# Aspects of Biochemical Engineering Prof. Debabrata Das Department of Biotechnology Indian Institute of Technology, Kharagpur

# Lecture – 19 Reactor analysis III

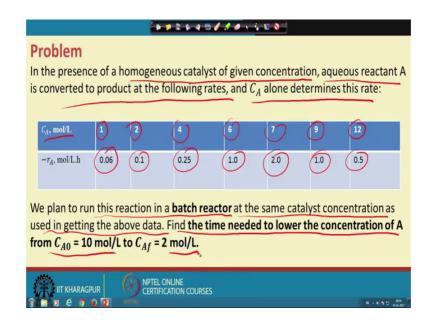
Welcome back to my course Aspects of Biochemical Engineering. In the last couple of lecture I try to concentrate on the Reactor Analysis. And this also this coming 2 lectures the todays this lecture and coming lecture also wild I will talk on mode on the reactor analysis, because I consider that this is very important to of the important for the reactor analysis, because I initially I pointed out you can remember that 1 of the major objective of this particular course to develop the expertise that to get a desired amount of product what should be the volume of the reactor.

So, until unless you do the reactor analysis properly you cannot find out the; what will be the volume required for getting a desired amount of product. Now in the last lecture you can remember that I tried to explain this continuous stirred tank reactor and the plug flow reactor in details and try to find out that, how you can calculate the conversion efficiency of the in the CSTR as well as in the plug flow reactor and also how you can find out the volume of the plug flow reactor that and continuous starting reacted now.

This particular lecture I try to concentrated on 2 different aspects 1 is the batch process that how you can find analyze the batch process, and second also I want to try to analyze the reversible reaction in the in the batch process that how we can analyze the reversible reaction.

So, these are the couple of things I want to take care in this lecture.

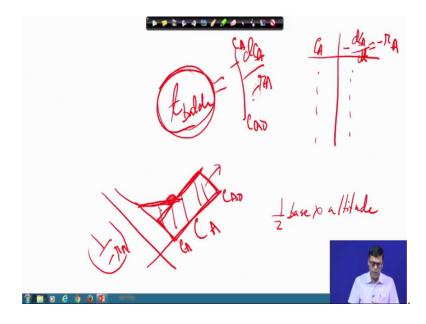
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Now, if you look at the first problem that we have that the; this problem says that in the in the homogeny homogenous catalyst of A of given concentration aqueous reactant a is converted to product at the following rates and C A is alone determine this rate. So, you know that what I want to know add at different C A value that you say 1, 2, 4, 6, 7, 9 and 12.

What is the rate; rate of the reactions this in a particular CSTR that in a batch process that they find out that what is the different rates, we plan to run the reaction in a batch reactor at the same catalyst concentration used in getting the above data find the time needed to lower the concentration of a from C A 0 10 moles per liter to 2 moles per liter.

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So, this is the; this problem if you look at this problem. So, we know t batch minus dcA this will be minus r A am I right minus r A. So, this is C A 0 to C A. So, in this problem what is happening the there they have given different value of C A and at the same time they also giving different value of the rate equation that that is giving there. So, from that we shall have to find out time of the batch process now how you can do that that that we can do it very easily that this is equal to minus r A.

So, if you plot 1 by minus r A versus C A. So, you will get some plot like this or this way or that way whatever is there. Now if you know the C A 0 value here and if you know how much of the C A C A should be converted, then area under this curve you can find out the volume of the time required for the batch process this you can easily find out now. Now how you can find how can calculate the area that is very important. So, what I can do I can make a straight line here. So, if you look at this this is what this is a rectangle and what is the area of rectangle is length versus breadth am I right this is length this is breadth. So, if you multiplies that you will get the area.

Now, you here you can you can put a straight line here. So, if you straight line they will find the triangles what is the area of a triangle half base into altitude. So, you can do this and this sum motion will be remaining that you can find out what the different-different squares 1 squared, if you know that what is the value of 1 square if you calculate the

number of square from that we can find out that total time required for there and then that gives you the idea of the time required for a batch process.

