Advanced chemical Reaction Engineering

Prof.H. S. Shankar
Department of Chemical Engineering
Indian Institute of Technology, Bombay

Lecture - 04
Design Equations – Illustrative Examples

We are looking at advance reaction engineering design equations.

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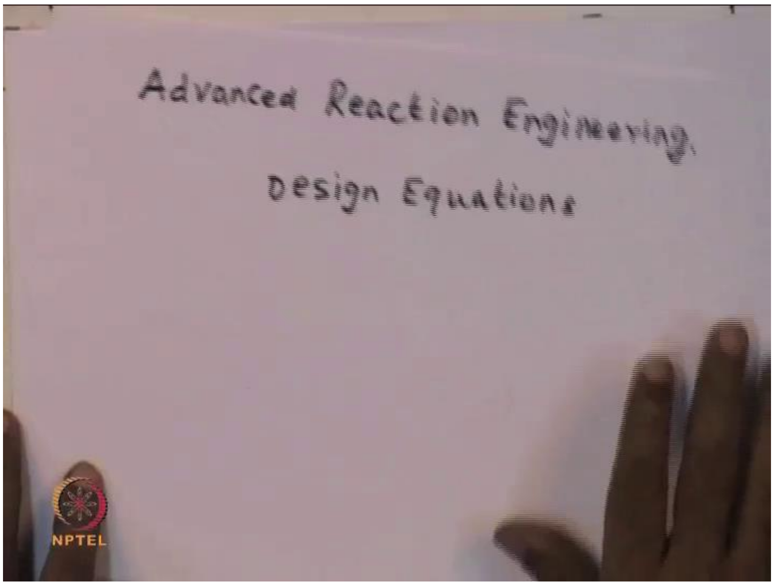

Advanced Reaction Engineering

Design Equations

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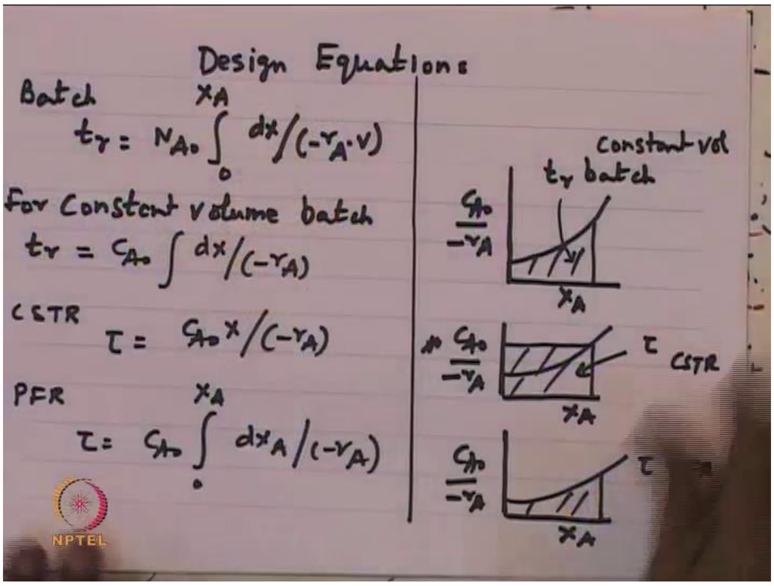

Design Equations

Batch

$$t_r = N_{A0} \int_0^{x_A} dx/(-r_A \cdot V)$$

For Constant volume batch

$$t_r = C_{A0} \int dx/(-r_A)$$

CSTR

$$\tau = C_{A0} x/(-r_A)$$

PFR

$$\tau = C_{A0} \int_0^{x_A} dx_A/(-r_A)$$

We are talking about design equations and we derived that the design equations for various situations, it will quickly run through all that. So, we said for a batch the reaction time is NA0 0 to XA dx by minus r a times v, we have derived this now, we can plot this if a constant volume batch. For example, then v you can take it out integral. So, that this becomes CA0 by minus of r A this what i plotted here CA0 by minus of rA versus XA.

This integral will be 0 and XA whatever, is area under the curve becomes the reaction time. On other words if you have a some data of your reaction it plotted in the form of CA0 by minus of RA versus XA simply area under the integral from 0 to XA gives you the reaction time. That is for a batch that is only for a constant volume batch now, if the volume does change due to various reasons then, appropriately we have taken in to account the effect of volume change which also we have done.

And you have done some exercises to illustrate this way now the 2nd situation. In fact, I have shown this here for the case of constant volume batch this, what you getting. Now if it is for a CSTR we have written the design equations also we are shown that the residence time for a CSTR is given as CA0 x divided by minus of RA. Once again we can make a plot a CA0 by minus of RA versus XA this data comes from our experiment. I am here to shown how to do the experiment and so on.

So, this data comes from our experiment. So, that you can plot this then, and then if you want to take the reaction from 0 to XA then the area under this rectangle you should this gives to the residence time for a CSTR. This is what is written here, residence time for CSTR is CA0 x by minus of RA which is the rectangle that you can see here. Once again the same data CA0 by minus of RA versus XA is used to find out the residence time for a CSTR.

Now we can do the same thing with the PFR. Once again we have derived little earlier that the residence time for a PFR is CA0 integral of dx a by minus of RA, when you plot CA0 by minus of RA versus XA. Once again area under the integral 0 to XA this area this is the resident time for a PFR. Notice here thus the residence time for PFR the integral the reaction time for a constant volume batch, which is given as TR.

The integrals are the same on other words we can look up on reaction time in a batch as equivalent to the resident time in a PFR they are the same because, it talks about the time of that the speed elements spend in the reaction environment. This something that we have understood based on whatever we have done.

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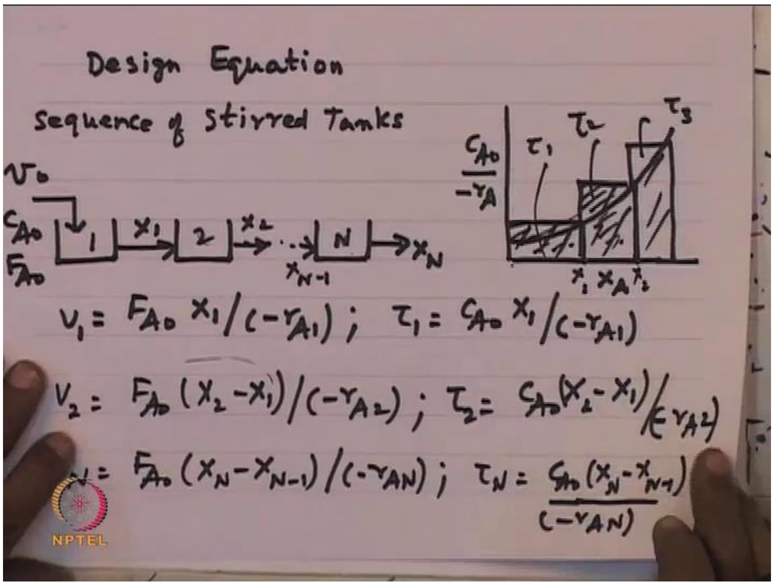

Design Equation

Sequence of stirred Tanks

$v_1 = F_{A0} X_1/(-r_{A1})$; $\tau_1 = C_{A0} X_1/(-r_{A1})$

$V_2 = F_{A0}(X_2 - X_1)/(-r_{A2})$; $\tau_2 = C_{A0}(X_2 - X_1)/(-r_{A2})$

$= F_{A0}(X_N - X_{N-1})/(-r_{AN})$; $\tau_N = \frac{C_{A0}(X_N - X_{N-1})}{(-r_{AN})}$

We can continue this and perhaps look at a more interesting situation something that could happen or it could have various other kinds of uses. Let us for examples look at a sequence of stirred tanks, what is the sequence of stirred tanks? Sequence of stirred tank is reactor 1, reactor 2, reactor 3 I will put 1 2 3 just to just to indicate that there are, so many tanks. Now, what is that we have? We have a reaction taking place in reactor 1, reactor 2, and reactor n. That means, fluid elements entering reactor 1, and moving to reactor 2, then moving on up to reactor n and coming out. Now, we have written the design equation for a CSTR I mean something that we write for quiet sometime.

So, accordingly I have written, what is the reactor volume? Reactor volume v1 is FA0 X1 by minus of RA1, what is reactor volume 2? FA0 times X2 minus X1 divided by minus of RA2. Notice here in a CSTR the reaction takes place in the exit conditions the reaction rates in exit condition has to be taken. FA0 X2 minus X1 is most of the component A that is undergone chemical reaction, divided by the rate of reaction gives you the volume of the equipment.

Now, we can put it into the form of residence time by dividing by volumetric flow at the inlet that gives you the residence time in stirred tank 1, residence time in stirred tank 2. Similarly this is reactor volume of stir tank n is FA0 XN minus XN minus 1 this is XN minus 1, what is entering here is x n minus of 1. Therefore, XN minus XN minus 1 multiplied by FA0 this is most of component a, that is been reacted divided by reaction rate this is the volume. And the residence time is simply you have divided by the volumetric flow.

So, you get CA0 XN minus XN minus 1 by minus of r AN. On other words tau 1 is CA0 X1 minus of RA1 tau 2 CA0 X2 minus X2 by minus of RA2. So, if we make a plot of CA0 by minus of RA something that we already said versus x. So, you get this curve, which is performance of the reaction now, if you look at this area this area going from 0 to X1. So, this area you can see is tau 1 you can see this area is tau 2 CA0 X2 minus of X1 you can say x, this is X2 minus of X1 divided by minus of RA2.

This is the residence time for reaction 2 reactor 2, and similarly residence time for reaction 3 and reaction n reactor 3 and reactor n and so on. So, on other words what we are trying to say in here is that, if you have a stirred tank a sequence of stirred tanks simply you have to construct these rectangles. And then area of those rectangles gives you the residence time plotted in the form of CA0 by minus RA versus X. So, what we are trying to say here is that, we could have situations in which the reaction kinetics is not very easy to determine. But what is not so difficult to determine? Are this kind of data CA0 by minus of RA versus X this kind of data is relatively easy to determine.

And therefore, it is relatively easy to determine, what is the reaction time that is required for a given extend of reaction? And that way you can use may be a number of stirred tanks or may be a 1 PFR and so on. To drive the reaction at the end point of your interest so, this is the point I was trying to clarify.

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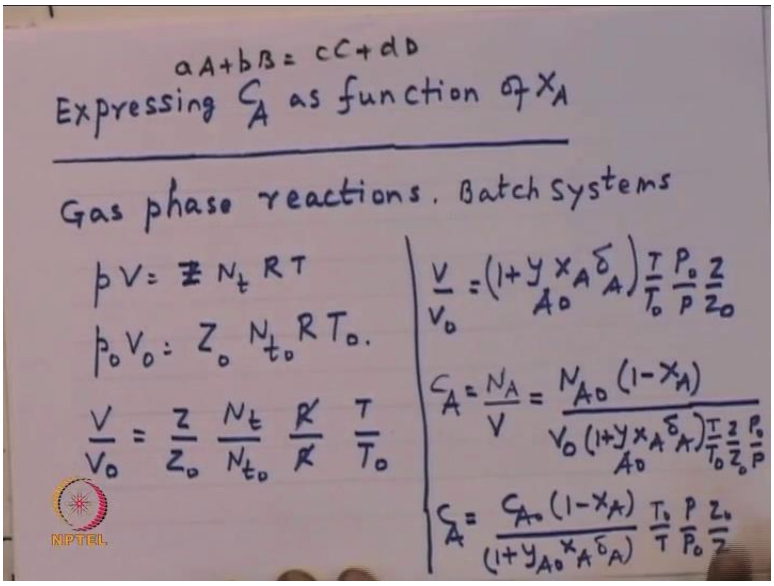

$aA+bB = cC+dD$

Expressing C_A as function of X_A

Gas phase reactions. Batch systems

$$pV = Z N_t RT$$

$$p_0 V_0 = Z_0 N_{t0} R T_0.$$

$$\frac{V}{V_0} = \frac{Z}{Z_0}\frac{N_t}{N_{t0}}\frac{\cancel{R}}{\cancel{R}}\frac{T}{T_0}$$

$$\frac{V}{V_0} = (1+y_{A0}x_A\delta_A)\frac{T}{T_0}\frac{P_0}{P}\frac{Z}{Z_0}$$

$$C_A = \frac{N_A}{V} = \frac{N_{A0}(1-X_A)}{V_0(1+y_{A0}x_A\delta_A)\frac{T}{T_0}\frac{Z}{Z_0}\frac{P_0}{P}}$$

$$C_A = \frac{C_{A0}(1-X_A)}{(1+y_{A0}x_A\delta_A)}\frac{T_0}{T}\frac{P}{P_0}\frac{Z_0}{Z}$$

So, our job now to determine, what is the relationship between concentration and conversion for a single reaction that is, what we are considering right now. If it is a gas phase reaction the reaction once again might be write down is a A plus b B equal to c C plus d D say as an example. So, what you got here is if it is a gas phase reaction this is gas law which is p v equal to Z N R T, Z is a complexablity factor. Now, at the initial state or at the entrance it is P0 V0 equal to Z0 NT0 RT it is a batch system.

