Principles of Polymer Synthesis
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Lecture – 25
Design of Chemical Reactors (Contd.)

Welcome back to the last class of this week. We have been talking about these chemical reactors, the design principles in general, and in particular how we can you know modify the equations for the design equations for different kinds of reactors in terms of conversion. And ultimately, some real problems of if you are carrying out a particular reaction in a particular reactor, what is the kind of you know parameters that are necessary to be controlled, so that you can get a particular amount of conversion. So, we are developing all these things step by step.

We started by talking about the rate law because for any chemical reaction that you do you need to know the rate law. So, that rate law basically tells you how the rate varies as a function of concentration. The second thing is that you have to find how the concentrations of these different species that are present in the system they vary as a function of conversion, these things you can find from the Stoichiometric table. And the Stoichiometric table you can construct individually for different kinds of reactors. And we already told that they have some similarity as far as the flow reactors and batch reactors are concerned. And when you combine these two things that is the rate law where the rate varies as a function of concentration and the Stoichiometric table which tells you how the concentration varies as a function of conversion, when we put them together you get an expression of rate as a function of conversion.

So, you basically have known you basically have now got the rate how it varies as a function of conversion so that you can construct those kinds of tables that I have already shown you. And a couple of problems we have worked out for CSTR. We will try to go back to those tables when we are doing other different problems mainly for the reason of simplicity and for the reason of comparison between different kinds of reactors. So, we will continue in the in the same vein today. So, let me first start by summarizing what we already know. So, the topic is the same design of chemical reactors that we are continuing the theme is the same for this particular week.

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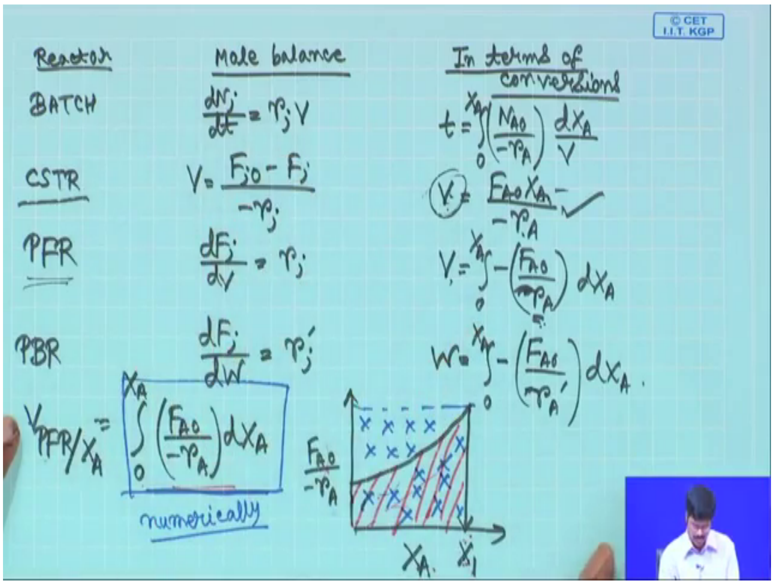

So, let me then write down this simplified thing for you means whatever we have understood until now reactor mole balance and then we have in terms of conversion this is at the heart of all the discussions that have gone on this week. So, the batch reactor, so for the batch reactor your mole balance was it is good to recap once in a while, so that you do not get lost the stream of inflow of all these information. So, in terms of conversion your t is basically 0 to X A N A 0 by minus r A into d X A by V excuse me, so that is batch.

So, if you are looking at CSTR then your mole balance equation is F v equals to F A 0 minus F j molar flow rate in molar flow rate out divided by rate of generation of the species j. And then this can be expressed in terms of conversion which is more practical for you F A 0 into X A divided by minus r A, we also constructed a ligand plot of F A 0 by minus r A versus X A in order to find out the value of V at a particular X A.

Now, PFR plug flow reactor the mole balance equation was d F j dV equal to r j and in terms of conversion here V equals to 0 to X A minus F A 0 by minus, so minus is already there r A into d X A. Now, this is inside the integral because the rate is also a function of conversion. And finally, for PBR packed bad reactor, you have d F k d W. So, as a function of the weight of the catalyst so that is equal to r j or r j prime if you so please r j prime. So, then that will be W equal to 0 to X A same form as PFR instead of d F w minus F A 0 divided by my divided by r A prime into d X A.