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Solution
Given data,
$C_{A0} = 10 \text{ mol/L}$ $C_{Af} = 2 \text{ mol/L}.$
We know that, $t_{batch} = -\int_{C_{A0}}^{C_{Af}} \frac{dC_A}{(-r_A)}$
The integration can be evaluated by graphical method or by numerical method. (area
under the curve of $C_A$ vs $\frac{1}{-r_A}$ between $C_{A0}$ and $C_{Af}$ )
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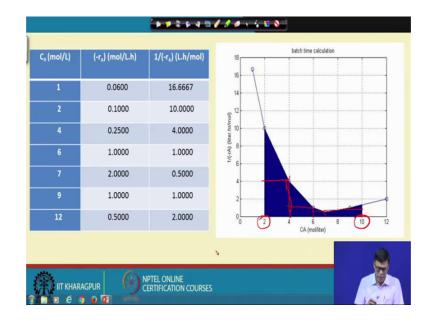
So, in this problem that to what is given in this problem what is given C A 0 is say 10 moles per liter and C A f is 2 moles per liter am I right and the batch as I showed you the batch time that is we calculated like this d C A by minus r A and C A 0 to C A f that we have. Now the integration can be evaluated by the graphical method or by numerical methods area under the curve is C A versus 1 by 1 by minus r A between C S 0 to C A f let us see how we have done that.

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			<b>* * * * * *</b>			
	C <sub>A</sub> (mol/L)	(-r <sub>a</sub> ) (mol/L.h)	1/(-r <sub>A</sub> ) (L.h/mol)	dea dea		
ľ	1	0.0600	16.6667	175 -14		
İ	2	0.1000	10.0000	12		
Ì	4	0.2500	4.0000			
Ì	6	1.0000	1.0000	-THA CA		
İ	7	2.0000	0.5000	~11		
İ	9	1.0000	1.0000			
Ī	12	0.5000	2.0000			
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So, this is a we have calculated in this problem we have the values of C A values given array value is given, but we shall have to convert it to 1 minus r A, because that that will reverse because your plot is what plot is minus r A by C A you know why because t batch is equal to minus d C A by minus r A; am I right.

So, this is this is 1 by r A and this is C A. So, you can you can until analysis 1 by r A you cannot draw this graph.



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Now, if we plot 1 by minus r A this is you can see minus r A is there and this is C A. So, we have we have this kind of plots.

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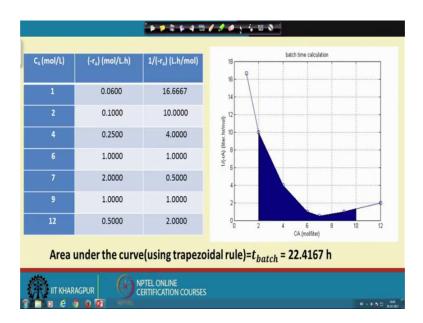
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Solution
Given data,
$C_{A0} = 10 \text{ mol/L}$
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We know that, $t_{batch} = -\int_{C_{A0}}^{C_{Af}} \frac{dC_A}{(-r_A)}$
The integration can be evaluated by graphical method or by numerical method.(area
under the curve of $C_A$ vs $\frac{1}{-r_A}$ between $C_{A0}$ and $C_{Af}$ )
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So, we have we so in this problem, If we look at the problem is that we shall have to reduce the 10 moles per liter to 2 moles per liter am I right. So, in this in this problem that. So, this is the. So, this is 10 moles per liter and this is 2 moles per liter.

So, this is the crop that we have and area under this curve you have to calculate. Now question comes how you can how you can do that, you can do this very very easily that is if you con you can considered this as the triangle, then you can consider from here to here you can consider the rectangle, then here you can consider the again triangle, again you can be rectangle like this you can do that and here you can do the you can do that.

