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

## Lecture – 17 Reactor analysis

Welcome back to my course aspects of biochemical engineering in the last lecture I try to discuss the different type of reactors and we have seen that we have different reactors is used both in the chemical and biochemical industries as for example, we have if you look at the mode of operation on the basis of mode of operation it can be have 3 different type of reactors one is called batch reactor another we have fed batch reactor and then we have continuous reactor and then we also come across the other different type of reactors like in the continuous reactor we have CSTR we have plug flow reactor and I told you that CSTR is very easy to operate.

But plug flow is little bit difficult to operate because during the flow there should not be any kind of back mixing that take place in the in the reactor radial mixing is permissible no not the axial mixing. So, that is the problem that we have and then I did we discussed the different other type of reactors like packed bed reactor expanded bed reactor fluidized bed reactor also we discussed the bubble column reactor nearly reactor and also I showed you what are the how the reactor looks in industrially that both in the biochemical and chemical processes.

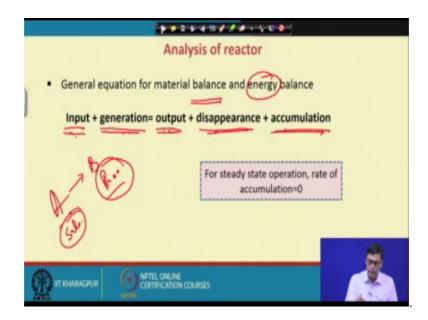
Now, today I want to discuss very important topic that is called reactor analysis now why the reactor analysis is required because to find out the volume of the reactor because. So, in the industry suppose I want to produce a certain amount of product there was suppose I i worked I personally work with citric acid industry and we produce 4 to 5 tons of citric per day now question comes that for the production of citric acid what should be the volume of the reactor how we can calculate. So, until unless you have the expertise you have the knowledge of reactor analysis you cannot do the analysis. So, through this lecture is totally deals with that now first let me discuss that

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Analysis of reactor
Reactor analysis
Material Energy balance
Substrate balance
Only one parameter can be considered for reactor analysis

That the analysis of the reactor we have we have the material balance we have substrate view you can see the substrate balance and the product balance and energy balance. So, 3 different way we can do that one is substrate balance another is product balance and the energy balance. So, we can we can do this balance of the equations that we can do then.

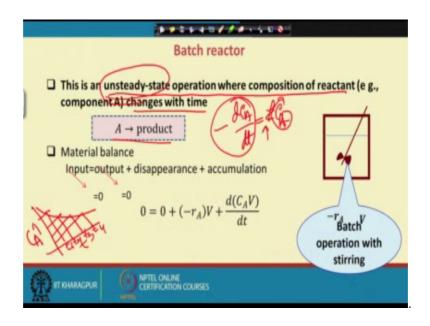
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If you look at the formula, because we considered basically the kind of formula that, what kind of equations we have for the reactor analysis. So, we have the input equal to plus generation equal to output plus disappearance plus the accumulation.

Now, now when you do any kind of reactor analysis we should always considered that you know that a particular one particular component as for example, suppose I want to produce a 2 b am I right a is the substrate and b is the product am I right. So, if me want to do the analysis we can do the analysis with respect to substrate. So, if you if you put the then rate of substrate input equal to rate of substrate generation rate of substrate output plus rate of substrate disappearance plus rate of accumulation this is the equation that we have. Now if you want to do the balance equation this is kind of balance equation am I right and if we write the balance equation with respect to product how we can write rate of product input plus rate of product generation equal to rate of product output rate of product disappearance plus the rate of product accommodation now we can we can we can write this balance equation with the respect to the energy also rate of energy input plus rate of energy generation plus rate of an equal to rate of energy output plus rate of energy disappearance plus rate of energy accumulation now first

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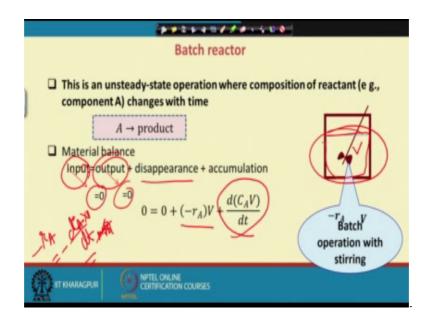
let me consider the batch reactor the batch reactor we want to apply this same formula in the batch reactor now what is batch reactor batch reactor is considered on steady state operation where the composition of the reactant keep on changing with respect.