Now, if you are looking at, so let us say we have already talked about CSTR in detail how to find out the volume for a particular conversion. If you want to do the same problem for PFR, the volume for a particular conversion, so let us say V PFR for a particular conversion of X A, what is the volume of PFR or plug flow reactor for the conversion of X A. So, that is equal to 0 to x a F A 0 by minus r A into d X A. So, again if you plot the same graph F A 0 by minus r A as a function of X A, so your plot is like this. So, let us say r as a function of X A.

So, let us say you are looking at a conversion of X 1, your question is at a conversion of X 1, if you have to have a conversion of X 1, then what is the volume of the plug flow reactor that you are going to use. Then it is immediately becoming apparent to you that it is basically the area under that curve that is important, this area under this graph gives you the volume of the plug flow reactor necessary in order to have a conversion of x 1 why this integral of 0 to say x 1 integral of this y d x. So, this is let us say this is y we are plotting against x. So, this curve the area under the curve is basically integral 0 to whatever value here y d x. So, this is the area under the curve nothing but the area under the curve. So, the area under the curve gives you the volume of PFR necessary to get a conversion of x 1.

But if you are looking at the same curve and if you are saying what is the volume of CSTR if you are using instead of a plug flow reactor, if you are using a continuously stirred tank reactor then what is the volume of CSTR that is necessary in order to get a conversion of X 1. So, that volume of CSTR that is necessary is nothing but this. So, from the graph itself, you can see that the volume of CSTR necessary in order to attain a particular conversion is basically higher than the volume of PFR necessary. So, you see the beauty of the mathematics here, it is nothing to be feared, but rather you try to get the physical meaning out of that what is useful for you. So, now, the question comes how do you determine this integral that poses a problem.

So, typically what we do is that we numerically evaluate these integrals. I will take you step-by-step through some of the most basic processes of numerical analysis to get the value of integral. It is necessary ultimately because even when you are looking for say polymerization and all you have to use the same kind of techniques same kinds of different equations that is at the heart of the chemical reaction we have to design. We are talking about ideal of course, ideal CSTR, steady state situation, and also we are talking about the temperature being constant say for example, CSTR. If it is isothermal situation temperature constant then all these things are valid. If you are talking about temperature changing then things will change, we would not to go into those kinds of complexities at least not for this course.

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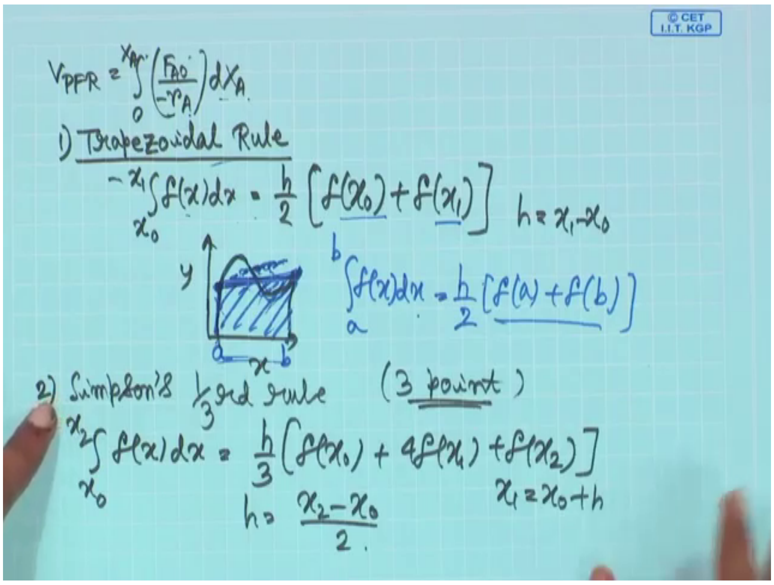

So, the problem then becomes essentially to evaluate this integral. So, evaluation of the integral is nothing but finding the area under the graph. So, one of the ways in which you can do that is trapezoidal rule a numerical process, basically this is a two point process. So, let us say so this is a two point process, you want to evaluate an integral x 0 to x 1 the functional form is f x d x, the same thing f x d x. So, this is f x d x because this particular thing is a function of x, which is the conversion that is why this is f x. So, function of x.