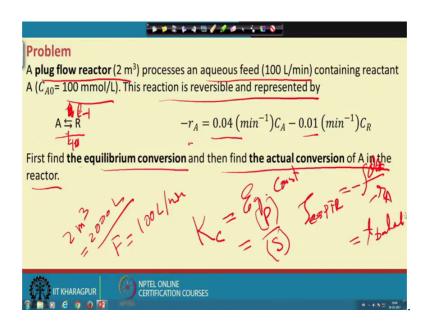
So, you can calculate the area under this curve maybe 1 2 3 4 5 6 and then you find out the t t batch what is the time that you required in the batch process.

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So, which is coming it will come around the 22.416 hours that from the graph we can find out these particular results.

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Now, let me go to the second may be interesting problem that is the; what you call reversible reaction and in the reversible reaction we know that, we have we have forward reaction in the backward reaction in the big BPSC reaction you assume this is irreversible. And this is the reversible reaction we have and in this in this reversible

reaction 2 things is very important 1 is equilibrium condition another normal condition normal operating condition.

And I told you here I want to highlight again that at equilibrium conditions that you have the equilibrium constant we call it equilibrium constant and equilibrium constant equal to what concentration of product by concentration of substrate am I right. Now this is the concentration of product this is the concentration of substrate. Now I told you that when you work with any kind of reversible process to increase the product concentration either you have to take the product out. So, there mode substitute convert to products or you have to at more substitute you can get the product.

So, let us see then how can and is this system now this is this is the plug flow reactor a plug flow reactor of capacity 2 cubic meter 2 cubic meter means what to give me remains 2000 liters am I right. Process I know the aqueous flow rate is what is the flow rate is there F is equal to 100 liter per minutes containing the reactant C A 0 value is given this is this is equal to 0.1 mole per liter this reaction is reversible and represented by this and the equation is minus r A is equal to 0.04 into C A. So, I want to into write it here this is this is suppose the k 1 and this is k minus 1 sorry the sign is given in different way.

So, let us assume this is k 1 and this is k backward is k minus 1 the k 1 is 0.0 4 and k minus 1 is 0.0 1 this I want to highlight this is say this is how you can you know the first find the equilibrium conversion and then find the actual conversation of a in the reactor. So, 2 things we shall have to find out in this particular problem.

What is the equilibrium condition; that means, under equilibrium condition what is the percentage of substrate that is converted and what is the actual substrate converted in this reacted. So, both the part both the portion that we shall have to solve in this particular program and by where the reactor that we are considering the plug flow reactor and we know the plug flow reactor expression and the batch reactor expression is same, because same integration that tau CSTR sorry tau plug flow reactor is what minus d C A by minus r A am I right and also this is equal to same as t batch so this same similar type of expression that we have.

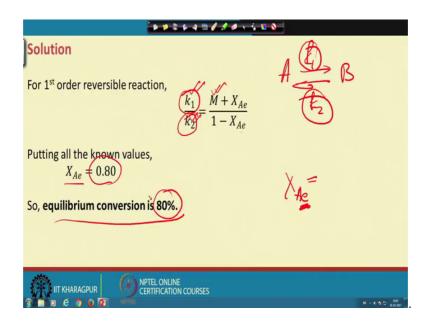
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Solution	
Given data,	
$k_1 = 0.04  min^{-1}$	
$k_2 = 0.01 \ min^{-1}$	
$C_{A0} = 100 \ \frac{mmol}{L} = 0.1 \ \frac{mol}{L}$	
$C_{B0} = 0$	
$E = 100 - \frac{L}{L}$	
$F = 100 \frac{L}{min}$ $V_{PFR} = 2 m^3 = 2000 L$	
$V_{PFR} = 2 m^3 = 2000 L$	
Thus, $M = \frac{c_{B0}}{c_{A0}} = 0$	
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Now, as I pointed out before that let me tell you again that when you solve any kind of problem first please write down the; what are the things that is given in the problem.