So, what I what I what I want to do that suppose there is a reaction a to product am I right. So, I can write ca with respect to time. So, it is keep on decreasing with respect to time. So, at different time at different time you have different ca value now if you if you

if you if you have the rate equation what is the rate equation dca by dt am I right equal to k into ca if you consider first order reaction now as your ca value k is constant, but as your ca value changes at different time this is t one this is t 2 this is t 3 this is t 4 they as the time changes your ca value changes as the ca value changes the rate of reaction changes we call it is a unsteady state operation. So, please unsteady state means that why the unsteady with respect to the substrate concentration substrate concentration is not uniform in the reactor as the time passes on substrate concentration keep on changing with respect to time.

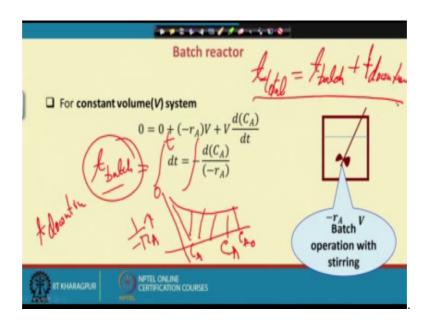
Now, now if you put this in the in this previous formula how we can write.

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That input the I told you in the batch system we take the material at a time allow it to react after the reaction is over you take it out. So, the input and output should be equal to 0 am I right this should be equal to 0 there is no continuous input continuous output from the process now what is the rate of disappearance rate of disappearance is minus r into v why minus r into v what is minus r minus r equal to minus dca by dt what is dca dca is the mass per unit volume am I right. So, so when you when you carry out the reactor reaction in the reactor you have to consider the liquid volume whole liquid volume you have to consider. So, you have to multiplied by v then you consider all the component that carrying out the take place in the take part in the reaction then this is the what is this is the rate of accumulation of a in the system. So, this is the dca into v into dt.

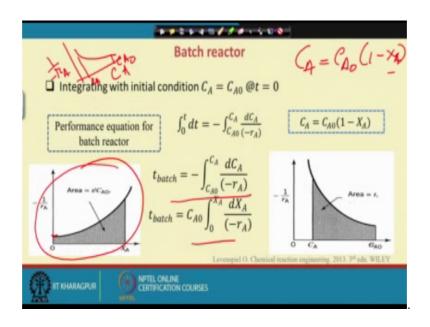
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Now, this equation I can I can write in this form dt equal to minus d dca into minus or this we can write now we can if you if you want to find out the batch time how we can do that how I can do I can do the integration here am I right I can do the integration with 0 to t. So, this is equal to t batch and this is equal to like this now if you want to calculate this how we can calculate. So, this is minus ra and this is ca and suppose that the correlation is like this then suppose this is equal to ca 0 and this is equal to ca. So, area under this curve is equal to t batch we can easily calculate the batch time like this now I can here let me point out one thing when you when you consider any kind of batch to batch process we should remember that the batch process the one per has for the material out and after taking the material you have to clean the vessel then again you have to refill the vessel it requires at some time and this time we call it downtime this way what do you what do you call it downtime. So, to what is the t total in the batch process total time equal to t batch plus t downtime.