So, this ratio gives you V by V0 is Z by Z0 NT by NT0 R cancels gas constant T by T0. Now essentially what we are saying now is that since we already derive the relationship between NT and NT0 from our sticheeometry. We know that our V by V0 written in terms of this ratio, which is already derived in the last class 1 plus yA0 is a mole fraction at the inlet.

XA is the extensive reaction delta A is the change in number of moles per mole of the reference component A. So, T by T0 P0 by P Z by Z0, on other words now, we are able to tell, what is the volume of the equipment? How it depends on the variable systems? Which is change in number of moles arising from number of moles changing because of reaction? And change in temperature definitely change in the pressure definitely change in the compressibility defector if any. Typically if concentration is, what we are interested in because, we want to express are reaction rate function in terms of concentration. We need concentration, which is simply NA divided by V now NA by definition NA0 times of 1 minus XA because, that is how we define conversion.

And V comes from the above equation as V0 times 1 plus YA0 XA delta A multiplied by the temperature T by T0, Z by Z0 P0 P. On other words using this relationship we are able to express concentration in terms of conversion XA. Similarly, we can do the same thing for components b, components c, components d and so on. Therefore, we can express the reaction rate function in terms of conversion. This is as far as the batch system is concerned, suppose we have a flow system; flow system means our previous relationship pv equal to ZNRT is replaced by p small v while small v is the flow rate through the system.

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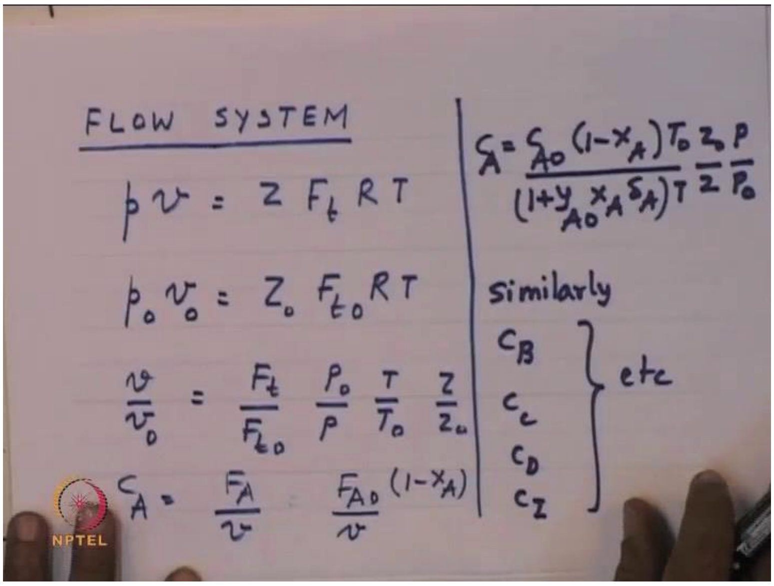

FLOW SYSTEM

$$p v = Z F_t R T$$

$$p_0 v_0 = Z_0 F_{t0} R T$$

$$\frac{v}{v_0} = \frac{F_t}{F_{t0}} \frac{P_0}{P} \frac{T}{T_0} \frac{Z}{Z_0}$$

$$C_A = \frac{F_A}{v} = \frac{F_{A0}(1-X_A)}{v}$$

$$C_A = \frac{C_{A0}(1-X_A)T_0}{(1+y_{A0}X_A\delta_A)T} \frac{Z_0}{Z} \frac{P}{P_0}$$

similarly

$$\left.\begin{matrix} C_B \\ C_C \\ C_D \\ C_Z \end{matrix}\right\} \text{etc}$$

So, we have P small v times Z FT R T, FT is a flow rate v is a molar mole volumetric flow. So, p0 v0 is Z0 Ft0 RT. Once again we get relationship very similar to, what you already talked this about? v by v0 in terms of FT by FT0 p0 by p T by T0 and z0. So, that now, we can express concentration CA as FA by v, FA is molar flow of A at any position and v is a volumetric flow. Therefore, by definition we know that FA FA0 times of 1 minus XA because, that is how we define conversion and v which is now coming from this equation as v0 times 1 plus yA0 X plus this relationship v0 this ratio FT by FT0, we already shown is equal to 1 plus ya0 XA delta A.

So, we are able to express concentration in terms of conversion. Similarly we can do for component B C D and I. So, what we have done is that, use the stoichiometry of reaction, and then using the stoichiometry of reaction, and the gas law we have been able to convert concentration in terms of conversion. So, that now we can substitute this CA function in the reaction rate function, and carry out the necessary integration or solution of the algebraic equations.

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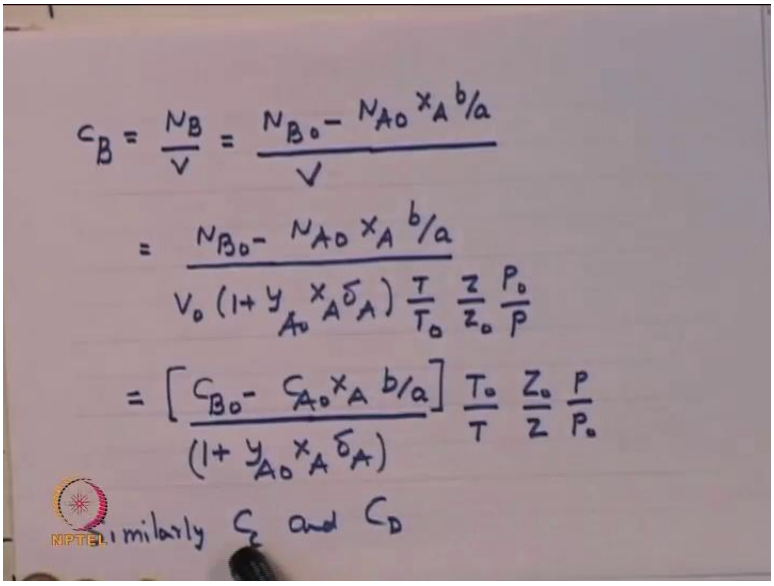

$$c_B = \frac{N_B}{V} = \frac{N_{B0} - N_{A0} x_A b/a}{V}$$

$$= \frac{N_{B0} - N_{A0} x_A b/a}{V_0 (1 + y_{A0} x_A \delta_A) \frac{T}{T_0} \frac{z}{z_0} \frac{P_0}{P}}$$

$$= \left[\frac{C_{B0} - C_{A0} x_A b/a}{(1 + y_{A0} x_A \delta_A)}\right] \frac{T_0}{T} \frac{Z_0}{Z} \frac{P}{P_0}$$

imilarly C_C and C_D

Now just like we have done our component A we can do for component B if it is a batch system it becomes NB by V. Once again we get nice relationship in terms of initial composition of component B and conversion XA CA0 and so on. Similarly we just like, what we got for CA and CB, we can do for CC and CD. So, what we want to now do I mean I quickly show you a problem sheet from which we want to look at 1 of these problems.

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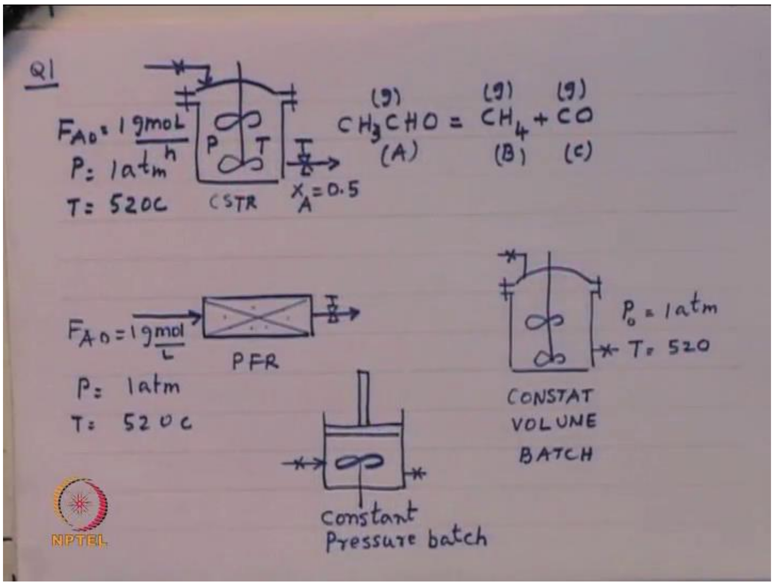

The problem you want to solve is that, we have a reaction which is acetyl de hide under going de composition in thermal giving you a methane and carbon monoxide. This reaction takes place at 520 degree c, it is at 1 atmospheric pressure we want to conduct this reaction to the extent of XA equal to 0.5, which is you want to convert 50 percent of it. We can conduct this reaction in a CSTR continuous input of component A continuous output is in CSTR, we can conduct this reaction in a PFR, where component A comes in and reaction goes out.

We can conduct this reaction in a constant volume batch reactor, we mean in the sense we put all the reagent inside close all the values and conduct the reaction at520 degree c or alternatively, we can also conduct this reaction in a constant volume batch reactor. How do you get constant volume you have a piston, which is able to move up and down depending up on changing in pressure inside.

Therefore, if we charge this acetyl-de-hide in this volume, and as a reaction proceeds there will be increase in volume, and it will keep changing the volume. So, that the pressure will keep changing, but volume will change, pressure will keep constant volume will change. On other words you can conduct this reaction in CSTR at constant pressure, in a PFR at constant pressure, in constant volume batch reactor or constant pressure batch reactor, what is you would like to do? Is to do perform a calculation to see, what is the size of the equipment or the reaction time? That you would require each of these reactor operation choices this is the problem you would like to solve.

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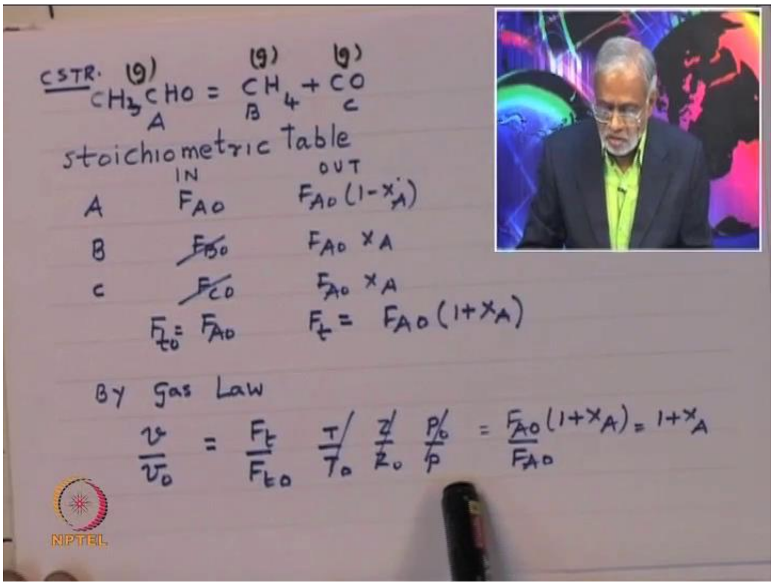

CSTR.

$$\underset{A}{\overset{(g)}{CH_3CHO}} = \underset{B}{\overset{(g)}{CH_4}} + \underset{C}{\overset{(g)}{CO}}$$

stoichiometric table

	IN	OUT
A	F_{A0}	$F_{A0}(1-x_A)$
B	$\cancel{F_{B0}}$	$F_{A0}\,x_A$
C	$\cancel{F_{C0}}$	$F_{A0}\,x_A$
	$F_{t0} = F_{A0}$	$F_t = F_{A0}(1+x_A)$

By gas Law

$$\frac{v}{v_0} = \frac{F_t}{F_{t0}}\,\cancel{\frac{T}{T_0}}\,\cancel{\frac{Z}{Z_0}}\,\cancel{\frac{P_0}{P}} = \frac{F_{A0}(1+x_A)}{F_{A0}} = 1+x_A$$

So, let us, how do you go about doing carrying out a solution to a problem like this of course, 1^{st} you have to write the stoichiometric to understand, what happens component A component b, component c, what do we start with? We are starting with pure component A, What goes in is pure component A. Therefore, B C that is no inert, these 2 are 0, what comes out? By definition we said whatever is the XA is extend of our conversion then, what comes out is given by FA0 times 1 minus of XA, how much B is produced by stoichiometry.

We can say, so much is produced and similarly, so much of C is produced. Therefore, the total number of moles that coming out of the equipment is FT is FA0 time of 1 plus XA, total number of moles you put in is simply FA0. So, what do you have? You are putting a FA0 moles, which is coming in? And, what goes out is FA0 times of 1 plus XA, which means the result increase in the moles because of chemical reaction. It is a gas phase reaction, so acetyl de hide is a gas these are all gases at the temperature of reaction.

