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Lecture – 18 Reactor analysis II

Welcome, to my lecture course, that is, aspects of biochemical engineering. In the last lecture you may remember that I tried to discuss how to analyze the different type of reactions. So, we have a basic formulation that we have that we shall have to remember before we analyze any kind of reactor that rate of input plus rate of that rate of input plus rate of that generation equal to rate of output plus rate of disappearance plus rate of accumulation.

Now, what I told you that, in case of the steady state condition, the rate of accumulation should be equal to 0. Now, what do you mean by steady state condition? When, the concentration in different portion of the reactor remain unchanged with respect to time. So, that is the steady stand that is only possible when a rate of accumulation is 0. So, this is the equation. So, our equation is the rate of input plus rate of generation equal to rate of output plus rate of disappearance plus rate of accumulation. So, this is the basic equation we have.

Now, when we analyze the reactor I told you we shall have to consider only one parameter; as for example, suppose we are using any kind of microbial system, so, we have 3 different things simultaneously take place. One is substrate degradation another is cell mass formation another is your product formation. So, we can do the analysis with respect to anything with respect to substrate. So, when we do the substrate balance then will be rate of substrate input plus rate of substrate generation equal to rate of substrate output plus rate of substrate disappearance plus rate of accumulation, same thing happened to products same thing happened to your cell mass.

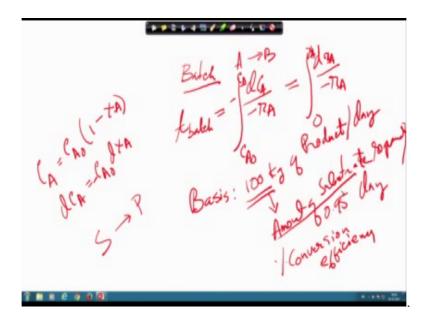
And, but you know if we can do the analysis with respect to energy also rate of energy input plus rate of energy generation equal to rate of energy output plus rate of energy disappearance plus rate of accumulation of the energy. So, this is the basic idea that a basic equation that we use for the analysis of the reactant and I told you that to have whatever reacted we have broadly it can be divided into 2 types; one is batch, another is continuous we use the fed batch reactor while we have the substrate inhibition problem. Now, in the batch reactor that we take the as I told you take the substrate at a time allow it to react after the reaction is over

you take it out, in between you are not putting anything to inside the reactor and you are not taking anything out of the reactor.

But, in the continuous system I told you that initially, particularly, if you look at CSTR first we operate in a batch mode, let the reaction take place. When the rate of reaction is maximum then we start feeding one and do not take the product from other end. So, for whatever flow rate we have the inlet that same flow rate will maintain in the outlet so that volume of the reactor remain constant.

Now, today, I want to discuss some kind of numerical problems so that your conception of the process will be very clear, because what we are interested? We are interested to know a couple of things, we are interested to know what is the percentage conversion take place during this process, also we want to know what is the volume of the particular reactor whenever you go for batch process, whenever you come go for continuous process.

Now, before we go to the PPT slides that let me show you something so that it can help you for understanding the process.



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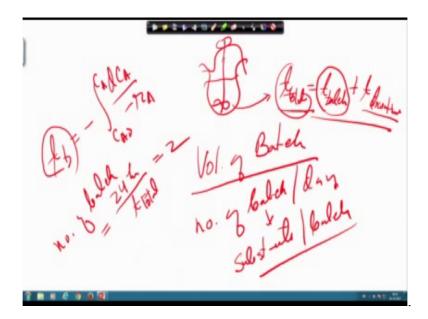
Now, I told you if you when you go talk about the batch process the t batch, I told you, this is equal to what this is equal to that minus dC A suppose the reaction is A to B divided minus R A. So, this is like this. Now, this is C A 0 and this is C A. Now, I told you C A equal to C A 0

into 1 minus X A; X A is the fraction of X that is converted. So, I can write C A d C A equal to C A 0; C A 0 is a constant I can write this is equal to X A.

So, this same equation we can write in the d x A form like this d x A by minus r A and they are 0 to x A, this is what we do. Now, suppose, when you talk about the design of the reactor first we shall have to have the basis and what is the basis, suppose we want a certain amount of product formation, let us assume we want to produce 100 kg of product. Once we want to know the 100 kg of product formation first we shall have to find out from the stoichiometry for producing 100 kg of product, what the substrate required. So, there will be some kind of stoichiometry between the substrate and the product formation. So, with respect to this stoichiometry we can find out amount of substrate required. Now, this might be this is with respect to day, am I right. So, per day you want to producer this also you can you can say per day how much substrate is required.