Am I right this is how we can get the get the total time required for the batch process

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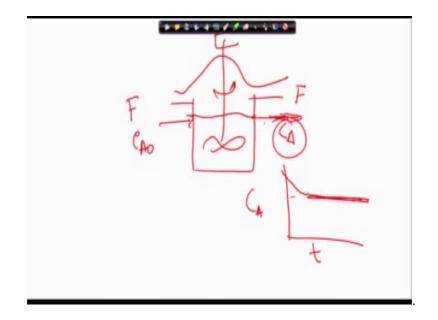


now this is exactly what I have done previously this is how we can find out and if the if your correlation is like this that we can we can find out this is ca 0 to ca and I i told you ca equal to what c is 0 into one minus xa. So, with respect to x a also you can do that the xa will be 0 to x in, but a one we should understand that when we have the correlation between minus ra by ca and that this correlation this is equal to ca 0 this is ca am I right, but now when you draw this coalition with respect to x then they you start 0 from here the same type of correlation will be like this

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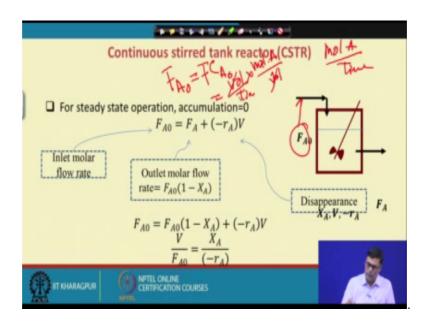
now let me let me talk about this continuous stirred tank reactor and I told you continuous stirred tank reactor is largely operated and is easy to operate and we here it is possible to establish the steady state conditions what is the steady state condition steady state condition means at a at a under steady state condition the concentration of the of the different component present on that of the reaction mixture remain constant. So, how it is possible now this is possible because let me explain that.

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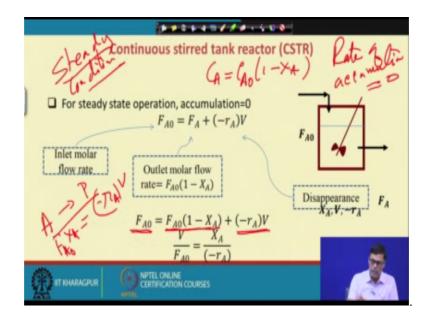
Suppose the suppose this is a CSTR am I right . So, so you operate a particular flow rate the particular substrate concentration when you when you run this process to you take out this is the materials time to time this is same flow rate you maintain here. So, this is ca. So, initially when you when you when you operate it you will find ca value might be get changing like this a time will come it is constant when it is constant we call it steady state because when this substrate concentration is remain unaltered then we call it in steady state . So, your material balance is the input equal to output the same that we have as we have done before input equal to output disappearance plus the accumulation

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now how we can analyze the reactor and this is if you if you if you if you consider here let us assume this is the fa fa is here fa is the moles of a per unit time you are feeding in the reactor now how you can write fa is fa 0 fa 0 is equal to nothing, but what you can write f into ca 0 what is ca f is the flow rate volume per unit time and this is ca is the moles of a per unit volume am I right this volume will cancel. So, it will be moles of a per unit time.

So, we can we can write that f a equal to fa 0 into one minus x a now ca equal to what.

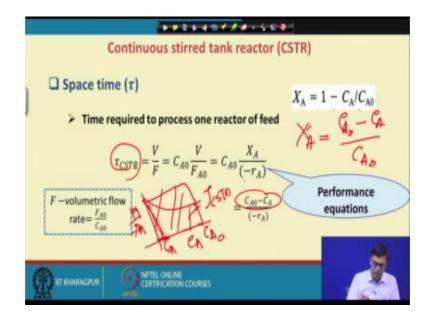


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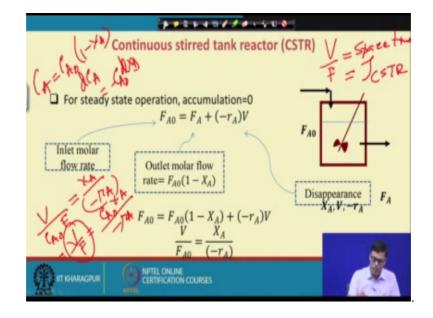
Ca equal to ca 0 minus one minus xa. So, similarly we can write that f a f a the molar output flow rate here will be equal to fa 0 into this. So, . So, this equation what we can write that f a f a is the input and f is 0 we do not have any generation because we are we are this a is the substrate am I right and it is producing product. So, there is the equation is that rate of input plus rate of degeneration is the rate of output plus rate of disappearance plus rate of accumulation now under steady state condition steady state condition what is steady state condition when the I told you when the substrate concentration will be uniform and this is this is possible when rate of accumulation is 0 when the rate of accumulation is 0 equal to 0 then and only then that is that your substrate concentration will be uniform. So, what will be basic equation rate of input equal to rate of disappearance.