So, the general thing here is that h by 2 into f x 0 plus f x 1. So, h is the distance between the two points which is basically x 1 minus x 0. So, it is nothing but saying if you have you are plotting y versus x, and you have a curve like this how to find out the area under the curve you approximate basically. So, you what you do is you generate a trapezoid. So, you generate a trapezoid like this. So, you generate a trapezoid like this sorry. This is a trapezoid. So, your curve is going like this. So, this is a trapezoid. Now, you find the area under the trapezoid and that is nothing but this. So, let us say this value here is b, and the value here is a, then integral a to b f x d x. So, this is an approximation of course, because this is this area is not exactly the same as the area under the full curve, but then again numerical analysis goes to an approximation of course for you.

So, this is a little bit you know not very clear. So, here is the curve. So, you are basically adding up these two points here. So, this is your trapezoid. So, the integral f x d x is nothing but h by 2 into f a plus f b h being the distance between the two. So, h being the distance between the two and f a, so f a plus h b these two value, so correspondingly this is the area of the trapezoid, so that is why it is a trapezoid rule. Now, we would not discuss this thing too much something more important that we will discuss is Simpson's what you say as one-third rule, this is basically a three point rule. So, whatever interval you have you basically divide that in equally spaced even number of intervals whatever spacing you have you basically divide that into equally spaced intervals.

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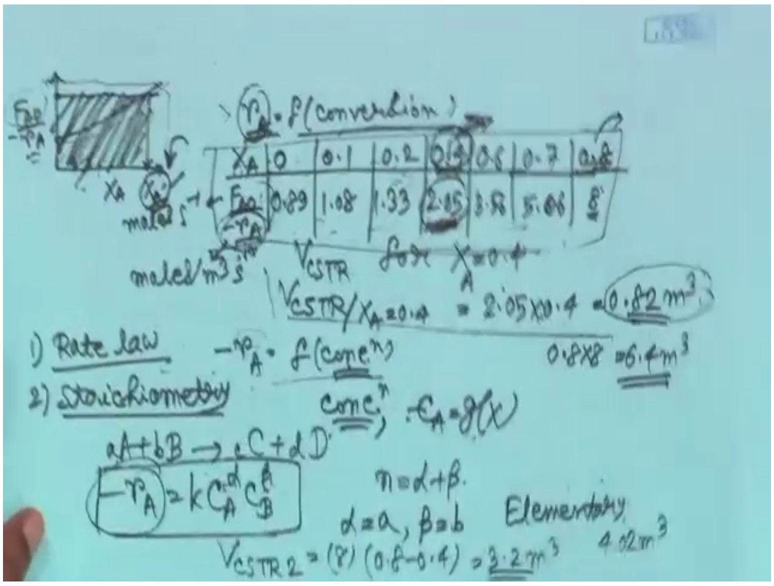

So, if you have to find the integration of the curve between these two points between these two points, then you divide that into equally spaced interval if possible. So, like that say. If you have 0, 0.1, 0.2, 0.4, suppose you want to find out the integral where the conversion is 0.4. So, for PFR then you have to find out the integral the area under the curve up to the 0.4. So, then this particular integral will become 0 to 0.4. So, it will be 0 to 0.4 F A 0 by minus r A into d X A. So, then you can divide this into two equally spaced interval 0 to 0.2. So, spacing is 0.2 the difference is 0.2, and 0.2 to 0.4. So, a difference is point two then you can use some of these rules.

So, equally spaced even number of intervals. So, these are equally spaced and what are the number of intervals two intervals are there. So, then you can use for example, Simpson's one-third rule. So, basically it becomes something like this x 0 to x 2. So, x 0 x 1, x 2, these are the three points. So, the total interval is 0 to x 2, you divide into two intervals, the total spacing is 0 to x 2, you divide into interval 0 to x 1 and x 1 to x 2 and these are equally spaced. And then the formula that you have is f x d x equal to h by 3 f x 0 plus 4 f x 1 plus f x 2; where x 1 is equals to x 0 plus h, and h is equals to x 2 minus x 0 by 2.