Now, from the stoichiometry we find out the theoretical amount of substrate required, but, in practice you might be requiring a little bit more. So, you have to divide by the percentage conversion efficiency. So, suppose percentage conversion efficiency is 95 percent. So, we divide by 0.95. So, this is how we can, but you know question come how you find the volume of the batch reactor.

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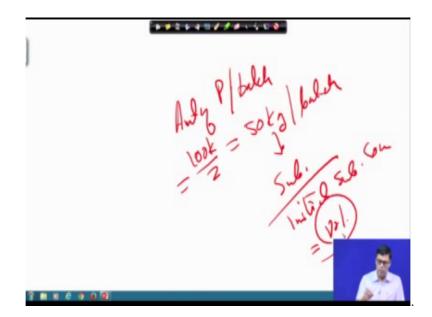


So, what we shall have to do, we know that the main bottleneck of the batch process is the downtime, because, suppose this is a batch and after the operation is over you have to take

the product out, again clean the vessel and then you have to refill the vessel. So, that requires some time. So, t total equal to t batch plus t down time. So, you know that, if we know. So, what I want to tell you that when you find out the volume of the batch reactor we shall have to first calculate how much batch we can operate per day? The number of batch per day, then from that we shall have to find out that how much substrate then we shall have to find out how much substrate is required per batch and then we can find out the volume of the reactor. So, when you want to find out t total what do you have to first you have to calculate t batch and I showed you the t batch is what t batch is equal to minus dC A by minus r A.

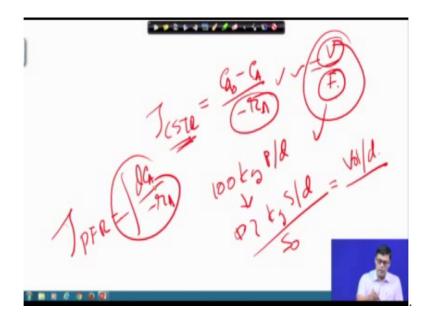
So, from that C A 0 to C A you can easily find out that you know what is this batch time required and you assume some down time and then you find t total. Now, number of batch how you can calculate? This is equal to suppose, per day you have given 24 hours, so, number of batch is the t total. Suppose, this is 2 and in the basis we have taken the 100 kg of product per day from that you can find out how much substrate is required per day.

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And, from that since we have 2 batches, so, amount of product per batch will be what? Per batch equal to 50 kg, am I right? 100 kg divided by 2, number of batches 2 if we assume this for per batch. So, from that you can find out how much substrate is required and if you know the substrate required then you divide by initial substrate concentration, you will get the volume. So, this is how you can find out the volume of the batch process.

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Now, if you look at the volume of the continuous process like tau CSTR is equal to what? is equal to C A 0 minus C A by minus R A. So, R A you can easily find out from rate of reaction, you know from the percentage conversion you can find out what is the C A 0 and C A value from that you can find out this is equal to what, V by F. So, F, you can find out from the amount of suppose we want to produce 100 kg of product per day. So, from that you can find out how much kg of substrate you required per day. So, if you know initial substrate concentration is 0, so, you can find out this is flow rate volume per unit per time.

So, you can put this value, you can put this tau CSTR, you calculate tau CSTR value you can find out the volume of the same thing happens, same thing applicable for tau Plug Flow Reactor; tau Plug Flow Reactor is what, this is same as batch process diviner the d C A by minus r A. So, if you know this and same correlation is whole good. You find out the F in the same way, you can find out the volume of the reactor.