So, k 1 value we can rate equation we can find out k 1 equal to points 0 4 minute inverse and k 2 is 0.0 1 minute inverse C A 0 you can easily calculate find out how much is the mole per liter C B 0 is 0 C B 0; means at the 0 hour the product concentration is 0 and flow rate is 100 liter per minute and plug flow volume of plug flow reactor is 2 cubic meter; that means, about 2000 liter. Now m if the ratio C B 0 by C A that is equal to 0 because at the at the initial point at 0 hour this product concentration is 0. So, m should be equal to 0. So, this is the input of the problem that we have and from that we can find out that, what is the equilibrium conversion that we have been this particular process.

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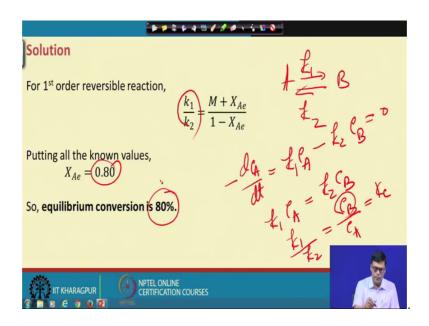


Now, if you go back to our expression that when we discuss the reaction kinetics then we discuss the reversible reaction in details and there we can find out that k 1 k 1 what is k 1 k 1 is the rate constant of the followed reaction, because if we write like this this is k 1 and this is k 2 this is k 2 for the backward reaction k 1 for the forward reaction.

Now, if you take the ratio k 1 by k 2 this is equal to m plus X A e what is the A e X A e is the fraction of a that is converted under equilibrium conditions that is that is called X e stands for equilibrium conditions and 1 minus A X into A e this this expression we have seen, we during this analysis of reversible reaction we have shown this expression please refer the refer this and then in this problem we know the value of k 1, we know the value of k 2 this M value is 0.

So, we can easily calculate the value of X A e and this is coming about 0.8; that means, equilibrium conversion of this process is eighty percent equilibrium conversion.

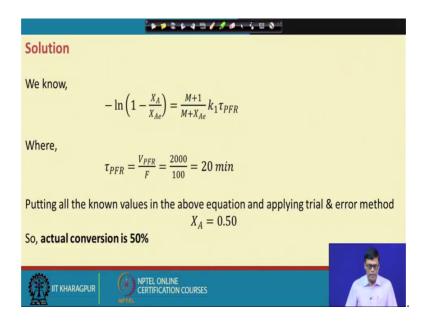
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Because again I am telling you that what do we mean by equilibrium conversion here suppose A B k 1 and k 2. So, if you if you look at minus d C A by dt this will be equal to k 1 into C A.

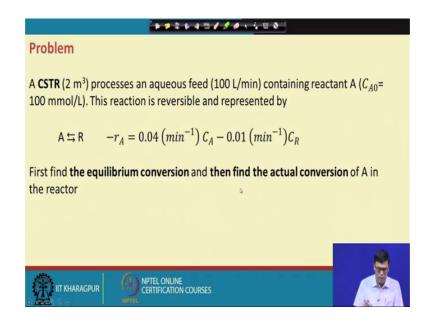
If you consider first order kinetics k 2 in to C B. Now under equilibrium condition this should be equal to 0. So, I can write k 1 into C A equal to k 2 into C B I can easily write. So, k 1 by k 2 equal to C B by C A this is equal to constant equilibrium constant now I write. This is what is written there C B equal to this and C A if we if we if we consider then then we can we can write this 1. So, you can put the equilibrium condition here then we can put this then we can calculate the value of X A e and that is the about 80 percent

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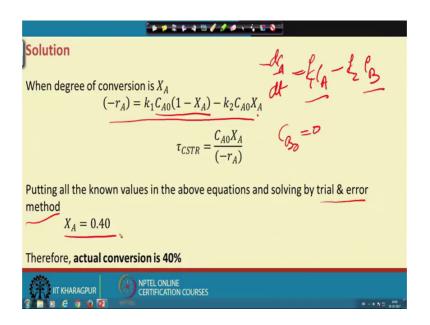
Now, next is that next problem is that let me go through that what I what I told you that in the next problem we shall have to find out the actual conversion of a in the reactor that you have to find out.