This is the rate of disappearance. So, if you solve this equation we will get the v this is b by f a 0 am I right into xa by this we can we can write this if we simple equation if we if we solve this equation we have this fa 0 fa 0 will cancel and f a 0 if it is cancels then it said the minus f a 0 into x a minus fa is 0 into xa you can take it this side f a 0 into xa equal to the minus ra into v now you can you can write v by fa 0 equal to x into this we can we can easily write it here now once

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we have we have done this then now if you look at previous equation we have seen the previous equation like this equation we get in the continuous stirred tank reactor am I right now this equation how you can write this is v by f now v I can write it here



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there is a what is v and what is the f a 0 I told you this is c a 0 into f am I right this is c a 0 into f equal to xa into minus ra now this is. So, so what a this is v by f equal to what equal to ca 0 into xa by minus ra can I write.

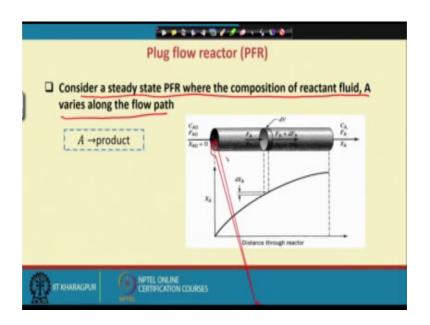
The if we if we can write like this now I have what I told you is that ca equal to ca 0 into one minus xa the dc a will be equal to what minus c a 0 into dxa now here you see that this is the this is the this is the xa that we have then and this minus ra that you get a get here that is that you can you can then what is this value this is nothing, but what you call space time this is what is the unit this is volume this is volume per unit time. So, this is called v by f v by f we call it space time for the CSTR now this is equal to how you express tau CSTR this is exactly we have done in the subsequent slide this is a tau CSTR equal to 3 by f ca is 0 v by fa 0 if this ca 0 into x a then what is the what is the ca 0 into xa it is c a 0 into because I i to what I told you this is the x a x a is equal to what c a 0 fraction of a that is converted in the c a 0 am I right. So, if it is like this. So, yeah this is the. So, ca 0 equal to c a 0 minus the x a that is c a 0 into xa plus ca 0 into ca the what we have writ10 here and this is like this now let me let me take the previous equation because plot minus ra versus suppose we have c a. So, we have this kind of plots.

Now, suppose we want to convert the c a 0 to ca. So, if you if you here the area under this curve is equal to tau CSTR because rectangle because I had to add as ca what is the rate of reaction is this one and at a c a 0 it is this one. So, so in this is this is the concentration different that the rate of reaction you multiplied you will get the tau CSTR this is how you can find out tau CSTR now this is.

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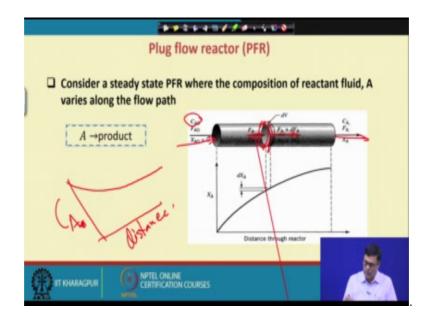
Exactly what the what they have mentioned here that it has been you can see that how here the area under this curve will be equal to tau this is equal to tau CSTR this we can calculate and it is very simple if you know the rate of reaction tau CSTR equal to c a 0 minus ca minus ra. So, if you know ra if you know c a 0 says it yeah we can easily find out that what is the tau CSTR now this is equal to tau CSTR is equal to what this is equal to v by f now if you know the flow rate though you can easily find out the volume of the reactor. So, that is exactly I am saying that this reactor and this is if you can do you can find out the volume of the reactor in any kind of production processes