So, we will have to apply gas law to understand how volume changes as the reaction proceeds. So, we have already shown little earlier that v by v0 is FT by FT0, T by T0 Z0 Z by Z0, P0 by P. It is the gas law statement we know this for from our early understanding of gas laws now, FT by FT0 you can see from here FT by FT0 is simply 1 plus XA.

Therefore, if the temperature of the reactor does not change this we maintain the temperature at constant at 520 c, and at the conditions the pressure also does not change much and therefore, this is 1 this is 1 this is 1 therefore, simply v by v0 is FT by FT0 from this stoichiometry relationship. We get v by v0 as 1 plus XA. So, what we are able to do is that, we are able to tell how volume volumetric flow changes as reaction proceeds. Now to be able to tell, what is the concentration?

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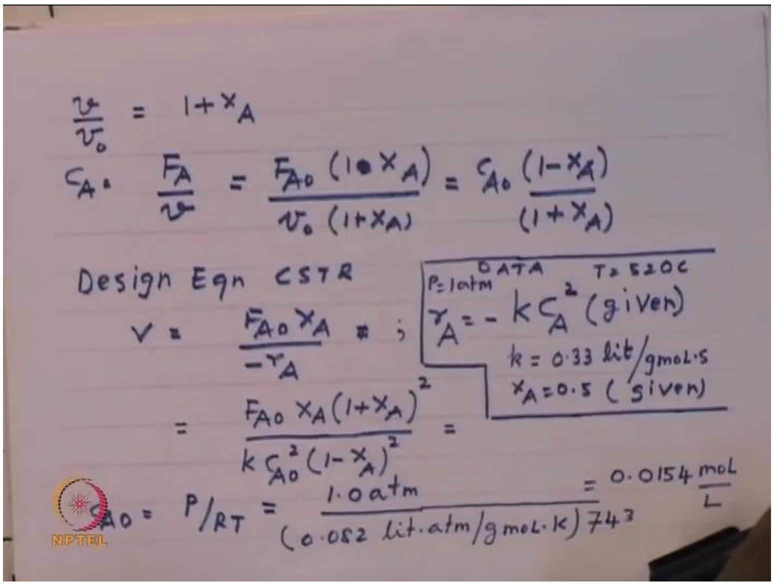

$$\frac{v}{v_0} = 1 + X_A$$

$$C_A = \frac{F_A}{v} = \frac{F_{A0}\left(1 \text{ [illegible] } X_A\right)}{v_0\left(1+X_A\right)} = C_{A0}\frac{\left(1-X_A\right)}{\left(1+X_A\right)}$$

Design Eqn CSTR

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

$$= \frac{F_{A0}X_A\left(1+X_A\right)^2}{k C_{A0}^2\left(1-X_A\right)^2} =$$

DATA

$P = 1\,\text{atm}$ $\quad T = 520\,\text{C}$

$r_A = -kC_A^2$ (given)

$k = 0.33\ \text{lit}/\text{gmol}\cdot\text{s}$

$X_A = 0.5$ (given)

$$C_{A0} = P/RT = \frac{1.0\,\text{atm}}{\left(0.082\ \text{lit}\cdot\text{atm}/\text{gmol}\cdot\text{K}\right)743} = 0.0154\ \frac{\text{mol}}{\text{L}}$$

We know concentration is FA by v if it is a flow system FA is FA0 times of 1 minus of XA, v now just shown is v0 times 1 plus XA. Therefore, we are now able to tell that concentration at any conversion is CA0 multiplied by 1 minus XA by 1 plus XA. So, in essence what we are been able to do now is that, you are able to express concentration in terms of conversion.

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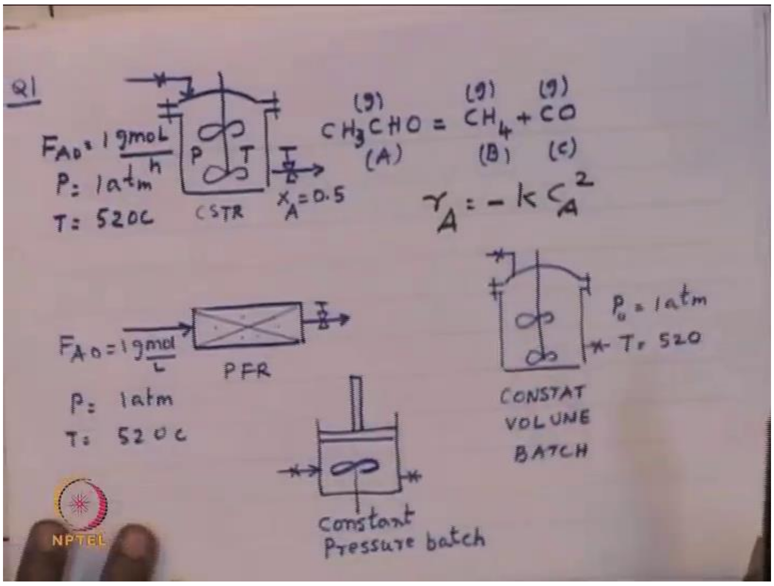

Now in this problem it is given here is a 2nd order reaction that is rA is given as minus k times c a square, it is given. It is given in the problem statement. So that, now we have that if design equation for CSTR we already done. So, that volume of the equipment is FA0 times XA times minus of rA. And what is minus of rA? Is simply from what we got here minus of rA is k times CA square.

So, that is what is done here CA is CA0 1 minus of XA 1 plus XA. So, I put here. So, you get minus of rA you taking signs in to account k times CA0 square 1 minus of XA whole square by 1 plus XA whole squared. So, the volume of this equipment is FA0 times all this, when you put all this numbers 1st you calculate concentration, which is p by RT calculate because 0.015 4 moles per litre at temperature of 520 c. So, what do we get? We get a reactor volume.

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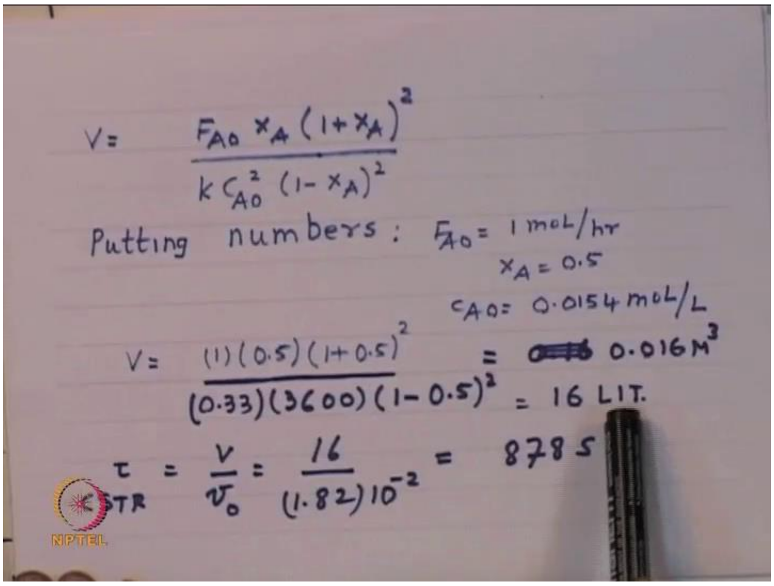

$$V = \frac{F_{A0}\, x_A (1+x_A)^2}{k C_{A0}^2 (1-x_A)^2}$$

Putting numbers : $F_{A0} = 1$ mol/hr

$x_A = 0.5$

$C_{A0} = 0.0154$ mol/L

$$V = \frac{(1)(0.5)(1+0.5)^2}{(0.33)(3600)(1-0.5)^2} = 0.016\,M^3 = 16 \text{ LIT.}$$

$$\tau_{CSTR} = \frac{V}{v_0} = \frac{16}{(1.82)10^{-2}} = 878\,s$$

We put all the number FA0 is 1 mole per hour, we want XA of 0.5 concentration, at CA0 is 0.0154. We can put all this numbers we get CSTR volume as 16 litres, and CSTR residence time is 878 seconds. We are looking at case 1, where we have a CSTR we want to get 50 percent conversion XA equal to 0.5, when at saying that to get 0.5 conversion. We need a residence time of 878 seconds the reactor volume should be 16 litres for this 1 mole per hour.

2nd exercise now, you want to do the same thing we want to do the same thing in a PFR at constant volume, which means you want to do this problem in a constant pressure PFR, where would be the molar flow is 1 gram mole per litre. Pressure is maintained at 1 atmospheric pressure temperature is maintained at 520 c, how do we do this?

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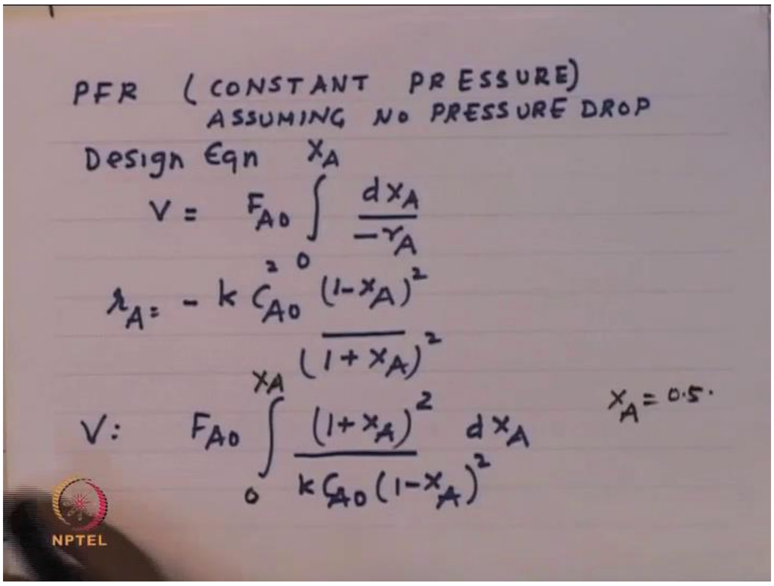

PFR (CONSTANT PRESSURE)
ASSUMING NO PRESSURE DROP

Design Eqn

$$V = F_{A0} \int_0^{x_A} \frac{dx_A}{-r_A}$$

$$r_A = -k C_{A0}^2 \frac{(1-x_A)^2}{(1+x_A)^2}$$

$$V: \quad F_{A0} \int_0^{x_A} \frac{(1+x_A)^2}{k C_{A0} (1-x_A)^2} dx_A \qquad x_A = 0.5.$$

We recall that our design equation for a PFR is simply FA0 integral 0 to XA dxA by minus of rA. We have done this earlier, what is rA? It is k times CA0 square 1 minus of XA by 1 plus XA. This also we are just now done because, we have derived CA in terms of conversion. So, simply what is the volume of the equipment? FA0 times 0 to you have to go from 0 to x xA and we notice that, we want xA of 0.5 in this case this what we want. So, we have put rate function here. So, we simply have to integrate this to find the value of the size of the equipment that is required to do this. Now, this is very simple integration i have done the integration.

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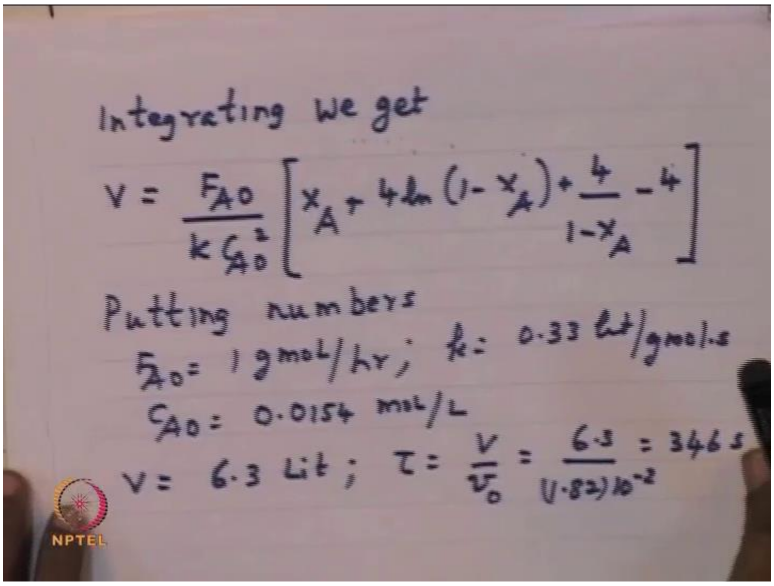

Integrating we get

$$V = \frac{F_{A0}}{k C_{A0}^2}\left[x_A + 4 \ln(1-x_A) + \frac{4}{1-x_A} - 4\right]$$

Putting numbers

$F_{A0} = 1$ gmol/hr; $k = 0.33$ lit/gmol.s

$C_{A0} = 0.0154$ mol/L

$V = 6.3$ Lit; $\tau = \frac{V}{v_0} = \frac{6.3}{(1.82)10^{-2}} = 346$ s

This how the answers look like that volume of the equipment is given by this relationship, and you can put all numbers FA0 is known CA0 everything is known. So, you can calculate the volume of the equipment to be 6.3 litres. Please recognize from the previous case when it use CSTR we got 16.0 litres now, the volume required is only 6.3 litres. And the residence time is defined as v by v0 is 346 seconds, we got 878 seconds last time, what are we saying; that means, when you use a CSTR as a reaction equipment, we require much bigger equipment widely use PFR you have much smaller equipment.