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Now, let us see how you can do that.

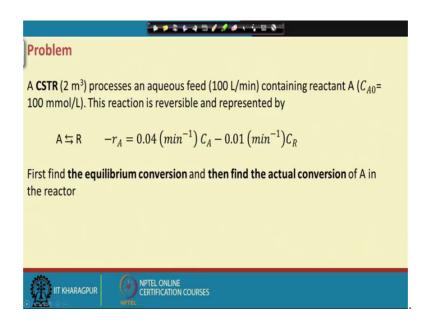
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Now this is the rate equation that we have because for the I have already done that this is equal to I what I showed you minus d C A by dt equal to k into C A minus k 1 into C A k 2 into C B I am right.

The k 1 equal to what k 1 equal to C A 0 into 1 minus X A and C B equal to C A 0 into a A X A because we considered C B 0 equal to 0. So, if you consider that is like this. So, now, tau CSTR equal to C A 0 into X A minus r X A. Now putting all the loan values in the above equation and solving the trial and error method that we can find out the value of X A. Now that you know that in this problem.

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In this problem that we shall have to we have here you can see that we have this is the CSTR volume and this is the flow rate aqueous flow rate.

So, from that we can easily find out the volume of the that you know tau CSTR that we can we can calculate the tau CSTR then if you know the tau CSTR and X A is X A 0 evolve know the v this the X A value you assume trial and error method and find out under what circumstances, the left hand side is equal to right inside and if you do that you will find that when X A equal to 0.4 then left hand side will be equal to right hand side and since it is 0.4; that means, the actual conversion is the about 40 percent that check take place .

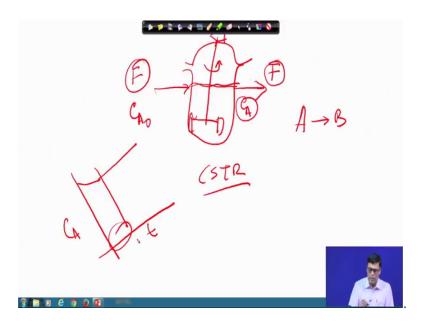
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Problem				
The aqueous deco	mposition of	A is studied in an expen	rimental mixed flow	reactor
(CSTR). The results in Table are obtained in steady-state runs. To obtain 75 %				
conversion of reactant in a feed, $C_{A0} = 0.8 \text{ mol/L}$ , what holding time is needed in a plug				
flow reactor?		ion of A, mol/liter		
	In Feed	In Exit Stream	Holding Time, sec	
0.6 mile	2.00	0.65	300	
N. Y.	1/2.00	0.92	240	
N Pri	2.00	1.00	250	
(AD O' ? ?	1.00	0.56	110	
4 0/-	1.00	0.37	360	
(x " )	0.48	0.42	24	
Lak .	0.48	0.28	200	
1262	0.48	0.20	560	
		NU NIE		

Now, let me go for the third problem that we have this is the aqueous the aqueous decomposition of a is studied in A experimental mixed flow reactor me, now here I want to want to tell you 1 thing that CSTR can be can be we can express in different way we can though it is say is the CSTR may continuous stirred tank reactors something we call it mixed flow reactor. Also when is used in the biological system we call it chemostat. So, basically all us CSTR continuous stirred rank reactor. So, different name we put for the CSTR because 1 is mixed flow reactor or chemostat when we use in the biological process and in the chemical process mostly we used either CSTR organics flow reactor.

So, this is the mixed flow reactor and we mentioned that is the CSTR the results in table are obtained in the steady state run and steady state run means here let me show you 1 thing that suppose this is CSTR.

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Now there is a flow with this is a inflow that this is a outflow and I told you this flow rate should be same.

Now, why should be same because if F is differed either volume will increase or decrease in the reactor. So, F should be same because we want to maintain the same volume in the liquid volume in the reactor liquid volume is the working volume liquid volume is considered as the working volume of the reactor, because we assumed the reaction take place only in the liquid phase and what I told suppose you want to carry out a reaction a to b and they want to carry out in this reaction.