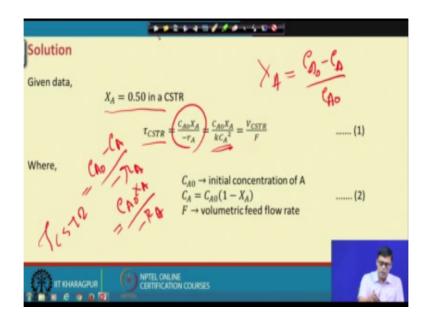
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Problem
A homogeneous liquid phase reaction
$A \rightarrow B$ $-r_A = k C_A^2$
Takes place with 50 % conversion in a CSTR.
(a) What will be the conversion if this reactor is replaced by a CSTR 6 times as
larger – all else remaining unchanged ?
(b) What will be the conversion if the original reactor is replaced by a PFR of equal
size – all else remaining unchanged ?
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So, now, let me take the first problem. The first problem deals with a homogeneous liquid phase reaction A to B and this is a second order reaction minus r A equal to k into C A to the power 2, take place with the 50 percent conversion in a CSTR. What will be the conversion if the reactor is replaced by 6 time as larger all else remains unchanged and what is the second part? Second part is that, what will be the conversion if the original reactor is replaced by the plug flow reactor and all else remains constant.

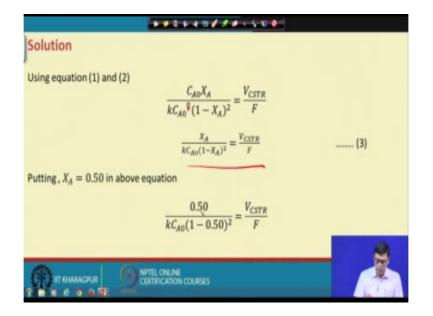
So, you have 2 different approaches is there. One, first case what we want to do, you want to increase the volume of the reactor of the CSTR 6 times and second case we want to replace the CSTR by plug flow reactor; 2 different approach, we want to find out how the conversion efficiency changes let us work on that.

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So, first, we have in this problem if you look at it is given here, what is given 50 percent conversion of substrate, am I right? A 50 percent conversion of substrate means X A is 0.5, what is the X A? X A I told you previously several times if this C A 0 minus C A by C A 0 this is X A. So, what is the equation that we have tau CSTR equal to, I told you tau CSTR equal to C A 0 minus C A by r A. Now, this is equal to C A 0 into X A by r A. So, this is how it has come and then this is the rate of reaction there k into C A squared and this should be equal to V by F, what I told you previously.

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Now, then we can analyze. We can analyze the reactor like this C A 0 into X in the k into C A 0, 1 minus X that you know that whole squared we can find out this is equal to this and finally, we can come this expression because C A 0, 1 C A 0 will cancel. So, one C A 0 will remain here. Now, put the value here you can 0.5 and 0.5, 50 percent conversion.

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Solution	
$\frac{2}{kC_{A0}} = \frac{V_{CSTR}}{F} \qquad (4)$	
(a) now, the CSTR is replaced by a 6 times larger CSTR	
From the equation (3) $V'_{CSTR} = 6V_{CSTR}$	
$\frac{X_A}{kC_{A0}(1-X_A)^2} = \frac{V'_{CSTR}}{F} = \frac{6V_{CSTR}}{F}$	
Putting $\frac{2}{kC_{A0}} = \frac{V_{CSTR}}{F}$ in the above equation	
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Then, we have here this equation we have 2 by k C A 0 V by F. Now, in this problem what is the first part, we want to increase the volume of the reactor 6 times am I right. So, C A, you are now new volume will be 6 into V CSTR; V CSTR was the previous volume is 6 time we want to increase. Let us assume the conversion efficiency at that time is the X A and this is like this is the question same equation we what we have written previously that we can write here.

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Solution
$\frac{X_A}{kC_{A0}(1-X_A)^2} = \frac{V_{CSTR}}{F} = 6 \times \frac{2}{kC_{A0}}$
Rearranging
$12X_A^2 - 25X_A + 12 = 0$
By solving
$X_A = 0.75, 1.33$
Here $X_A \neq 1.33$ as $X_A \gg 1$
Therefore, $X_A = 0.75$
∴ conversion will be 75 % if the reactor is replaced by 6 times as larger CSTR.
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Then, this equation we can write the expression like this is equal to 6 because V CSTR by this we have already written. This is equal to 6 into 2 by k I can show you, this is what we have written now. So, this is what.