We will come back to this within a minute now one issue that we would always like to know because there is a change in volume, and we are calculating our residence time tau as v divided by v0 where v0 is the volumetric flow at the inlet. But the fact is that because of the volume change the volumetric flow is increasing, in this case. Therefore, the actual time of residence inside the equipment is different from, what we have found out is based on v by v0. So, it is interest to us actually find out, what is the residence time? That is experienced by the fluid elements, how do we do this?

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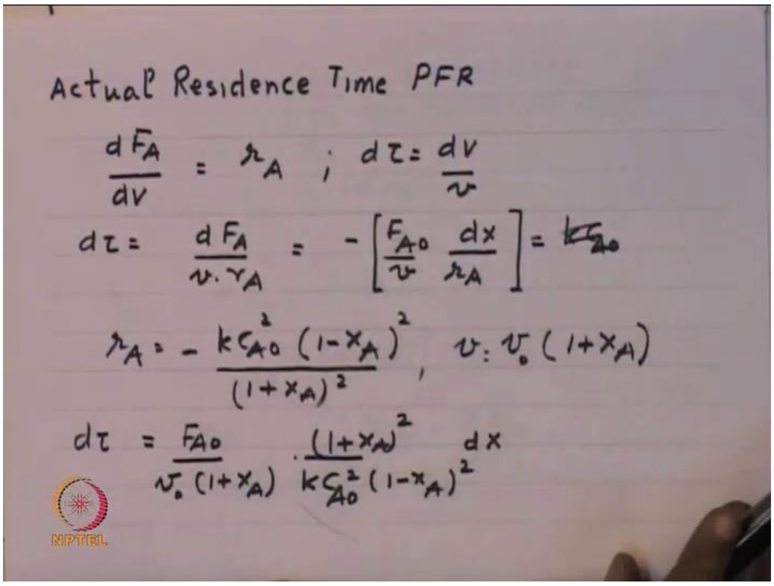

Actual Residence Time PFR

$$\frac{dF_A}{dV} = r_A \; ; \; d\tau = \frac{dV}{v}$$

$$d\tau = \frac{dF_A}{v \cdot r_A} = -\left[\frac{F_{A0}}{v}\frac{dx}{r_A}\right] = \cancel{kC_{A0}}$$

$$r_A = -\frac{kC_{A0}^2(1-x_A)^2}{(1+x_A)^2}, \quad v = v_0(1+x_A)$$

$$d\tau = \frac{F_{A0}}{v_0(1+x_A)} \cdot \frac{(1+x_A)^2}{kC_{A0}^2(1-x_A)^2}\, dx$$

Then we derive, what we call us actual residence time that is required for this equipment, how do you define actual residence time d tau which is the actual residence time is simply d tau is dv by v; that means, if we take elemental volume dv divided by the volumetric flow at that position that gives the residence time for the differential element.

Therefore, we can use the design equation for PFR which is dFA by dv equal to rA, and then simplify this, and get what we call as actual residence time in terms of the rate function and so on. We already derived all these things in our earlier class therefore, this basically gives us, what is the actual residence time now in terms of other measure properties like XA and so on.

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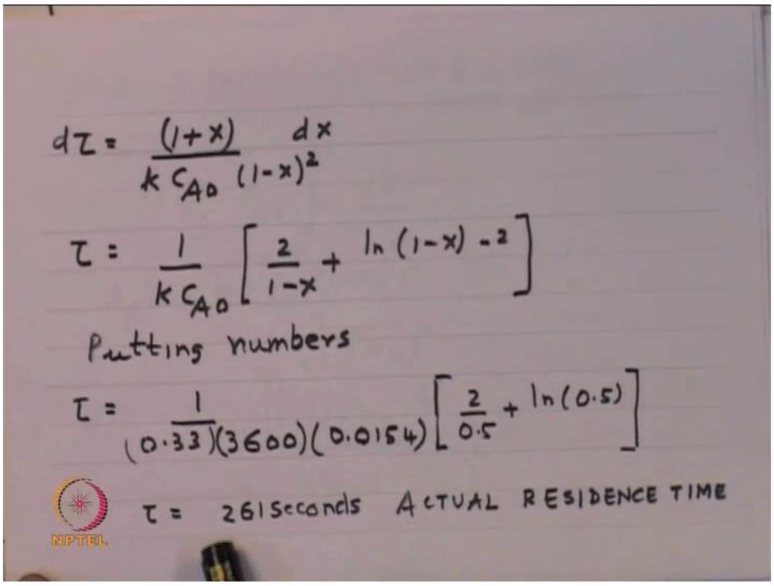

$$d\tau = \frac{(1+x)}{k\,C_{A0}\,(1-x)^2}\,dx$$

$$\tau = \frac{1}{k\,C_{A0}}\left[\frac{2}{1-x} + \ln(1-x) - 2\right]$$

Putting numbers

$$\tau = \frac{1}{(0.33)(3600)(0.0154)}\left[\frac{2}{0.5} + \ln(0.5)\right]$$

τ = 261 seconds ACTUAL RESIDENCE TIME

This can be integrated, and we get a result like this it says that the actual residence time in a PFR while, there is an increasing in volume can be integrated to get this function, where x is the extend of reaction or conversion. You put to a number x is 0.5, we know that k is known, and CA0 is known, I put all the numbers here, you get actual time of residence is 261 seconds, what are we saying? what we are saying is that; if we have a plug flow reactor entering at 1 mole per hour and then temperature is 520 because of this reaction.

Even though the residence time based on inlet molar flow is 346 seconds actual time of residence is only 261 seconds because of, the fact that there is an increasing in volume or increase in volumetric flow rate as the reaction procedure. The next issue that we would look at is, what happens suppose you conduct the reaction in a constant volume batch reactor, how does it look? Let us see how it looks

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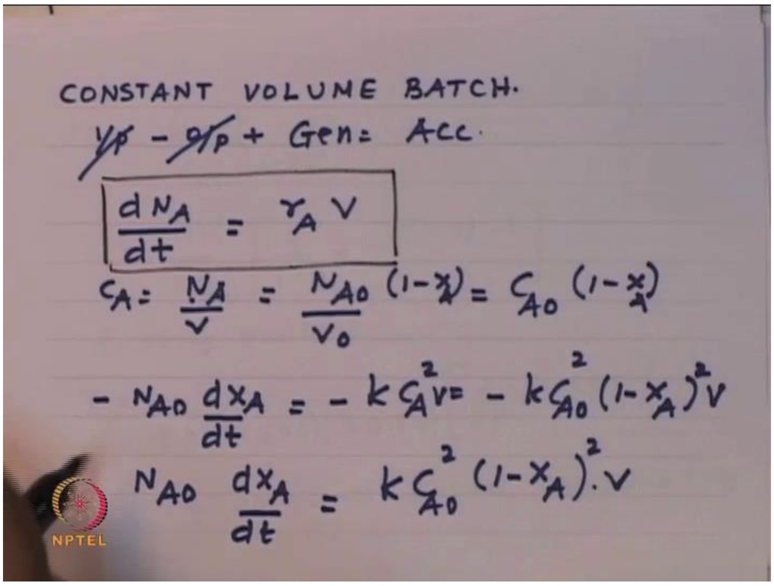

CONSTANT VOLUME BATCH.

$$\cancel{I/P} - \cancel{O/P} + Gen = Acc.$$

$$\boxed{\frac{dN_A}{dt} = r_A V}$$

$$C_A = \frac{N_A}{V} = \frac{N_{A0}}{V_0}(1-x_A) = C_{A0}(1-x_A)$$

$$-N_{A0}\frac{dx_A}{dt} = -kC_A^2 V = -kC_{A0}^2(1-x_A)^2 V$$

$$N_{A0}\frac{dx_A}{dt} = kC_{A0}^2(1-x_A)^2 . V$$

Now, our constant volume batch reactor we have look at the design equation for batch input output generation accumulation there is no input there is no output therefore, this is dNA by dt. This is the statement of material balance for a batch reactor something that we have done. Now, once again CA is what? NA by v and since the constant volume batch therefore, v is v0 therefore, CA becomes CA0 1 minus of x a.

Please notice that the function CA for a constant volume batch CA0 1 minus XA. But for the case that there is a constant pressure we have the effect that we have already shown. Now you can substitute NA in terms of NA0 and so on. Finally, that you kind of equation that we have to solve this is the kind of equation that we have to solve. Notice here, that this kind of equation looks very different from what we have done for a constant pressure batch. So, we can put all the numbers, and then integrate and so on.

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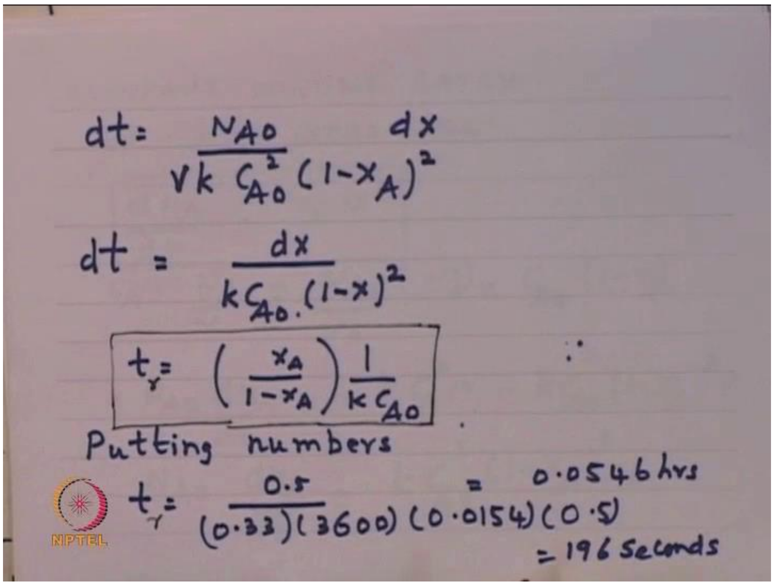

$$dt = \frac{N_{A0}\, dx}{V k\, C_{A0}^2 (1-x_A)^2}$$

$$dt = \frac{dx}{k C_{A0}.(1-x)^2}$$

$$\boxed{t_r = \left(\frac{x_A}{1-x_A}\right)\frac{1}{k C_{A0}}}$$

Putting numbers

$$t_r = \frac{0.5}{(0.33)(3600)(0.0154)(0.5)} = 0.0546 \text{ hrs}$$

$$= 196 \text{ Seconds}$$

We will get for a constant volume batch reaction time is given by XA by 1 minus of XA times 1 by k CA0. So, this is the integrate form for that case then there is a constant volume batch. Please notice that the final result we get for a constant volume batch quiet different from, what we got for other 2 cases we are considered. If you put a numbers you find, that the reaction time for a constant volume batch is 196 seconds, what are we saying? What are we saying is that; when we do this in the case this is for a constant pressure for CSTR, this is for constant pressure for PFR. Then we also looked at what is the actual residence time here now, we are looking at constant volume batch reactor for this case you find that the reaction time for a conversion of 0.5 is about 196 seconds much lower than these 2 cases we consider so for.

So, the reaction time required for a constant volume batch is only 196 seconds. Let us see what happens if we conduct this same the reaction in a constant pressure batch, how do you get constant pressure? We get constant pressure by, providing a piston which is able to move up and down depending on, changes in pressure inside keeps the volume changes keeping the pressure constant. So, what do we do? You allow the volume to change because of the piston able to move. So, we are looking at case of constant pressure variable volume, this is the case of variable volume, let us quickly run through this how it looks.