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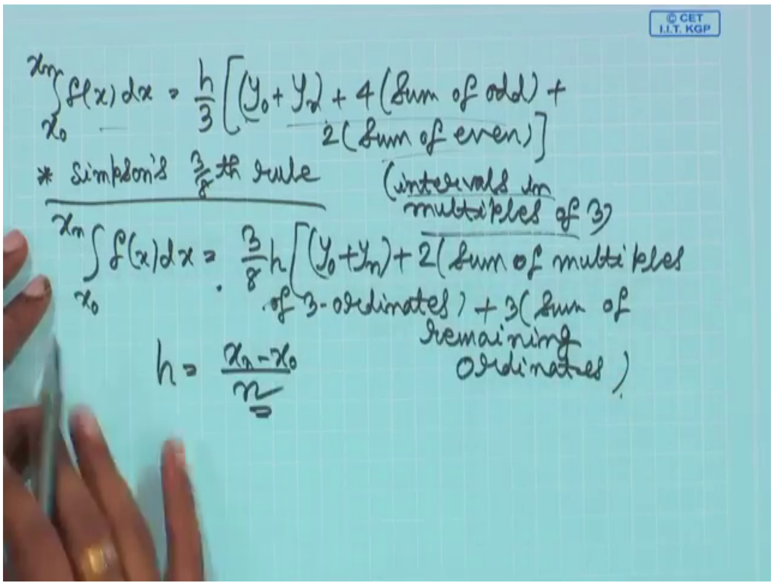

And in general the form of the Simpson's one-third rule will be x 0, let us say you are integrating from x 0 to x n f x d x that will be equal to h by 3 into y 0 plus y n. So, the first ordinate and the last ordinate plus 4 into sum of all ordinates plus 2 into sum of even actually you do not need to remember all these things you know these things are already documented. So, when that interval is there when you find out when you have what is the power of this. if you have to have this kind of problem, if you have this kind of problem, then you find out for yourself which rule to use and all those expressions for the rules these are already in the literature. So, you find out you put it there and you can get the conversion value that is why it is important.

But you need to know that such things exist that is why I am just writing down all these things. Then there is another form Simpson's, so this is basically you are using your

Simpson's one-third rule for equally spaced intervals even number of equally spaced intervals, but you may not always be able to have even number of equally spaced intervals. So, you can use what you call as Simpson's three-eighth rule also. Just look at it as some of the techniques that I am introducing. So, basically then it will be fine for you.

So, look beyond again some of these expressions and try to understand why we are using them, these are just tools, but you need to understand the tools in order to use them effectively for your own purpose that is important. So, Simpson's three-eighth rule basically it is the intervals in multiples of 3, if you can manage to have intervals in multiples of 3, then you can use this in multiples of 3, then you can use this Simpson's one-third rule.

So, the general form of this rule is x 0 to x n again this is the whole range f x d x equals to 3 by 8 into h into again this is the first ordinary, this is the last ordinate plus 2 into sum of multiples of 3 ordinates, because your multiples of 3 those ordinates you just take plus 3 into sum of remaining ordinates. And here h is x n minus x 0 by n where n is the number of intervals. So, if you can manage to split this whole range in the problem, whatever range is there suppose you are talking for about 0.4, so you are trying to find out four from this particular table, what is the plug flow reactor or volume with a conversion of 0.4 for 40 percent.

So, then you can actually see that you can all the data that you have from there you can divide this whole range into two equally spaced intervals 0 to 0.2, and 0.2 to 0.4 then you can only use Simpson's one-third rule like this you have to look at some of these situations. So, and sometimes you may have to use both of them together for certain region you have to use one of them, and for the other part you have to use the other one . So, in combination of that you may have to use that.

So, what we will do now is the following. So, let us say we are going for the same table. Again we are trying to find out what is the volume of plug flow reactor for this particular system that is necessary in order to get 40 percent conversion X A and this is F A 0 by minus r A, all these values are there. And we have already found out what is the V CSTR - volume of CSTR or continuous stirred tank reactor necessary for 40 percent conversion that is 0.82 meter cube that was the volume of CSTR necessary.