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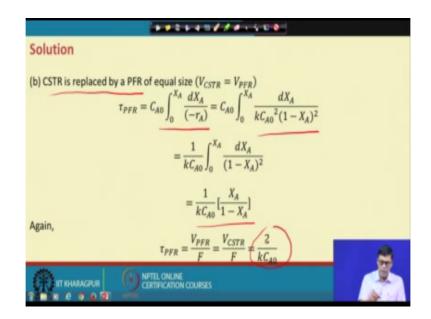
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Putting $\frac{2}{kC_{A0}} = \frac{V_{CSTR}}{F}$ in the above equation	-
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So, this is we had we have calculated previously this is the new approaches that we have this is equal to this. Now this equal to what, this equal to 2 by k C A 0. So, this we can do it here.

So, this is how it has come. So, we can shop this quadratic equation we find 2 values one is 0.75 and 1.33. Now, more than conversion, if it is the more than 100 percent is not possible,

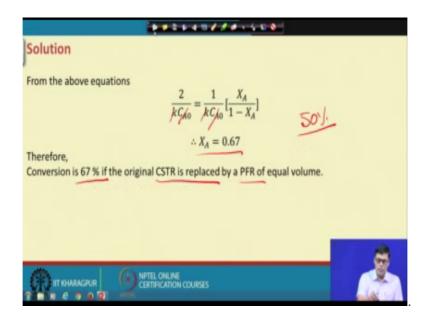
so, we take 75 percent. So, X A is the 75 percent when we replace by the. So, previously the conversion was 50 percent and when you increase the volume of 6 times then conversion will be 75 percent. So, this is how we can solve this equation.

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Next part is very interesting that, if you what are you saying that if a CSTR is replaced by the plug flow reactor. Now, what is the expression for plug flow reactor is this one. So, we can solve this equation like this because we know this is the k into C A 0 square 1 minus X A whole square. So, this will come here and then we can this is equal to V by f and this is equal to that in case of CSTR it is like this. We told that everything is remain constant. So, we can equal to like this if everything is constant how it what will be the conversion in the plug flow reactor.

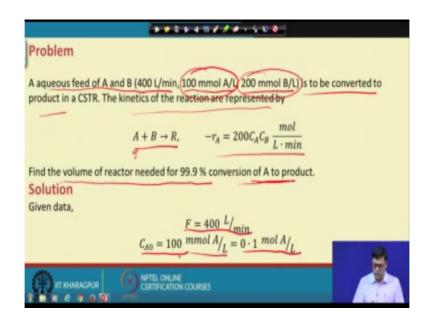
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Now, if we equilibrate this then we find this 2 by k into C A 0, 1 by k into C A 0, X A 1 minus X A equal to then we can solve this equation this will cancel, this will cancel then only one equation one unknown we can easily solve the X A value.

So, we find the 67 percent will be the conversion if we CSTR replaced by the plug flow reactor. So, initially that in case of CSTR is 50 percent conversion, now if you replace the same thing by the plug flow reactor, it is increased to 67 percent. So, you give this some kind of impression that, how what happens if the CSTR is replaced by the 6 times CSTR, the volume of the reactor is replaced by increase by 6 time, how the conversion efficiency changes. And, second case we try to find out if the CSTR is replaced by the plug flow reactor, how the conversion efficiency changes.

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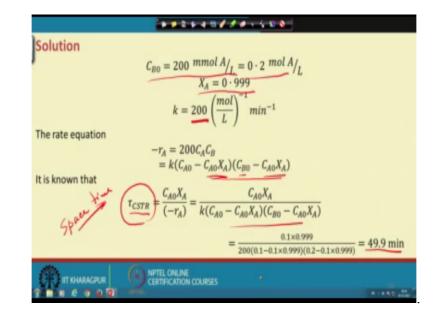


Now, next problem also very important let us work with the next problem. This is like this is you see the aqueous feed A and B, this is a feed flow rate is given 400 liter per minute and what is the A concentration, 100 millimoles A per liter and what is the B concentration 200 millimoles B per liter and to be converted in the CSTR. So, here I want to tell you one thing that when your reaction is A plus B equal to R; that means, that indicate 1 mole of A react with 1 mole of B to give the 1 mole of R.

So, this is the stoichiometry is like this. So, here in this particular case, your concentration of A is less as compared to concentration of B. So, limiting factor is the A that we should remember. So, the kinetics of the represented by this equation, so, find the volume needed for 99.9 percent conversion of A. Since this is the limiting factor, this problem is there to convert ninety 99.9 percent of A, what should be the volume of the brief. Previous problem was that what is the percentage conversion efficiency, now in this problem we have given that if we know the percentage conversion efficiency, what will be the volume of reactor, let us see how we can solved it.