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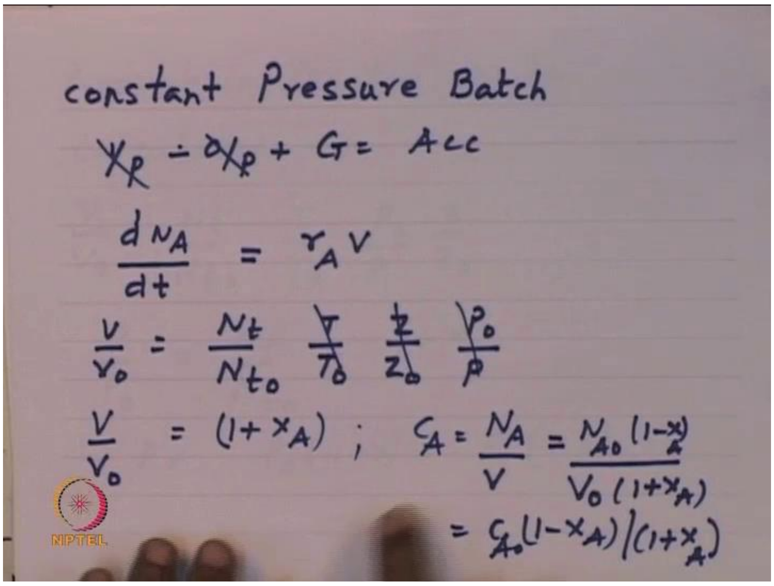

constant Pressure Batch

$$\cancel{R} - \cancel{P} + G = Acc$$

$$\frac{dN_A}{dt} = r_A V$$

$$\frac{V}{V_0} = \frac{N_t}{N_{t0}} \cancel{\frac{T}{T_0}} \cancel{\frac{z}{z_0}} \cancel{\frac{P_0}{P}}$$

$$\frac{V}{V_0} = (1+x_A) \; ; \quad C_A = \frac{N_A}{V} = \frac{N_{A0}(1-x_A)}{V_0(1+x_A)}$$

$$= C_{A0}(1-x_A)/(1+x_A)$$

So, once again we are writing the material balance, there is input output generation accumulation there is no input because, the batch process there is no output because, the batch process. Therefore, generation equal to accumulation therefore, dN by dt equal to r AV. Once again v by v this gas law will hold temperature does not change, compressibility changes are not important there is no change in pressure because, we are keeping the pressure constant. Therefore, v by v0 that mean change in volume of this equipment is NT by Nt0, we have shown from our stoichiometry the NT by NT0 is1 plus XA.

Therefore, volume of the reaction equipment divided by the volume at 0 time is 1 plus XA. Now, what is concentration? We said concentration is number of moles divided by volume, number of moles is NA0 times of 1 minus XA. Therefore, we get that CA at any conversion is CA0 times of 1 minus XA by 1 plus of XA, something similar to what we already got for constant pressure case earlier. So, we get the same kind of result CA is CA0 1 minus of XA by 1 plus XA. Now, we know, what is the rate function? Rate function we can therefore, substitute from our, we can substitute for rA rate functions are known therefore, we can substitute integrate this to find out solution, that is what have been done.

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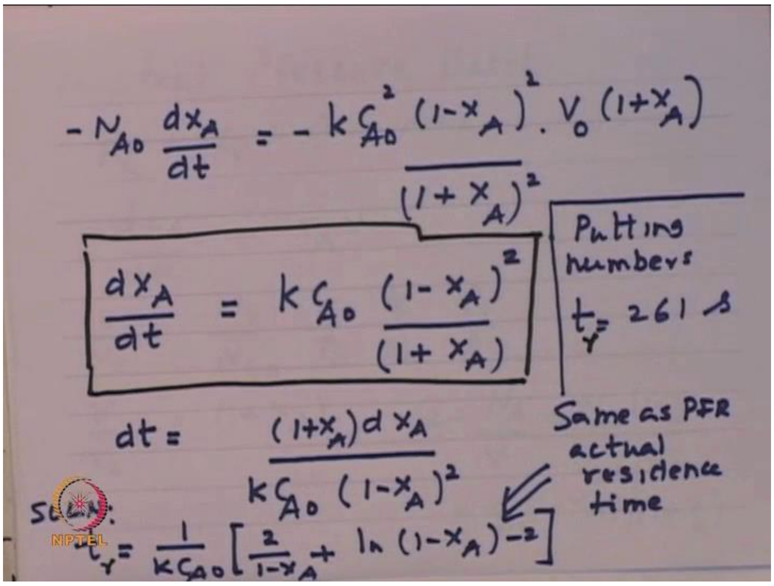

$$-N_{A0}\frac{dX_A}{dt} = -kC_{A0}^2\frac{(1-X_A)^2}{(1+X_A)^2}.V_0(1+X_A)$$

$$\boxed{\frac{dX_A}{dt} = kC_{A0}\frac{(1-X_A)^2}{(1+X_A)}}$$

$$dt = \frac{(1+X_A)\,dX_A}{kC_{A0}(1-X_A)^2}$$

Soln:

$$t_r = \frac{1}{kC_{A0}}\left[\frac{2}{1-X_A} + \ln(1-X_A) - 2\right]$$

Putting numbers

$t_r = 261$ s

Same as PFR actual residence time

So, left hand side dNA by dt replace like this, the right hand side rAV is replaced like this. So, that you get d by dt of XA is given by this relationship. So, our result will come from the solution of this equation for the case of constant pressure variable volume batch, when you integrate this, this is the result you get. On other words for case of constant pressure variable volume batch reactor answer we get, is reaction time equal to this result. And you will notice that this is the exactly the same result we got for the actual residence time in a PFR, on other words the result we are getting for a actual residence time in a PFR, and for constant pressure variable volume batch is identical. Therefore, when you put all the numbers you get the actual time that is required t \r is equal to 261 seconds that is we got for the case of actual residence time in a PFR. So, what are we saying? what we are trying to say is a following this is important.

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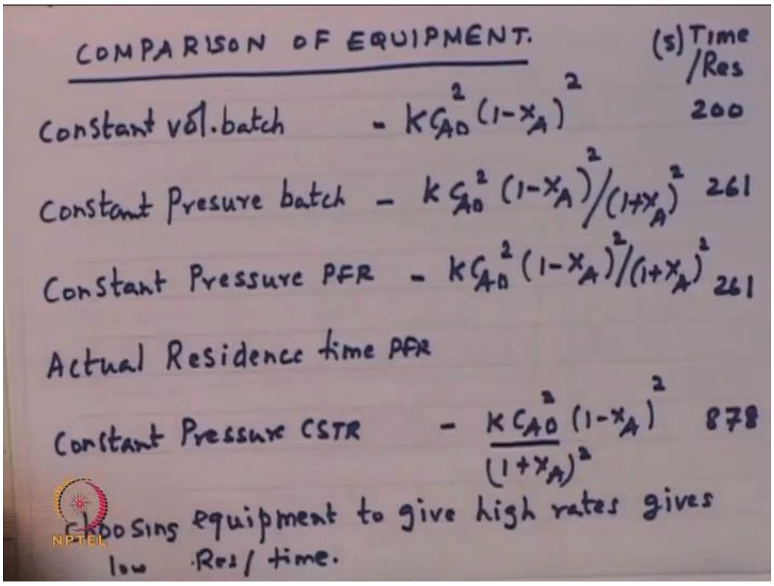

COMPARISON OF EQUIPMENT. (s) Time /Res

Constant vol. batch - $kC_{A0}^2(1-x_A)^2$ 200

Constant Presure batch - $kC_{A0}^2(1-x_A)^2/(1+x_A)^2$ 261

Constant Pressure PFR - $kC_{A0}^2(1-x_A)^2/(1+x_A)^2$ 261

Actual Residence time PFR

Constant Pressure CSTR - $\frac{kC_{A0}^2(1-x_A)^2}{(1+x_A)^2}$ 878

Choosing equipment to give high rates gives low Res/ time.

We have the problem we are trying to solve is this; you have a reaction, which is undergoing decomposition to give you a methane and carbon monoxide. You conduct the reaction in a constant pressure CSTR, you conduct the reaction in constant pressure PFR, you conduct the reaction in constant volume batch, and then you conduct this one in the case in a variable volume constant pressure batch.

There are 4 cases, notice here the initial pressure is 1 atmosphere, pressure would change because of the reaction now to understand this, what I have done is; just looking at how the different equipment would perform constant volume batch, constant pressure batch, constant pressure PFR, constant pressure CSTR. I just set out here, what is the rate expression that we are getting for each case, for each case, what is the rate expression that we are getting? If you look carefully you find that constant volume batch the rate expression is k CA0 1 minus XA whole squared, while in the other cases there is a denominator 1 plus XA whole squared.

On other words in a constant volume batch the rate at which the chemical reaction occurs is always much higher than the rate at which the chemical reaction occur, if it is a constant pressure batch. And because the fact that the reaction rates are much higher in a constant volume batch, the time of residence a time of reaction is much slower, compared to the constant pressure batch. Similarly if you look at a constant pressure PFR, once again we find that the reaction time is higher than constant volume batch. The reason is the rate expression is itself to shows you very clearly that, the rate of chemical reaction in constant pressure PFR is much lower than the rate of chemical reaction in constant volume batch, that is why you get a higher time of reaction.

Now, if you look at a constant pressure CSTR our rate expression is if you see carefully is such that is much lower than the other, and therefore, you find that the reaction time is very large. So, what are we trying to tell? What we are trying to say is that; in our reactor design we must take care to see that the rate expression that we would choose of the equipment that we would choose, should have very high reaction rates at every point of the equipment, that is important at ever point of the equipment.

And that is why because, it is very favourable in constant volume batch we get very small reaction time it is not, so favourable in a CSTR. Therefore, we get very high reaction time. Therefore, choice of equipment really depends up on, how well we understand the reaction kinetics. So, that we can maximize or minimize, maximize the benefit or minimize the size of the equipment that we use for our application. Let just quickly recall, what we are said? What we are said is that we have a reaction.

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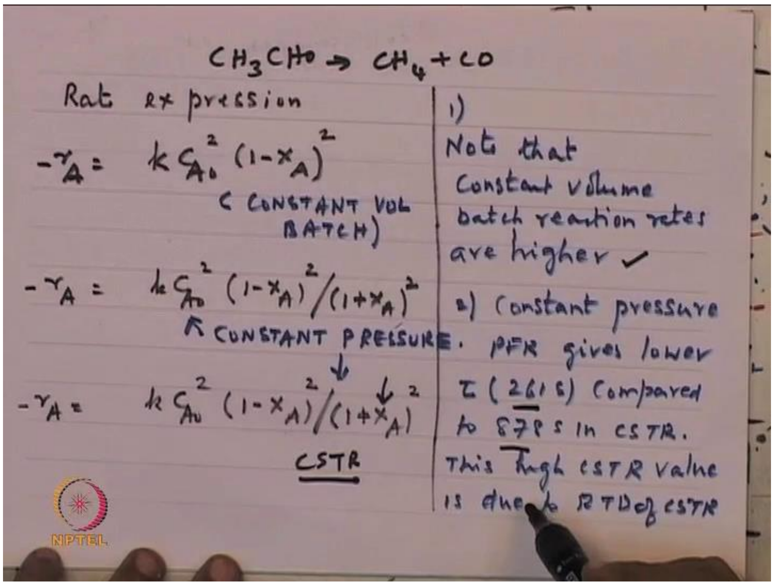

$CH_3CHO \rightarrow CH_4 + CO$

Rat ex pression

$-r_A = k C_{A0}^2 (1-x_A)^2$

(CONSTANT VOL BATCH)

$-r_A = k C_{A0}^2 (1-x_A)^2 / (1+x_A)^2$

↖ CONSTANT PRESSURE.

$-r_A = k C_{A0}^2 (1-x_A)^{\overset{\downarrow}{2}} / (1+\overset{\downarrow}{x}_A)^2$

CSTR

1) Not that Constant volume batch reaction rates are higher ✓

2) Constant pressure PFR gives lower τ (261 s) Compared to 878 s in CSTR. This high CSTR value is due to RTD of CSTR

And this in this reaction, we are trying to look at, what is the performance of various kinds of devices for a given reaction? The reaction for our interest is we wrote this reaction as acetyl de hide CH3CHO giving you CH4 plus CO, correct CH4 plus CO. Now, we look at various devices I just summarise this, just to bring your attention in some important features, what we are shown through our calculations? Is that constant volume batch reactor has the rate expression, if you see the rate expression for a constant volume batch, and compare this with constant pressure batch, this also a constant pressure CSTR.

The rate expression shows very clearly that the reaction rate that we can achieve, in a constant volume batch is much higher than the reaction rate that you will get in constant pressure, and then, and in a constant of CSTR. Both the cases the reaction rate are less because, the rate expressions are like that. Therefore, if we can actually utilize a constant pressure constant volume kind of batch equipment we will get a higher reaction rates.

There is one important point that we trying to get across, the 2ndpoint we trying to get across to you is that even if you having a constant pressure process for example, a constant pressure PFR, and a constant pressure CSTR. Now the both cases the reaction rate expressions are the same, but notice that the residence time is 261 for a PFR and 878 for a CSTR, how do you explain this? We explain this by recognizing that there is a fundamental difference between CSTR and a PFR because, the residence time are very different.

On other words CSTR because, it operates at exit conditions of conversion to exit conditions conversion the reaction rate that we achieved in a CSTR is that of the reaction rate at exit. While in a PFR the reaction rates are at the instant position at which the reaction taking place. On other words, even though the reaction rates expressions are the same, PFR has a much higher average reaction rates compared to CSTR. This point must be born in mind in the choice of reaction equipment, so this one example that you would like to recognize. Now the another example we would like to take to illustrate how our system would perform, when there are certain important changes taking place in the equipment.