And we know from this graph, so we actually have already found out that it is the area under the curve that gives you the PFR volume, but this is the area for this rectangle whole rectangle that gives you the CSTR volume. So, basically you will have a value lower than this when you calculate this thing. So, you can use Simpson's one-third rule for this thing here.

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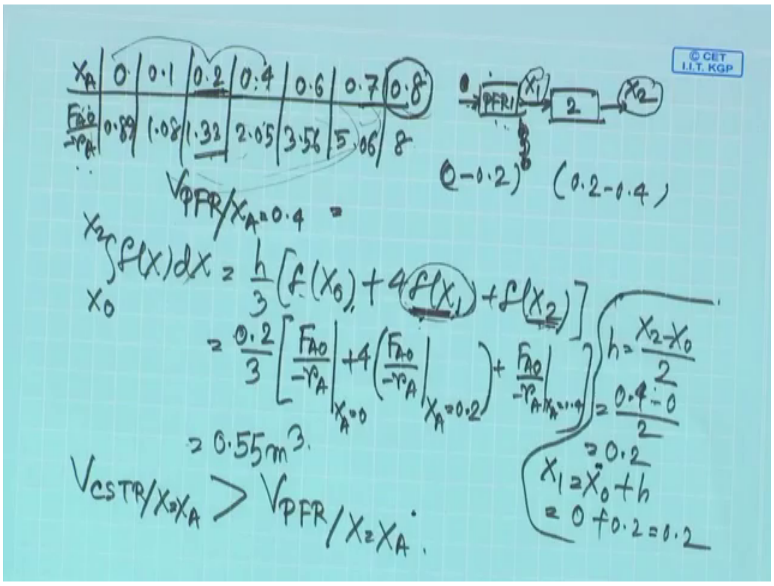

So, let me do this for you. So, I will just write down this expression again X A and then if you have F A 0 by minus r A 0, 0.1, 0.2, 0.4 and then you have 0.6, 0.7, 0.8. So, this is F A 0 by minus r A is 0.89 as I told you we can find this out because you know how r A changes as a function of conversion we have already discussed this. 0.1 is 1.08, this is 1.33, 2.05, 3.56, 5.06 I suppose and this is 8. So, the question was obtain the volume of PFR necessary for a conversion of 40 percent. So, then this is. So, you can actually have two equally spaced interval as I told you. So, two equally spaced interval for this. So, you can apply Simpson's one-third rule. So, one interval is 0 to 0.2, and the other interval is 0.2 to 0.4.

So, Simpson's one-third rule, so if you look at the expression for Simpson's one-third rule that was this when you have two intervals specifically that was this is general form also, but here this is necessary. So, this is x 0 to x 2 f X dX this is the integral you want to find out and that will be equal to h by 3 let me write down the formula again f X 0 plus 4 f X 1 plus f X 2. So, if you are putting these values here, so what is the value of h, h is nothing but X 2 minus X 0 divided by 2, because 2 is basically the number of intervals you have. So, that is here X 2 is 0.4, X 0 is 0 and 2 is there. So, this is 0.2, so this is 0.2.

Now, what is the value of x 1 that is necessary because f x 1 is basically the value of F A 0 by minus r A where x equals to X 1. So, what is the value of X A that corresponds to the value of f X 1 that you have to find out. So, X 1 is nothing about X 0 plus h, X 0 is 0, and h is 0.2. So, X 1 is 0.2. So, f X 1 is nothing but f 0.2, so that means, this value is the value of F A 0 by minus r A at x a equals to 0.2, so there is 1.33. Same way f X 2 also you can find out because f X 2 is the value of F A 0 by minus r A at x equals to 0.4. So, then if you put all these values here, this will be 0.2 by 3. So, f X 0 is basically the value of F A 0 by minus r A at x a equals to 0 plus 4 into f X 1 is the value of F A 0 by minus r A at X A equals to 0.2 plus f X 2. It is the value of F A 0 by minus r A at x a equals 2.4 ok. So, if you calculate this thing, it becomes 0.55 meter cube.