Now, first, let us say whenever we solve any kind of equation I request all of you that please write down all the data that whatever given data is given you write down one after another. Here, in this problem you see that flow rate is 400 liters per minute this is the flow rate, volumetric flow rate and what is the C A 0 concentration 100 millimoles of A, this I can

easily convert it in moles of A per liter because this is millimoles if you divided by 1000 then it will be 0.1 moles of A per liter.

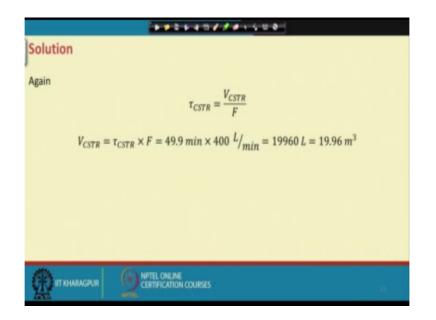


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Now, second case is that if you C B similarly, you can calculate and find out 0.2 moles of A per liter. So, we try to convert this millimoles to moles at the then X A the conversion efficiency is 99.9 percent. So, X A value will be 0.999 and here k value in this equation is already given 200 moles per liter inverse and minute inverse. Now, if you put these values here that here with this equation we have 200 in C A minus this and this is the conversion of A take place.

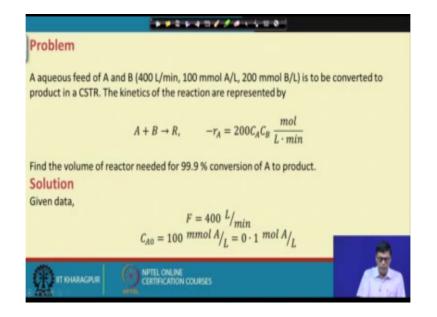
So, this is to be deducted with C B because this is the equal molecular reaction and then we can find out the tau CSTR. Tau CSTR is the space time of CSTR, I told you space time. Space time means that you know the time you are allowing the particular volume of the reactor, volume of the liquid to reside in the reactor. So, what is the space time you are you giving? Though this is equal to C A 0 into X A and this is the rate equation I can put it here and then we put the data, all the data you can find out tau CSTR. This is coming about 49.9 minutes. So, this is how we can calculate the time required for CSTR.

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Now, once you know that tau CSTR, now our equation, what is our equation? Our equation is tau CSTR equal to V CSTR by F. So, if we already know if V is 400 liter per minute and time we have now. Sometime let me, tell you sometimes some when you when you give this unit, you should be very careful, what is the flow rate of this unit. Sometimes if it is in per day or per hour and your tau CSTR is in minute. So, you have to convert into per minutes and then you multiply this you will get the volume of the reactor. Now, I repeat the problem, but for a CSTR.

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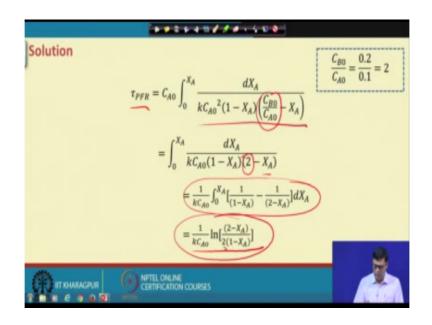
So, let us say that this is conversion that this is with respect to CSTR, now we want to show the similar type of things that we have when we can go for plug flow reactor when previously we are talking about the CSTR.