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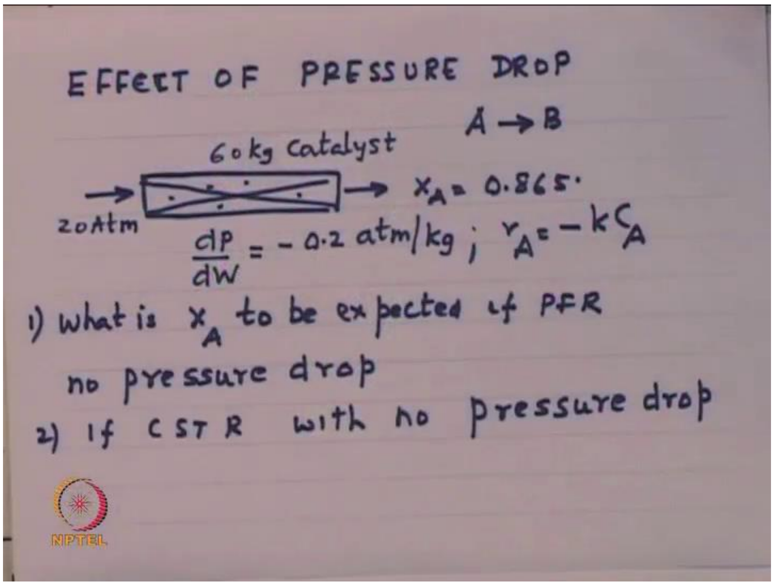

EFFECT OF PRESSURE DROP

$A \rightarrow B$

60 kg Catalyst

20Atm → → $x_A = 0.865$.

$\frac{dP}{dW} = -0.2$ atm/kg ; $r_A = -kC_A$

1) what is x_A to be expected if PFR no pressure drop

2) if CSTR with no pressure drop

For example, the problem we would like to now address is there is a plug flow reactor. The plug flow reactor in which there is a reaction a going to b, reaction a going to b, and this plug flow reactor contains a catalyst. Now, what comes in? The feed is coming in at 20 atmospheres and because of pressure drop the pressure that goes out is less than what is coming in, and then the pressure gradient that we are expecting in this process is given as dp by dw is minus of 0.2. On other words, as fluid moves the pressure drops at this rate dp dw is minus of 0.2 keeps on decreasing.

And because of, decreasing in pressure we expect some effect on the process that is what we would like to quantitatively understand and evaluate, what are we saying? That the rate of chemical reaction is given as minus of k times CA 1st order reaction, when k is a rate constant, rate constant is given everything is given. Now, what is being said in this problem is that; you in an experiment in which you have feed coming in feed going out and so on. You experiencing as 86.5 percent conversion.

Now, what is asked of you is; what do you expect to see if there was no pressure drop, you understand that those no pressure drop, what do we expect to see? That is 2nd point is that instead of using a PFR, if we had used a CSTR, what do we expect to see? That mean you have got some data based on in your experiments where you find 86.5 percent is the conversion because of this pressure gradient, and you would like to know suppose, by some design of the catalyst you could have substantially eliminated this pressure drop due to this catalyst, what is the likely benefit you will see in this equipment PFR or alternatively? Or alternatively, what is the likely benefit you would see if you add a CSTR, this is the question we are trying to answer. Let us see, how to understand this? Now, our data says that 86.5 percent conversion using the existing equipment while there is a pressure drop in this dp dw is point two. So, we have to 1st model this equipment to understand, what are the features of this equipment that we are using? What is it say?

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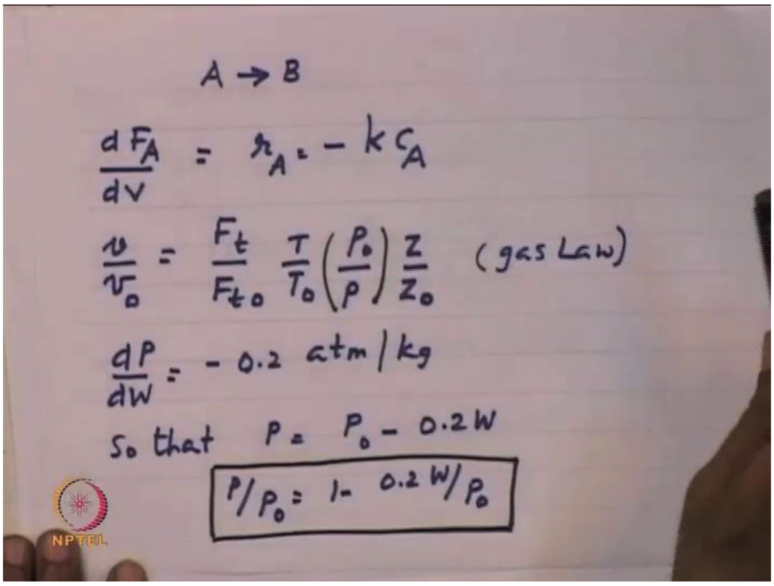

$A \rightarrow B$

$$\frac{dF_A}{dv} = r_A = -kC_A$$

$$\frac{v}{v_0} = \frac{F_t}{F_{t0}} \frac{T}{T_0} \left(\frac{P_0}{P}\right) \frac{Z}{Z_0} \quad (\text{gas Law})$$

$$\frac{dP}{dW} = -0.2 \text{ atm/kg}$$

So that $P = P_0 - 0.2W$

$$\boxed{P/P_0 = 1 - 0.2\,W/P_0}$$

dFA dv ((Refer Time: 35:02)) PFR equation ka which is minus of k CA 1st order reaction. Now, it is a gas phase reaction therefore, our gas law will hold v by v0 FT by FT0, T by T0, P0 by P, Z by Z0. This is gas law, we know from our problem statement that pressure changes because it is of the pressure gradient dp dw minus of 0.2. So, that when we integrate this, you get that the pressure at any point is pressure at the inlet multiplied by 0.2 times w. That means pressure keeps on decreasing by this relationship, so that; if you want p by p0 we get this relationship.

So, why are we writhing this relationship? We are writhing this relationship because; we know that our volumetric flow depends on pressure. So, how the pressure changes accordingly our volumetric flow is affected, and volumetric flow is affected we know concentrations are affected. So, you find you will find the pressure will have an effect on concentration and therefore, it will have an effect on rate of chemical reaction. So, it is that effect that we want to quantitate in this problem. So, what are we saying? What are we saying is that df da d v is ra which is minus of k CA. Now, we have been given catalyst w, so it is not volume that is given, what is given is wait of catalyst. So, you have to express this in terms of data that is given.

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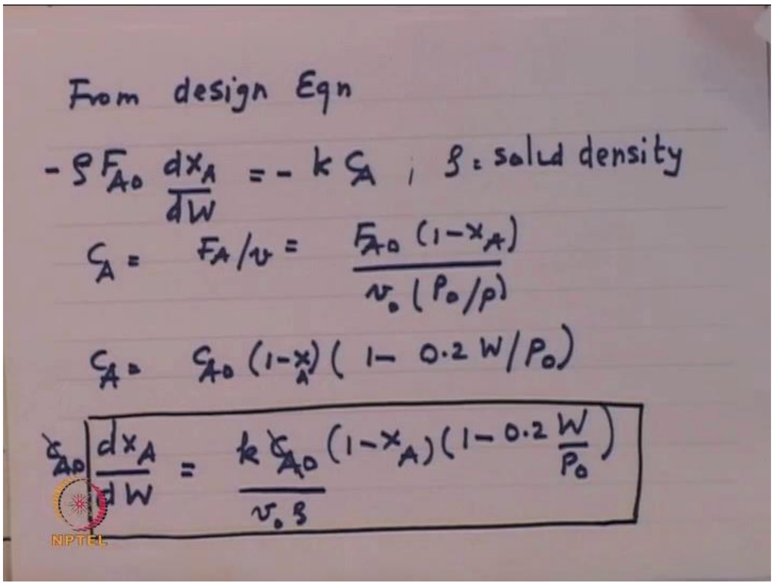

From design Eqn

$-\rho F_{A0} \frac{dx_A}{dW} = -k C_A$; ρ = solid density

$C_A = F_A/v = \frac{F_{A0}(1-x_A)}{v_0 (P_0/P)}$

$C_A = C_{A0}(1-x_A)(1-0.2W/P_0)$

$$\cancel{C_{A0}}\boxed{\frac{dx_A}{dW} = \frac{k\cancel{C_{A0}}}{v_0 \rho}(1-x_A)\left(1-0.2\frac{W}{P_0}\right)}$$

That is what is done here; volume is expressed as w divided by rho is volume, so I put rho on numerator. So, we have this equation, which tells you the 1st our what is called us our design equation. So, CA is what? We said CA is FA by v, but FA is what FA0 of 1 minus of XA from stoichiometry. And, what is v? We said just now from here v by v0 is what P0 by P what is; that means, this relationship appears here when you substitute this in to this relationship, we find v by v0becomes our v becomes v0times P0 by P. So, this effect of volume v by v0, what is v equal to? v0 times P0 by P, T by T0 is 1, Z by Z0 is 1, FT by FT0 is 1, because there is no change in volume due to reaction.

So, but there is change in volumetric flow because of, pressure variation that is the effect we are trying to quantitate. So, what are we got here? Concentration in any position is FA0 times 1 minus XA comes with stoichiometry, while volumetric flow changes because pressure variation is v0 times P0 by P. So, that now, we see the concentration CA is written as CA0 1 minus of XA multiplied by this term which takes into account the effect of pressure drop. Now, we can substitute all these things in to our design equation here. So, that we get d by dv d by dw of XA rated which conversion changes with weight of the catalyst, is given by k times rho times v0, where are we? This how it comes you are substituting for CA here, so it comes relationship like this where k by v0 rho which you do not know XA is given as 0.85 for this particular case of PFR. So, if you integrate this if you integrate this; this equation essentially tells you how the PFR that we have got in our experiment performing. That is what has been done.

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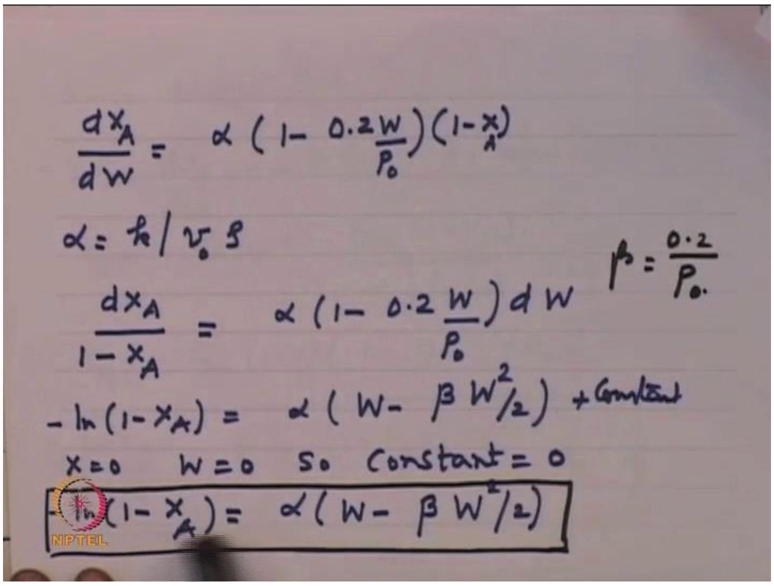

$$\frac{dx_A}{dW} = \alpha\left(1 - 0.2\frac{W}{P_0}\right)(1 - x_A)$$

$$\alpha = k / v_0 \rho$$

$$\beta = \frac{0.2}{P_0}$$

$$\frac{dx_A}{1 - x_A} = \alpha\left(1 - 0.2\frac{W}{P_0}\right) dW$$

$$-\ln(1 - x_A) = \alpha\left(W - \beta W^2/2\right) + \text{Constant}$$

$$x = 0 \quad W = 0 \quad \text{So Constant} = 0$$

$$\boxed{-\ln(1 - x_A) = \alpha\left(W - \beta W^2/2\right)}$$

Then we find that when we integrate this we get a relationship like this. This is the final result we get, when we integrate the final result we get is for this PFR containing 60kg of catalyst 1 minus of XA is multiplied alpha times w minus beta and so on. While beta is what beta is beta is; beta equal to 0.2 I mean mention beta is 0.2 by P0 that is beta. So, XA is given, what is alpha? Alpha is this which is unknown P0 is known, so this quantity is known beta by P0 is known. Therefore, we can substitute the value of XA coming from our experiment that is what I have done.

