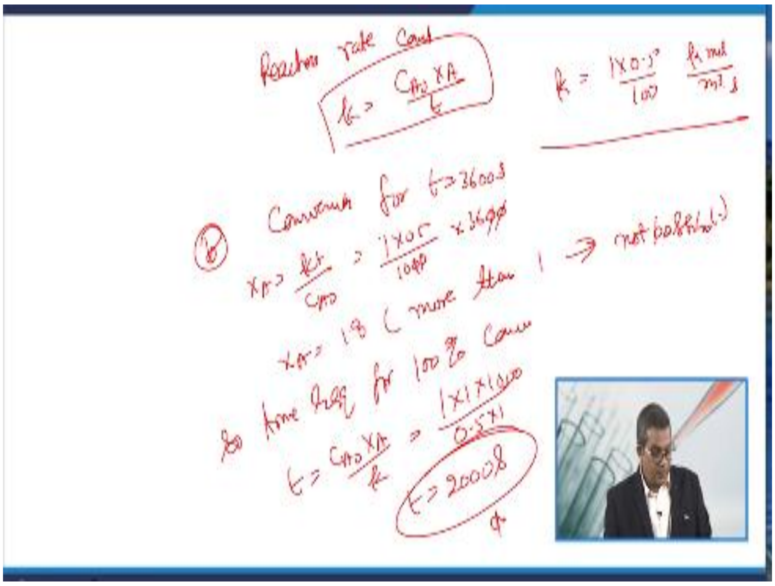

Reaction rate Const

$\boxed{k = \frac{C_{A0} X_A}{t}}$

$k = \frac{1 \times 0.5}{100} \frac{k\,mol}{m^3\,s}$

(b) Conversion for $t = 3600\,s$

$X_A = \frac{kt}{C_{A0}} = \frac{1 \times 0.5}{1000} \times 3600$

$X_A = 1.8$ (more than 1 → not possible)

So time req for 100% Conv

$t = \frac{C_{A0} X_A}{k} = \frac{1 \times 1 \times 1000}{0.5 \times 1}$

$\boxed{t = 2000\,s}$

So, when we are talking about the reaction rate constant, then k is equal to C_{A0} X_A upon t. So, k is equal to 1 into 0.5 upon 1000 that is kilo mole per metre cube second. So, we can write k like this. Now, let us talk about the second part that is conversion for t is equal to 3600 seconds. Now, X_A is equal to k t upon C_{A0} that is equal to 1 into 0.5 divided by 1000 into 3600 that is X A is equal to 1.8 that is more than 1, which is not possible.

So, the time required for 100% conversion t is equal to C_{A0} X_A upon k that is equal to 1 into 1 into 1000 upon 0.5 into 1 and t is equal to 2000 second. So, that is all of the reactant A will be consumed or converted into the product after 2000 second. So, conversion after 3600 would be 100% and that is my answer.

Solution:

$$-\mathrm{r_A} = \mathrm{k} = \frac{-dC_A}{dt}$$

$$-dC_A = \mathrm{k}dt$$

On Integration of the above equation for t=0 C_A=0, t=t C_A = C_{Ao}

$$-\int_{C_{A_o}}^{C_A} dC_A = \mathrm{k}\int_0^t dt$$

$$-(C_A - C_{A_o}) = kt$$

$$-[C_{A_o}(1 - X_A) - C_{A_o}] = kt$$

$$[C_{A_o}X_A] = kt$$

$$\frac{[C_{A_o}X_A]}{t} = k$$

$$\mathrm{k} = \frac{0.5\times1}{1000}\ \mathrm{kmol/m^3.s}$$

For t=3000s

$$\frac{tk}{C_{A_o}} = X_A = (1 \times 0.5/1000) \times 3600$$

=1.8 (More than 1 which is not possible)

So time required for 100% conversion

$$\frac{[C_{A_o}X_A]}{k} = t = \frac{1 \times 100}{0.5} = 2000\mathrm{s}$$

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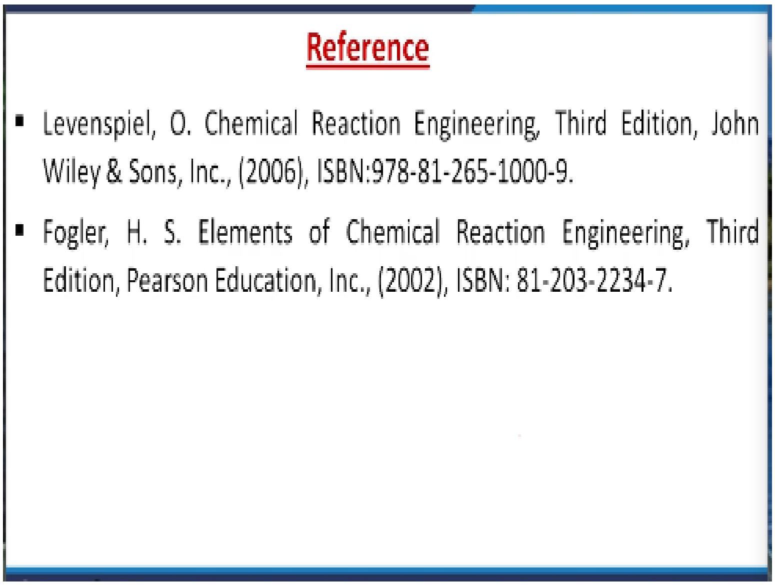

Reference

- 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 discussed the various problems related to the plug flow reactor and the CSTR. And again, for the theoretical part, you may refer to the lectures as well as the references given in this particular slide. Thank you very much.