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P	roblem
Re	epeat the previous problem but for a PFR. $1_{DTR} = -1_{RD}$
S	olution (ADU-TA)
Tł	olution he rate equation $-r_{A} = 200C_{A}C_{B}$ $C_{A} = C_{A}LA$
It	is known that $\begin{cases} k(C_{A0} - C_{A0}X_A)(C_{B0} - C_{A0}X_A) \\ \int X_A C_{A0} dX_A & \int X_A \\ \int X_A C_{A0} X_A & \int X_A \\ \int X_A \\ \int X_A C_{A0} X_A & \int X_A \\ \int $
	$\tau_{PFR} = \int_{0}^{X_{A}} \frac{C_{A0} dX_{A}}{(-r_{A})} \neq C_{A0} \int_{0}^{X_{A}} \frac{dX_{A}}{k(C_{A0} - C_{A0}X_{A})(C_{B0} - C_{A0}X_{A})}$
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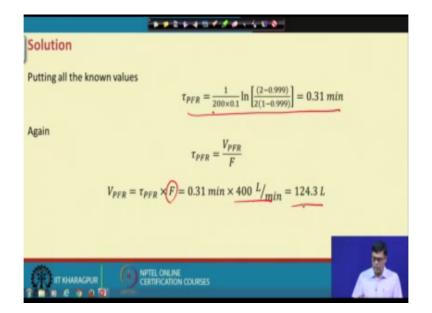
Now, in the plug flow reactor your rate constant will be the same. The rate of reaction is same that we can express like this. Only your expression is like this, I told you this is tau plug flow reactor is equal to minus d C A by minus R A. So, this R A is same that d C A I told you what is C A? C A equal to C A 0 into 1 minus X A. Now, if you do d C A is equal to minus C A 0 into d X A, this is exactly. So, here there is minus sign, so, this will be removed this will be plus minus will be plus this is minus r and minus r value I can take it from here and put it in this equation like this.

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So, next we can we can find out here that tau plug flow reactor equal to C A integration 0 to X A you know d X A and this is the equation that we can write only we can take the common of C A 0. So, that this ratio will come C B 0 by C A 0 and this ratio at the initial stage is 2, we know that one is 200 millimoles another is 100 millimoles and X A is the percentage called that you know fraction converted, then this equation if we solve it will come in this form. So, it is you can see it this is if you have then if you do the percent differentiation of this you will get this particular expression this is 1 by k C A 0 ln 2 X A by 2 into 1 minus X A.

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Then, we if we put that then values here, now if you look at previous equation that we have a tau CSTR that the k into k value is known and C A 0 is known. So, this value if you put all these values we put it here, then we will get the tau plug flow reactor. The tau plug flow reactor we can easily calculate. This is coming about 0.31 minutes. So, I can just show you previously, that when you in case of CSTR, we calculated it is coming quite high 49.9. Now, it is coming quite less actually. So, volume also is coming quite less this is when you calculate this with the flow rate, the flow rate is basically same in the continuous system then we can find.

So, we find that volume of the plug flow reactor is much less as compared to that of the CSTR. So, in this particular presentation what I try to point out, I try to point out 2 important aspects, that how to analyze the batch as well as the continuous reactor and how to calculate the conversion efficiency of the continuous process. Only one thing I can highlight that in case of CSTR, there is we have continuous stirred tank reactor. So, it is main purpose of the excitation to make the homogeneity in the reaction mixture, but in the plug flow reactor, the liquid flow from one into others and when it flow one form there is no axial mixing there might be radiant mixing. So, that is the if you have that pattern your expression is change and with that we find out that percentage conversion for the same type of reaction is different when you go for CSTR as well as plug flow reactor.

And, only the batch reactor problem I did not solve in this particular lecture, that I am going to solve in the coming lectures, that I just show you how you can find out the volume of the reactor. Now, volume that when you calculate the volume of the reactor I want to emphasize that first you have to find out that how much product is to be produced per batch and how we can find out because here from the first you have we shall have to calculate, what is the total time required for the batch process. Now, total time of a batch process is nothing, but batch time plus your downtime. Downtime is nothing, but idle time and this comprises of time required to take out the liquid from the reactor and cleaning the vessels, refilling the vessels, because this is called downtime and other way we can call it also idle time. Why idle time, because during this time we assume no reaction take place.

So, this time is to be added with the total time and when you get the total time. So, if we suppose we have a basis that we want to produce 100 kg of product per day, so, 1 day comprises of 24 hours. Now, if your total time is 12 hours, the number of batch per day will be 24 by 12 that is 2 batches. So, per batch you have to produce 100 by 2 that is 50 kg of

product per day. So, if you know the how much product you have to produce per batch then from that you can find out how much substrate is required per batch. How you can find out? You can find out from the stoichiometry of the reaction.

Also, now stoichiometry of the reaction will give you the theoretical requirement, but in practice the 100 percent conversion is not taking place. So, we can we can assume some conversion efficiency of the process and from that we can find out that what is the exact amount of substrate required per day. Now, when you find out their exact amount of substrate equal per day then if you divide by initial substrate concentration then you will get the volume of the reactor.

Thank you very much.