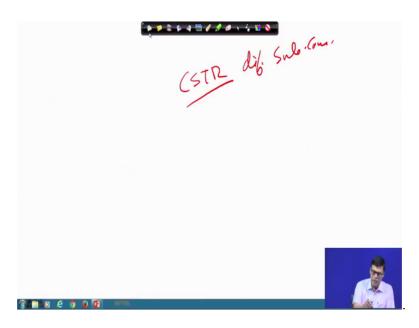
So, what we shall have to do we shall have to first you have to run this process in the batch mode let the reaction take place when is maximum then you fluid the flow rate. Now as soon as you give the flow rate that here you have C A 0 am I right and this is here we have C A. Now if you look at that concentration that with respect to time and that concentration of C A it maybe little bit change with respect to time this is outgoing C A concentration will be changed a time will come it is constant and when it will be constant then we call is steady state condition.

So, in this problem they are talking about and this requires sometime this is the time required for to attend the steady state conditions.

So, this is the exactly what it is mentioned here that the runs of the table are obtained in steady state run to obtain that 75 percent conversion of the reactant in the feed steam 0.8 moles are what holding time is required in a plug flow reactor.

So, that is the that is the 75 percent of this means that is C A 0 suppose it is 0.8 mole per liter then if you considered the 75 percent how much will be remaining that is 1 forth am I right. So, C A will be there will be 0.8 into 1 by 4 that is 0.2 mole per liter this is mole per liter am I right. So, you have to find out that that will to obtain 75 percent conversion of the reactant what holding time is required in the so you have we shall have to find out tau plug flow reactor tau plug flow reactor we shall have to find out in the.

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So, in this problem what is given in this problem that in this problem we operate CSTR at different substrate concentration different substrate concentrate and different you see that a in this problem that in the feed stream you have this in the existing is this. So, this is the this is this is given there in the feed stream and existing is like this and holding time is like this.

Now, now 1 thing I want to point out in the as per as per this CSTR is concerned.

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Problem				
The aqueous dec	omposition of	A is studied in an exper	rimental mixed flow re	actor
(CSTR). The result	ts in Table are	obtained in steady-stat	e runs. To obtain 75 %	
		d, C <sub>A0</sub> = 0.8 mol/L, what		
flow reactor?	Concentration of A, mol/liter		Holding Time,	Holding Time
	In Feed	In Exit Stream	sec	
LX,	2.00	0.65	300	
PNIN	2.00	0.92	240	
	2.00	1.00	250	
	1.00	0.56	110	
$\lambda$	1.00	0.27	260	
sc (o pa)	1.00 0.48	<u>0.37</u> 0.42	360 24	
	0.48	0.28	200	
C	0.48	0.20	560	

That in the CSTR when you calculate tau CSTR equal to C A 0 minus C A by minus r A am I right. So, you can the feed stream is there and this is there. So, if time is required. So, you can find out already you can find out the minus r A value, you can find out at different substrate concentration you can calculate the minus r A value this is and what is the substrate to concentration you have to assume you have to assume this because I told you under steady state conditions after a concentration it remain the unchanged.

So, this is the which at different substrate concentration what is the r A value is given. Now once you have that so C A 0 value is this 75 percent conversion so what I told you that C A should be about 0.2 mole per liter am I right.

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Solution
Given data Given data Here, holding time = space time = $\tau$ For the data given $\tau_{CSTR} = \frac{C_{A0} - C_A}{(-r_A)}$ $(-r_A) = \frac{C_{A0} - C_A}{\tau_{CSTR}}$
Now from the given data we can obtain following table
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And CSTR is like this. So, this is the things that we have this already we have we know this this is minus r A for this CSTR we know that.