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Now, let me discuss another reactor to a continuous reactor what you call plug flow reactor now what is the plug flow considering the steady state plug flow where the composition of the reactant of the fluid varies along the path now in case what is happening that you know liquid this is you can you can find out this is this is this is the this is the tube tubulary I told you this is a basically it is a tubular reactor the liquid is

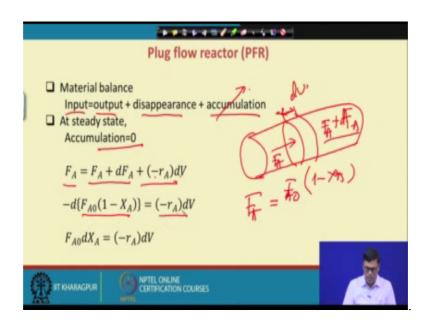
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passing through the tube am I right it is passing like this now when it pass it like this that a concentration of ca keep on changing with respect to time. So, if you if you make a

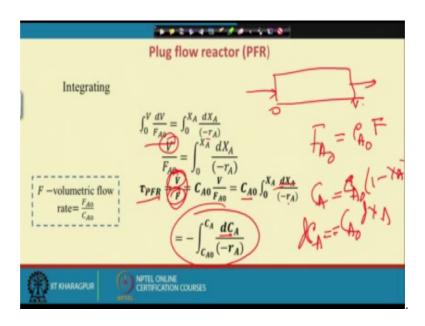
profile that you find ca 0 ca concentration not ca 0 ca concentration keep on changing with respect to distance like this you keep on changing with respect to distance. So, naturally that now here what we can do the analysis of the plug flow reactor we shall have to assume a differential segment in the particular reactor the small segment that we can consider in the reactor and we can we can do the material analysis across the segment. So, we let us assume the fa the moles of a that is entering here and what is going out that fa plus df a and volume of the this segment is d db that we have .

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So, what you can write material what is the material analysis we have rate of input equal to rate of output rate of dips disappearance accumulation the under steady state condition rate of accumulation is equal to 0 this as we mentioned. So, what is the rate of input fa across the differential segment what I told you this is this is the tubular reactor and we assume a differential segment here am I right. So, it is coming fa and going out what f a plus df a and what is the volume of the segment volume of the segment is dv that we have now if you if you have fa the fa is the input and f a plus dfa is the output am I right this is the output and what is the rate of reaction minus ra into dv. So, this I can write that fa will fa will cancel now what is the fa fa fa I can write like this f a equal to fa 0 f a 0 one minus xa that is the that the exactly what he has writ10 there and this is equal to minus ra into dv now this we can write that this is fa 0 into dx a equal to minus ra into dv . So, so we have we have this equation if you if you look at the previous equation is like this.

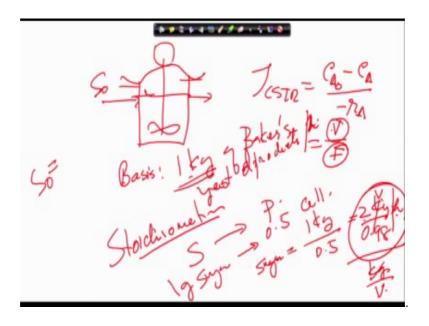
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So, we can write dv. So, what we can write dv by d fa 0 f a 0 I can take it here. So, there dx a minus ra am I right. So, that is exactly what is writ10 here d dv by f a 0 the da by minus ra am I right.

So, this is. So, if you if you do the this is the plug flow reactor and the this is the 0 volume this is the v volume. So, you can you can integrate from 0 to v value and naturally dv will be v and fa 0 is constant it will comes out and this will be like this now what is fa 0 I told you fa 0 is equal to c a 0 into f am I right. So, I can write v by f equal to c 0 into this is this is ca 0 into this dxa by this and again I i I told you that a ca equal to what ca equal to ca 0 one minus xa now dx d ca is equal to what minus ca 0 ca 0 is constant d xa now here this is ca 0 and d xa is there. So, we can we can write this in the form of d x a. So, this will be minus this is minus there were plus is there. So, it should be minus. So, this equation we can come across this equation this is equal to again v by f. So, if we find out the tau plug flow reactor then we if we find out the f value we can find out the volume of the reactor f is the volumetric flow rate now how you can find out the volumetric flow rate let me explain that.