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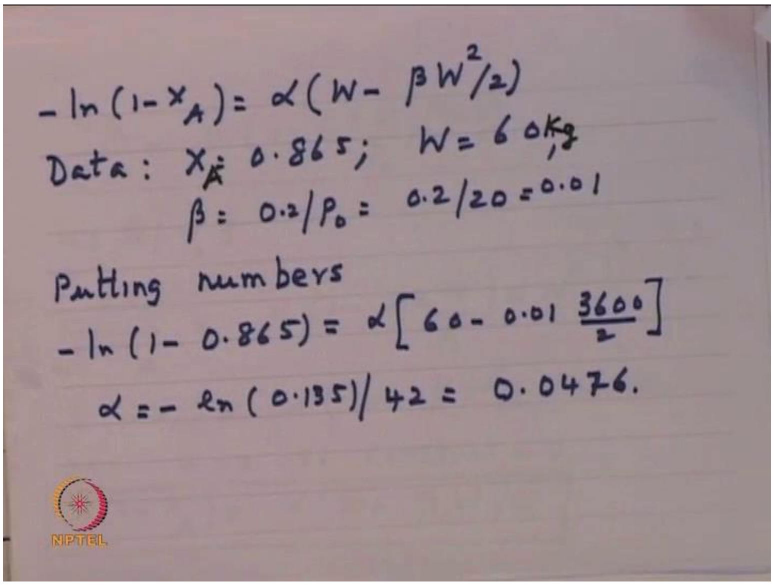

$-\ln(1-X_A) = \alpha(W - \beta W^2/2)$

Data : $X_A = 0.865$; $W = 60$ kg

$\beta = 0.2/P_0 = 0.2/20 = 0.01$

Putting numbers

$-\ln(1-0.865) = \alpha\left[60 - 0.01\,\frac{3600}{2}\right]$

$\alpha = -\ln(0.135)/42 = 0.0476.$

But, I have done here is that in this solution I substitute the data which XA is given XA not X, XA is 0.865, w is given so many kg, beta is given P0 is 0.01 everything put all the number, and find out, what is the value of alpha that is appropriate to our experiment. So, essentially what we have done, so for is that; from the data that is given to us we have calculated, what is the value of parameters that describes this data

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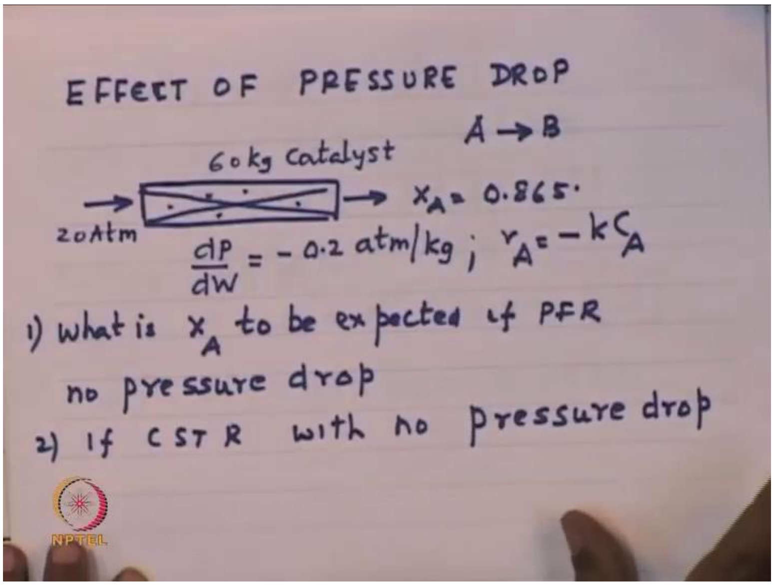

EFFECT OF PRESSURE DROP

A → B

60 kg catalyst

20Atm → → $X_A = 0.865$.

$\frac{dP}{dW} = -0.2$ atm/kg ; $r_A = -kC_A$

1) what is X_A to be expected if PFR no pressure drop

2) If CSTR with no pressure drop

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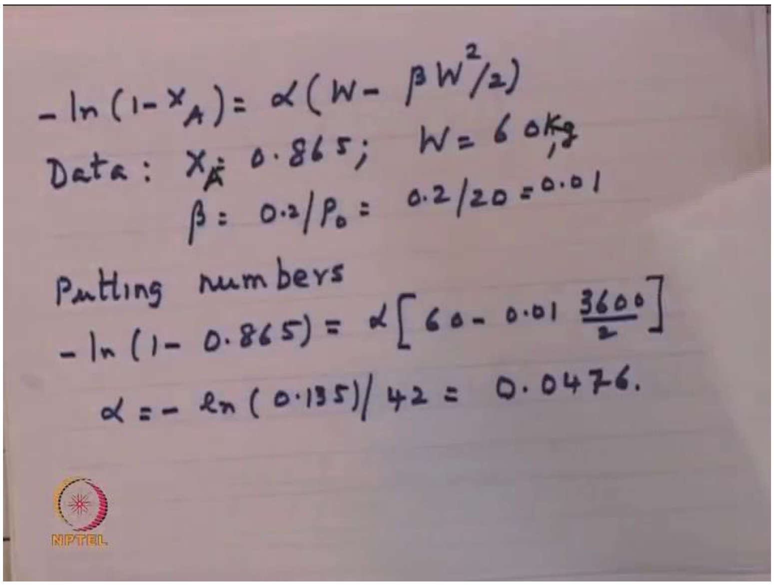

$$-\ln(1-x_A) = \alpha(W - \beta W^2/2)$$

Data: $x_A = 0.865$; $W = 60$ kg

$\beta = 0.2/P_0 = 0.2/20 = 0.01$

Putting numbers

$$-\ln(1-0.865) = \alpha\left[60 - 0.01\,\frac{3600}{2}\right]$$

$$\alpha = -\ln(0.135)/42 = 0.0476.$$

Our parameters are alpha is the parameter of the process alpha is equal to 0.476. So, what are we done? What you have done is that; we have taken a problem in which data is given XA is 0.865 weight of the catalyst is given pressures are given. So, we characterize this in terms of what is the value of alpha that is responsible for this kind of chemical reaction. Now, the question is now the alpha is known we can answer the question that we want to answer, what happens if there is no pressure drop? What happens if we instead of using PFR if we use a stir tank? We are straight to answer the question.

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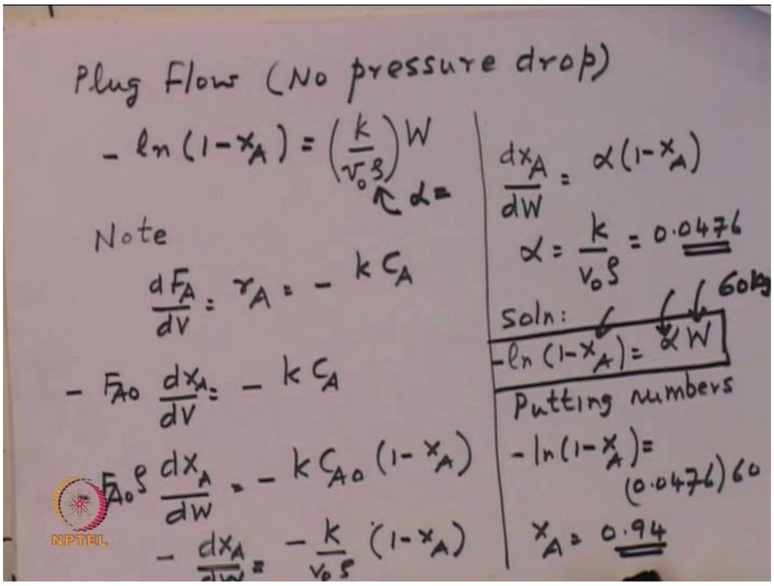

Plug Flow (No pressure drop)

$$-\ln(1-x_A) = \left(\frac{k}{v_0\rho}\right)W \quad \alpha =$$

Note

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

$$-F_{A0}\frac{dx_A}{dV} = -kC_A$$

$$F_{A0}\rho\frac{dx_A}{dW} = -kC_{A0}(1-x_A)$$

$$-\frac{dx_A}{dW} = -\frac{k}{v_0\rho}(1-x_A)$$

$$\frac{dx_A}{dW} = \alpha(1-x_A)$$

$$\alpha = \frac{k}{v_0\rho} = \underline{\underline{0.0476}}$$

Soln: 60kg

$$\boxed{-\ln(1-x_A) = \alpha W}$$

Putting numbers

$$-\ln(1-x_A) = (0.0476)60$$

$$x_A = \underline{\underline{0.94}}$$

So, suppose if we have a plug flow reactor there is no pressure drop for which this value of alpha is known, this is alpha which is known in this case given as 0.0476. Therefore, what we simply find out integrate this, when you integrate this you find that our PFR, in the absence of pressure drop is given by this relationship, this is the solution. Our solution is this, and what is the value of XA? If I ask you alpha is known because, alpha is 0.0476, w is known which is 60kg.

Therefore, you can find out what is the conversion that you would expect if there was no pressure drop. Now, the context to this question is the important, why are we looking at the case of no pressure drop? It tells us that what was 86.5 when there is a pressure drop actually become 94, when there is no pressure drop. On other words, there is considerable benefit in a process to significantly reduce pressure drop by a suitable design of a catalyst that is the point being made. The 2nd question that we are trying to answer is suppose instead of using a PFR, we have to use stir tank; that means, what is a stir tank?

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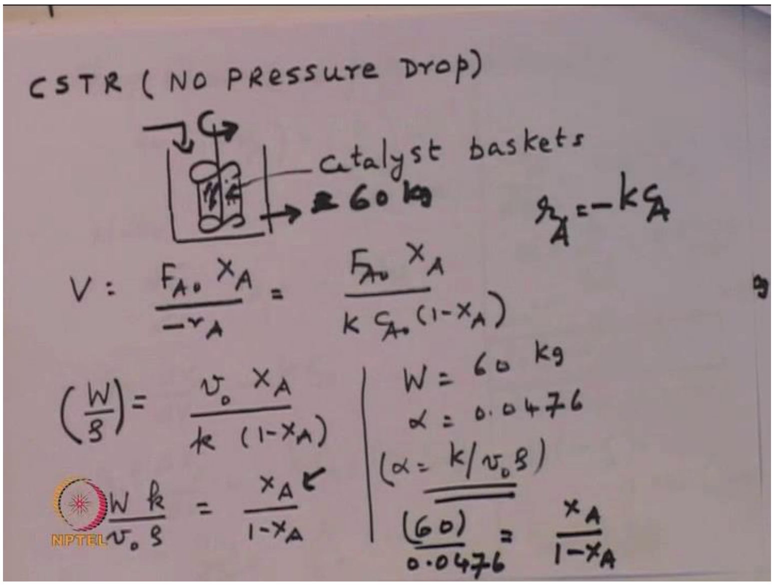

CSTR (NO PRESSURE DROP)

$r_A = -kC_A$

$$V = \frac{F_{A0}X_A}{-r_A} = \frac{F_{A0}X_A}{kC_{A0}(1-X_A)}$$

$$\left(\frac{W}{\rho}\right) = \frac{v_0 X_A}{k(1-X_A)}$$

$$\frac{Wk}{v_0\rho} = \frac{X_A}{1-X_A}$$

$W = 60$ kg

$\alpha = 0.0476$

$(\alpha = k/v_0\rho)$

$$\frac{(60)}{0.0476} = \frac{X_A}{1-X_A}$$

You have a catalyst a 60kg of catalyst you want to support in on a basket; that means, you have a spinning basket, in to which you have to support a 60kg of catalyst it is not a very difficult thing to do appropriately design the stir tank and so on. Once you do that you are able to put your feed your feed comes in, and your feed goes out product go out and your reactor design equation is v equal to FA0 XA by minus of rA. So, that you can put all your rate functions here, rate function rA is we have just now been shown that r a is minus of k times CA. So, 1storder process therefore, you can find out, what is the weight of the catalyst in terms of parameters in the system? What are the parameters of the system here? Alpha is given therefore, you can find out what is the extent to which you can write the reaction, what is the value of XA? What is the value of x a?

Let me do this calculation for you w 60 and then v0 alpha is alpha is k by k by v0 that is 0.0076 0.0476 equal to XA by 1 minus of XA. So, you can find out value of XA. So, what we are saying is that, we can find out the value of XA as you know the alpha values. So, the problem that we are try to solve is in the absence of pressure drop, there are significant benefits are achieved if we have a plug flow reactor without pressure drop. Now, the idea of doing what is called as the CSTR is the spinning basket is something that very important that you should recognize.

Now, generally to be able to get good data on kinetics on a catalyst it is important to have temperature around the catalyst to be uniform. And, spinning baskets give you very good temperature uniformity, and this is what makes spinning basket reactors extremely valuable for catalyst evaluation, how well the catalyst perform under various condition to get good kinetic data, so that you can model the kinetics properly which you can use for design. So, you will find that CSTR data is what generally useful from the point of view of trying to get good kinetic data for design. Have you set this about pressure drop there are few things that I would like to try you tension from the point of view of pressure drop in a process.