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·	C <sub>A</sub> (mol/L)	$1/(-r_A)$ (L.s/mol)	a (2Ca
	0.65	222	7 - 00
	0.92	222	DFel -Th
	1	250	U.
	0.56	250	/
	0.37	572	N
	0.42	400	XID
	0.28	1000	-PA 0.2 Cm 0.8
	0.2	2000	102 Ch
			1

Now, we can easily find out C A value at different C A value what is the 1 by r A or first we calculate the r A value then we calculate the 1 by r A value. So, this we can have that now we know the plug flow reactor when you tau plug flow reactor is equal to minus d C A by minus r A am I right. So, now here you can you can again plot minus 1 by r A into

C A and that C A that you are I do not know what kind of plot you have to find out and suppose this is a 0.8 mole per liter and this should be 0.2 mole per liter.

So, you have to find out area under this curve. So, you can found out the value of tau plug flow reactor this is how you can calculate.

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Solution	
We know	IN Som
	$\tau_{PFR} = -\int_{C_A}^{C_A} \frac{dC_A}{(-r_A)} \frac{dC_A}{2} \frac{dC_A}{dC_A}$
Here,	
	$C_{A0} = 0.8 \frac{mol}{L}$
	$C_A = C_{A0}(1 - X_A) = 0.8(1 - 0.75) = 0.2 \frac{mol}{L}$
The integration c	an be evaluated by graphical method or by numerical method.(area
under the curve of	of $\frac{1}{-r_A}$ vs $C_A$ between $C_{A0}$ and $C_A$ )
Area under	the curve(using trapezoidal rule)= $\tau_{PFR} \neq 300$ s
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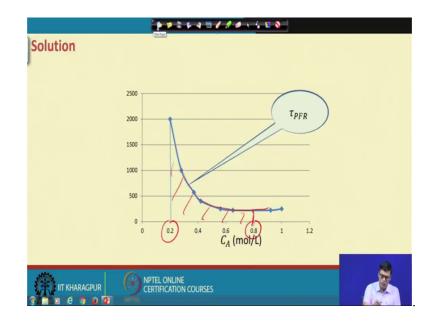
Now, this is there equation this is C A value you can calculate and this is the about 0.2 I showed you and then we have when you calculate the this area under this curve area under this curve when you calculate 1 by r A versus C A that you know, we can find out this is tau plug flow reactor and this is coming about 300 seconds.

So, you can easily calculate. So, this problem I considered very interesting problem in the sense that how the batch data can be utilized for finding out the time required for the operation of the plug flow reactor. Because when you when you operator a continuous stirred tank reactor then you find after infinite time when the steady state condition reach your substrate con concentration remain constant, at that particular concentration of what is the rate of reaction is there you can easily find it out from this equation tau CSTR equal to C A 0 minus C A by minus r A.

So, if you know that. So, different C A value you can get the r A value and if you know the r A value you can find out minus 1 by r A value and if you then you plot minus 1 by r

A value by C A you the area under this curve will give you the value of tau plug flow reactor.

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So, this is this is how you can find out here you can see that this is the kind of curve we got and this is 0.8 and this is 0.2 the area under this curve you can find out that this is this is what we call tau plug flow reactor .

So, what we what we learn from this particular lecture we learn that how to find out the batch time. And I told you that to find out the batch time what either you to go for numerical techniques or computational techniques or better you go for and graphical analysis and since the batch time is equal to minus d C A by minus r A.

So, if you plot 1 by minus r A by C A and area under this curve will we can easily if I calculate and find out that for the conversion with 75 percent 80 percent 90 percent substrate conversion how much time is required you can easily calculated. Now in case of reversible reaction we come across that 2 thing 1 is; what is the equilibrium, the conversion with that equilibrium condition what is the percentage conversion of the substrate.

How we can calculate and also if the normal reversible reaction at time t what will be the conversion that you have, but only in case of reversible reaction I told you that 2 strategy we maintained to increase the product concentrated product formation in the reactor

either as soon as the product formed, if you take it out more substitute convert it to product or you add more substitute in the reactor so that you will get more product in the reactor. Now in the last problem is very interesting how I try to find out how from the data of the CSTR can be utilized for the operation of plug flow reactor.

Thank you very much.