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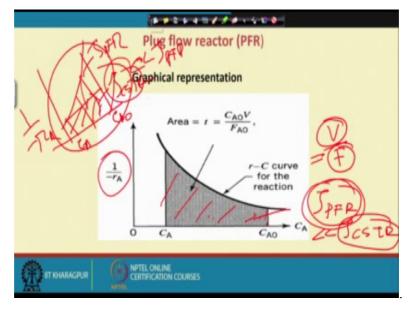


Suppose let me let me first assume, but the suppose this is the CSTR there is the input and output am I right then what is the equation that we have we have equation is that tau CSTR is equal to c a 0 minus ca minus ra and this is equal to v by f now suppose the one industry produce let us assume basis what is basis is let us one kg of bakers yest production bakers yest production per day let us assume the per day or whatever you have per hour you can you can say per hour whatever you have now if we assume that and then first we shall have to find out the stoichiometry what is stoichiometry that how much of substrate gives how much of product the in case of bakers yest suppose you have. So, you use the sugar as a raw material sugar the one gram of sugar produces approximately point 5 gram of cell.

So, suppose for one kg of bakers yest how much sugar is required sugar is required this is the one kg divided by point 5 this is equal 2 kg am I right 2 kg event now 2 kg the one kg bakers yest you want to produce per hour that mean 2 kg bakers yest is required part hour, but provided your conversion is hundred percent, but usually your conversion cannot be hundred percent maybe ninety 5 percent ninety 8 percent. So, again you divide by that factor make a may be ninety 8 percent. So, this is the exact amount of substrate that is required for your system now if you have if you know what is the initial substrate concentration here. So, if you if you divided by any what is the initial substrate concentration the kg per unit volume. So, kg will cancel volume will go here their volume per unit time. So, volume you can put it here flow rate you can put it that volume

per unit time is the flow rate and this then you can easily find out the volume of the reactor similarly you can do this same thing you can do in case of plug flow reactor this is how you can find out the volume of the reactor and here in the plug flow reactor when you do the correlate that you know previously you can remember that when we talk about the CSTR the area under this curve.

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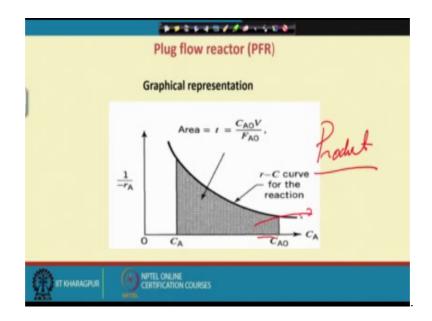
The area under this curve this is this is like this area under this curve we call it this is tau CSTR am I right, but now in case of plug flow reactor when is the area under this curve is we call this is called tau plug flow reactor though; obviously, if you order any kind of reaction if you have the correlation between one by ra versus ca you have this kind of pattern I can easily say that tau CSTR will be much less than tau CSTR. So, naturally if the if the tau CSTR is less then this is equal to what v by f the f is more or less constant in a in a particular continuous system. So, if a if you want to produce a definite amount of product.

So, v of the reactor volume of the reactor directly proportional with the space time of the plug flow reactor. So, as it is decreases the. So, your volume of the reactor will be will be less. So, we will go for if the correlation is like this then we will go for the our choices plug flow reactor, but if we have other type of correlation like this then if you if you look at that c a 0 ca the area under this curve it you have tau CST, but area under this curve will be tau plug flow reactor. So, in that

particular if you have correlation like this minus ra by the ca 0 then we will go for our choice will be tau CSTR.