And as we have already shown you before, so the for the same conversion of 40 percent if you are using a continuous stirred tank reactor you need a higher volume 0.82 meter cube if you are using a PFR which is a plug flow reactor you require lesser volume. So, graphically also we have shown. And when you do the calculations also these become apparent. So, then in general, we can write V CSTR for a particular conversion X equals to X A will be higher than V PFR for a particular conversion X equals to X A.

So, the final thing that we would like to do here, I mean we could go on and on and we can do lot of expressions here, but one thing you should remember is that we are using a technique these tools. So, this particular workout that I have done is later on if you find a problem where you have designed the reactor which reactors to use and so on and so forth.

What is the volume of the reactor, then you can go to some of these numerical approximations, and you can use them, so I am telling you how to use them, you do not need to remember the expressions of those say Simpson’s three-eighth rule that is there. But you need to keep in mind how many intervals you can divide it into, and then what kinds of techniques you can use correspondingly whether you will use Simpson’s one-third rule or whether you will use Simpson’s three-eighths rule, so that is the thing here.

Now, if you are say for example, if you are looking at this particular thing, say if I ask you, if you are using two PFRs two plug flow reactors in series and you are trying to achieve 80 percent conversion, and the outlet from the first plug flow reactor is giving you 40 percent conversion. Then what is the volume of the two plug flow reactors? It is a similar question to when you are having to CSTRs in series and the outlet of the CSTR one has a 40 percent conversion, so that is the then the inlet input for the CSTR 2 and the outlet for the CSTR 2 is giving you 80 percent conversion. In this case you can just rephrase this same question for PFR.

So, if you are considering the same question for PFR, then the total volume of PFR suppose 0. So, in the first PFR, PFR 1, your inlet your conversion is 0. So, it is coming out as say the conversion is X 1 suppose. This is the input for PFR 2, and the output is X 2. So, suppose I want to get a final conversion of X 2 the intermediate conversion is X 1 after it leaves the first PFR then what is the total volume. The total volume will be the volume of the first one, which is 0 to 1, 0 to I will just write down it in a new page.

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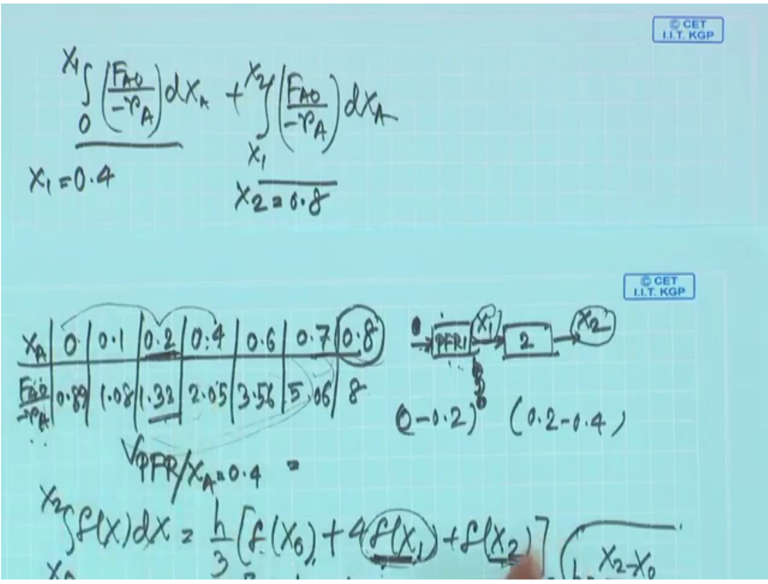

So, what will be the total volume. So, the volume of the first PFR will be 0 to X 1 into F A 0 0 to x 1 integral F A 0 by minus r A into d X a plus X 1 to X 2 this is the second volume of the second PFR F A 0 by minus r A into d X a. So, the problem essentially reduces to finding out the two the two integrals where X 1 is equals to 0.4 and x 2 is equals to 0.8. And you can immediately see that when x 1 equals to 0.4 already we have done this particular calculation, you can have a Simpson's one-third rule, because you can divide into two equally spaced intervals 0 to 0.2, and 0.2 to 0.4.