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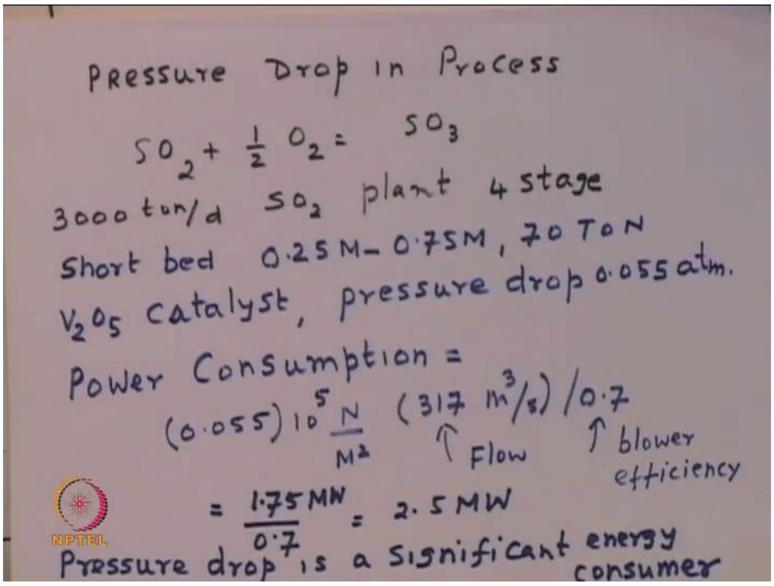

Pressure Drop in Process

$SO_2 + \frac{1}{2} O_2 = SO_3$

3000 ton/d SO_2 plant 4 stage

Short bed 0.25 M – 0.75 M, 70 TON

V_2O_5 catalyst, pressure drop 0.055 atm.

Power Consumption =

$$(0.055)10^5 \frac{N}{M^2} \underset{\uparrow \text{Flow}}{(317\ m^3/s)} \underset{\uparrow \text{blower efficiency}}{/0.7}$$

$$= \frac{1.75\ MW}{0.7} = 2.5\ MW$$

Pressure drop is a significant energy consumer

As take an example here the example is that suppose, we look at sulphur dioxide reaction, sulphur dioxide giving you sulphur trioxides so2 plus half o2 to get so3. The very old process running may be for last 150 years when it is a pent oxide catalyst is well known. I just taken some data from 3000 tonne per day so2 plant the plant itself is in 4 stages I mean after every stage sulphur trioxide produced is taken for absorption and the it is put back.

So, what is called as double contact double absorption process, but our concerned here is something else typically, the beds are about 0.25 to 0.75 meters thick and about70 to 80 tonnes of catalyst what is used, and the pressure drop that is observed as 0.055 atmospheres. This typical pressure drop that we see in the sulphur dioxide plant now, a 3000 tonne per day sulphur dioxide plant because, of nitrogen is coming in along with oxygen and so on. So, the actual flow at the reaction conditions is around 317 cubic meters per second.

So, large flow you have a pressure drop of 0.055 atmosphere I have put it in terms of Newton’s and if we take the efficiency of blower to be about 70 percent about typical, you find that the energy that is required to actually pump this gases into the system require, 2.5 mega watts. The point I am trying to put across to you is that the energy that is required to overcome pressure drop is a very significant part of our cost. And therefore, any work that we can do to take care of this pressure drop is would be extremely valuable. So, is how in a sulphur dioxide plants we are spending about 2.5 mega watts of energy to be able to push the gases through the system, all because of pressure drop.

So, just to sort of emphasize the point that anything we can do to design catalyst might a great advantage from point of view of energy consumption of course, from the point of view of cost as well. That is the point I trying to put across. So, let us just summarize what we are trying to say in the exercise is that, we have looked a design equations for idealized cases, and then we are set that the design equations various choices exist. And these choices, gives you various kinds of reactor design, and these reactor design give you know give you various kinds of performance, and those performances has implications in terms of costs and so on. And I took the example of pressure drop to illustrate, how designs must look for catalyst which is not very high in terms of pressure drop.

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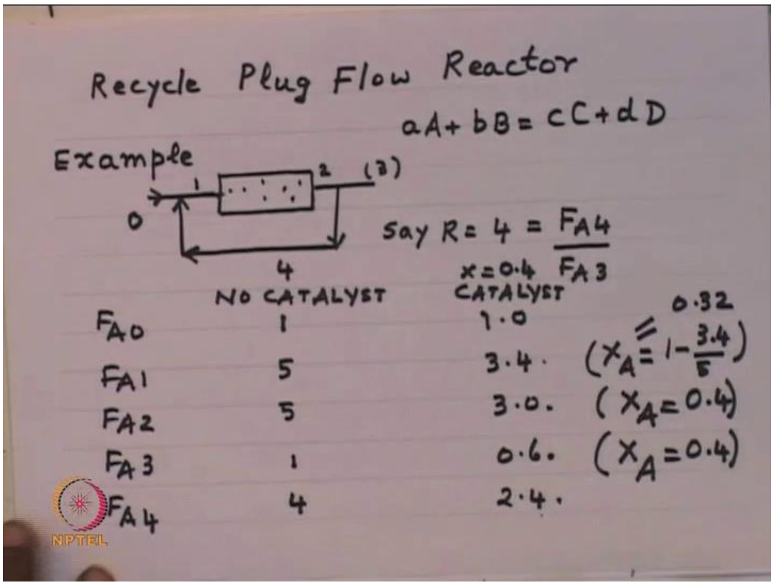

Recycle Plug Flow Reactor

$aA + bB = cC + dD$

Example

Say $R = 4 = \frac{F_{A4}}{F_{A3}}$

	NO CATALYST	$x = 0.4$ CATALYST	
F_{A0}	1	1.0	
F_{A1}	5	3.4.	$(X_A \overset{0.32}{=} 1 - \frac{3.4}{5})$
F_{A2}	5	3.0.	$(X_A = 0.4)$
F_{A3}	1	0.6.	$(X_A = 0.4)$
F_{A4}	4	2.4.	

We will go to the next item now, suppose instead of looking at what is called as plug flow reactor we put a recycle. Let us say, we are considering a reaction aA plus bB going to cC plus dD this is their reaction we are considered. Now, our interest in trying to understand is recycle are meaning, why do we recycle? Generally the recycle that you will find in process industry is mostly because, you want make better use of this of the energy here, because it is hot we want to make use of heat that one reason. Of course, there are some other reasons for looking at recycles that before we do that let us just look at the recycle from a more fundamental point of view.

We want to set up design equation therefore, you want understand how to handle recycle. So, to illustrate this what i have done I just put down suppose there was no catalyst; that means, you have a recycle ratio taken an example here, let say the recycle ratio is 4, how do you define recycle ratio? moles in stream 4 to moles in stream 3 its define that way. Recycle ratio is defined as moles in stream 4 divided by moles in stream 3, there are some people who define this volume volumetric flow in stream 4 divided by volumetric flow in stream 3 instead of moles people might define in terms of volume, but you should careful here because, temperatures at 3, temperature at 4 may be different therefore, those ratios are carefully looked at.

Therefore, I have taken recycle ratio in terms of moles f a moles at 3 to moles at moles at 4 to moles at 3. Now I ask you suppose there is no chemical reaction there is no there is no catalyst here therefore, we are putting a recycle ratio of 4, what are the flow rates of various points? Now, it stands to reason FA0 if it is 1 what is FA3 it has to be 1. Because, you know whatever goes in must come out. Now, what will be FA4? 4 times of this, so I put 4 here, what is FA2 and FA3? I put the numbers.

On other words, what we are trying to say here is; when there is no chemical reaction on other words, when there is no catalyst in the reactor the molar flow rate through the system at position 1 and position 2, position 1 is 5 and position 2 is 5, why is position 2 is5? Because there is no reaction, why is position 1 is 5? There is no reaction. But the important point is that we should bare in mind is that the fluid that entering at position 1 is 5 units, 5 units are entering. Now, let us say what happens to flow rates at all these position when the extend of reaction is about 40 percent of XA is 0.4. If I say that we are entering at 1 mole per hour 1 mole per whatever the number may be per hour per second whatever, is 1 if I say that the conversion is 0.4, if I ask you, what is coming out at position 3? You will say it is 0.6, why? Because 40 percent is conversion.

So, if I say conversion is 40 percent as we said mention here how much is coming out at position 3, clearly it be 0.6 because 40 percent is converted. Now, if I say that is recycle ratio is 4 how much is FA4 you will say it is 2.4, 4 times 0.6, how much is FA2? What will you say? It is FA3 plus FA4 therefore, it must be 3, what is the FA1? What will you say? FA1 is FA0 plus FA4, FA0 is 1 FA4 is 2.4 therefore, FA1 is 3.4. This comes out from our material balance, so on the basis of numbers that I have given you will find that the flow rate at position 1 is 3.4 flow rate at position 3 is 0.6 position 2 is 3.0.

The question that i want to ask you is, what is the conversion? It at position 1 what is the conversion at position 2? How would you answer this question? What is the conversion at position 1? What is the conversion at position 2? A simple answer you would give me is between position 2 and position 3 there is no chemical reactor. Therefore, we should expect that the conversion at position 2 at position 3 must be the same. So, that means, at position 2 conversion should be 0.4 position 3 also conversion should be 0.4. Here, we know that the conversion is here we know the conversion is 0.4 any way based on our physical understanding. We want conversion here also to be 0.4, how can you make conversion here 0.4? By an appropriate choice of our reference.

If we chose high as our reference; that means, if we chose 5 units as our reference on the basis of which will define conversion inside the recycle loop then clearly we find that conversion here at position 2 is 0.4, what I am trying to get across to you is that; whenever you looking at a recycle device, the choice of reference inside the recycle device is important. And that choice should be the moles of component A entering at position 1, in the absence of reaction because, our reference is always on the basis of absence of reaction, how much is going into equipment in the absence of reaction? We know that at position 1 5 units entering in the absence of reaction you can see here, 5 units are entering in the absence of reaction, moment reaction took place the amount of coming here is 3.4.

Therefore, what I want to ask you is that; what is the conversion that is appropriately define in the presence of reaction at position 1? Now, you will tell me that in the absence of reaction 5 units are entering, in the presence of reaction is only 3.4 therefore, conversion at position 1 is 3.4 divided by 5 1 minus. So, conversion here it would be 1 minus 3.4 divided by 5. This would be the conversion, why divided by 5? Because5 is the unit that was entering in the absence of reaction, 3.4 is in the presence of reaction, and 1 minus this is the conversion. So, what is it? 5 3.4 divided by 5. So, this becomes 0.32. So, this becomes 0.32. So, what are we saying?

What we are saying is; when we have a recycle device we need a proper reference to be able to work inside the recycle device. To work inside the recycle device we must have a proper conversion, as we can see in the slide that inside the recycle device if we define conversion on the basis of 5 units, you find conversion at point 1 is 0.32 conversion at point 2 is point 4 conversion at point 3 is also point 4 showing that as we go from point 2 to point 3 the conversion remains consistent with our understanding. So, this is the most important point in the recycle device, we must choose conversion which is consistent across point 2 and point 3. Similarly conversion at point 1 is consistent with respect to, what enters at position 1 in the absence of reaction which in this case is 5 units, but expressed in terms of our variables, what we are saying is that;

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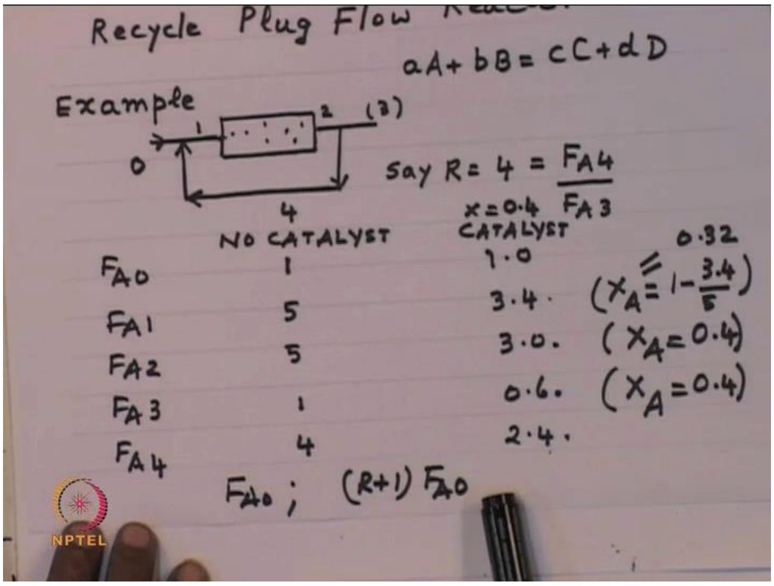

Recycle Plug Flow

$aA + bB = cC + dD$

Say $R = 4 = \frac{F_{A4}}{F_{A3}}$

$x = 0.4$

	NO CATALYST	CATALYST	
F_{A0}	1	1.0	0.32
F_{A1}	5	3.4.	$\left(X_A = 1-\frac{3.4}{5}\right)$
F_{A2}	5	3.0.	$(X_A = 0.4)$
F_{A3}	1	0.6.	$(X_A = 0.4)$
F_{A4}	4	2.4.	

F_{A0} ; $(R+1)F_{A0}$

If FA0 is entering the process, what enters recycle system is R plus 1 FA0, what we are saying is that; what enters the reactor what enters the reactor in the absence of chemical reaction is R plus 1 FA0, when R is 0 then, what is entering is FA0, when R is finite, what enters the reactor in the absence of chemical reaction is R plus 1 FA0. Therefore, inside the recycle loop our reference for defining conversion should be r plus 1 FA0, we take up more of this, when we meet next time.

Thank you.