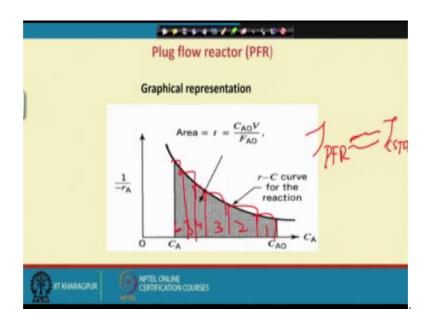
Now, I have one observation here because we want to share with you now what is this situation you try to think over that now as the substrate concentration decreases one by ra increases one by ra increases means that ra decreases as the you imagine the situation in the reactor when the substrate degrades decreases substrate concentration decreases the rate of reaction also decreases and why it happens it only happens when there is a product formation. So, so, but this kind of correlation is valid when there is a product inhibition in the system.

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This is product inhibition am I right. So, in case of product inhibition we go for what choice this plug flow reactor now goes a since I told you the plug flow reactor is very difficult to operate am I right now how is it possible question comes is this possible to replace the plug flow reactor by CSTR answer is this how it can be done now here if you look at here if we put the multiple plug CSTR like this the multiple CSTR what will be the area of the CSTR is like this. So, 1, 2, 3, 4, 5, 6. So, if you if you if you if you considered multiple

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CSTR in series then you will find tau plug flow reactor is almost is the almost equal to not exactly equal to tau CSTR if you have multiple CSTR in series which can be easily operated.

Now, here I have I have given an example.

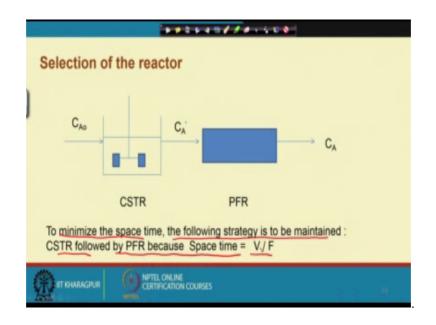
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)	Selection of the reactor In case of the following reaction: $A \rightarrow B$ The correlation between (1/-r <sub>A</sub> ) vs. C <sub>A</sub> is given below:
	PFR U/4.) J.F.P. J.CSTR
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Suppose how is like the reactor suppose there is a reaction a to b and you have correlation one by ra versus c a is like this. So, we I i have identified 3 2 different zones

this is zone and this zone now here you get clearly you can find out here area under this curve this will be what tau CSTR am I right this is tau CSTR and. So, will, but here the total area here will be tau plug flow reactor. So, ca 0 to ca dash we with that you know our tau CSTR will be much less than tau plug flow reactor. So, we will go for our preference should be tau CSTR now here situation will be different ca dash to ca the area under this curve this curve will be will be tau CSTR and this is this area under they said this will be tau plug flow reactor. So, this is much less as compared to tau CSTR. So, we' will go for plug flow reactor. So, what I have writ10 here

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That in that particular what is about choice first ca 0 should be passed through the CSTR.

So, that it converted to ca dash and then it passed through the plug flow reactor you will go to the ca to. So, what I have writ10 here to minimize the space time the following strategy is to be maintained the CSTR followed by plug flow reactor because the space time is equal to v by f the if the if the time in the overall space time is reduced in the particular reaction then volume of the reactor will be very less and if the volume of the reactor is less our cost involvement of the process of is less this is how we can select the reactor now in this say in this particular lecture I try to discuss that how we can find the batch time of a batch process and how you can I i told you batch process is an example of the unsteady state reactor and if you go if you wanted to have the steady state re reaction only it is possible in the continuous reactor, but one thing I want to highlight that steady state conditions will be prefill at infinite time you know I mean instantaneously it cannot be done it you have to run it for quite some time until and unless is at in the steady state and after. So, we try to analyze the CSTR we try to analyze the plug flow reactor and we have seen that plug flow reactor is suitable for the product inhibition reaction and, but plug flow reactor can be replaced by the multiple CSTR because I showed you that how it can be multiplied and finally, I showed you that what is the strategy we should have for selecting the different reactor in a particular reactions.

Thank you very much.