Similarly, from 0.4 to 0.8, for the second integral for the derivation of second integral, where X 1 is 0.4 and X 2 is 0.8, what you can do is that here also incidentally you can divide it into two equally spaced interval 0.4 to 0.6 and 0.6 to 0.8. The spacing being 0.2 between the two and 0.2 between these two, and you can apply the Simpson's one-third rule again. You can actually work it out yourself. And also what you can do is that you can then try to play around with this, and let us use you can use only one PFR only one plug flow reactor in order to get to 80 percent conversion.

We did this correlation with CSTR. For the same total conversion, if you split it up between two CSTRs, then the total volume of CSTRs necessary is basically lower than the individual CSTR that was used for the overall conversion. In this case, here you can do the same treatment for plug flow reactor and I will not show you this will be a homework for you, you can actually show these that suppose you want to get 80 percent conversion at the end. And you are using one PFR so that your inlet your conversion is 0, outlet your conversion is 80 percent. If you integrate you get the volume, if you use to PFRs the first one the outlet is 0.4 that is 40 percent yield already achieved. The second one is 40 percent yield after this in this composition is the inlet input for the second one and outlet output is 0.8.

So, if you now split it up into two reactors to achieve the final goal of 80 percent conversion, it can be shown no matter how many PFRs split it up into the overall volume that you have to use is the same. Whether you are using sever al PFRs to achieve the same yield or whether you are using one PFR to achieve the same, the total value is the same.

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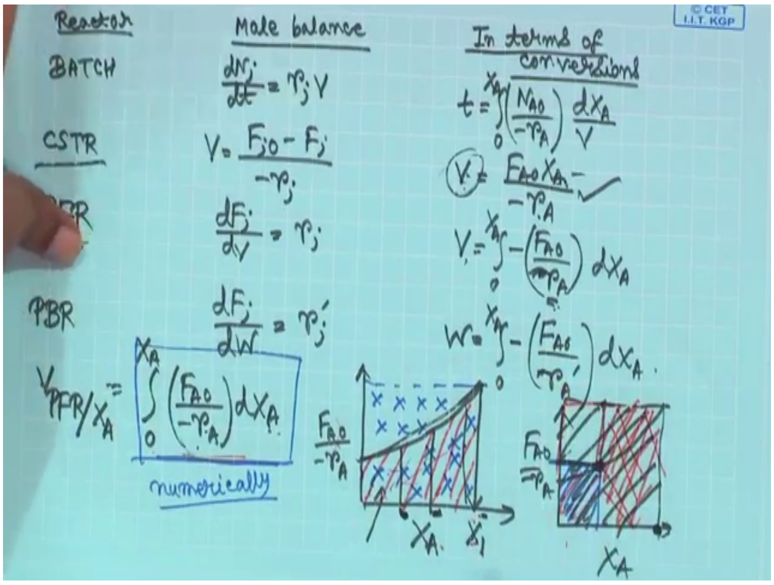

Because ultimately what you are trying to get if you look at the graph it becomes clearer for you if you look at the graph, so it is the area under the curve. So, no matter how many divisions you make. So, maybe the first PFR will give you a conversion here up to this; second PFR this is the inlet conversion I mean this is the inlet composition, and this is the outlet conversion; third PFR this is the inlet composition this is the outlet conversion. So, everything will fall under this curve. So, overall volume will be the same.

But this is not the case when you are talking about say your CSTR, because when you are talking about your CSTR if you are plotting F A 0 by minus r A versus X A, you have this kind of graph. So, this is the area under the curve, when you are using only one CSTR to achieve this conversion. If you are using more than one CSTR, suppose you are eating two CSTRs, you start with this conversion suppose. So, for the first CSTR, the area under the curve will be this. For the second one, you start with this input and you get this output. So, the area under the curve will be this. So, this total area is basically excluding this particular area that means, the total volume this area is equal to volume in this case the total volume necessary will be lower than the volume of the individuals CSTR, if you are using only one CSTR. So, graphically also you can show this thing.

So, what we will do is we will stop here today. And in the next class, we will talk about the chemical reactors a little bit more, a couple of problems we will do, may be one of the problems will be related to polymers and that is all that we will do as far as the principles of chemical reactors are concerned. So, and afterwards we will start talking about industrial preparation of polymers as the topic once we finish the talk of chemical reactors.

So, till then thank you and goodbye.