Principles of Polymer Synthesis
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Lecture – 22
Design of Chemical Reactors

Hello and welcome back to this NPTEL course on Principles of Polymer Synthesis. In the last class, we have just finished discussing about radical chain polymerizations. And basically the last class dealt with the living radical chain polymerization and principle thereof. And as promised at the end of the last class, today the topic for the lecture number 22 is the design of chemical reactors. So, this is the class where we now sufficiently deviate from what we have been talking about until now, we had been talking about the principles of really the principles through which that that govern the synthesis of polymers stay polymers radical polymers we talked about the kinetic analysis.

And we also talked about how to control the molecular weights and so on and so forth for different kinds of system. And then we also talked about when you have more than one monomers present specially for radical polymerization, how you can know the composition of the what you call as copolymers. And finally, we also said how you can narrow down the molecular weight distribution and you can specifically choose the compositions that you want you can control the compositions of polymers. And therefore, the properties of the polymers we have given several examples of that by introducing a new class of radical polymerization called living radical polymerization.

So, in this class, we start to bear of completely from what we have been talking the overall theme or it might look like to start with. So, in that we are going to talk about the principles of chemical reactors. So, the idea here is to introduce chemical reactors to you. So, reactors are basically containers or vessels in which you are doing chemical reactions that is why the name chemical reactor comes into the picture. So, what has that to do with polymers because polymers also you are preparing actually in chemical reactors. So, in order to ultimately go towards the final theme of this particular course, where it will be about elaborating on the structure property relationship of polymers. We have now until talked about how to create the structures the synthesis aspect of that we did not cover everything, but whatever we covered we covered in sufficient details.

So, afterwards the course will involve towards how the structure cofound the properties. So, again we will talk about synthesis of industrial polymers, industrial important polymers, how to create those structures and what are the properties that are coming out of those structures. So, it is then important to know a little bit about chemical reactors, the reactors in which this polymerization actually take place. So, we may not go into the details of how the polymer reactions are cofound as per as the chemical reactors design is concerned. But at least in this course we want to introduce the basics of the design principles of chemical reactors. And in order to do that, we will in general talk about chemical reactors the mention of polymer will come and intermittently at least in the initial classes.

Then we will start to talk about you know for specific chemical reactions, how you can design your chemical reactors. So, that the general design so called design equations. So, there will be some mathematics involved, but you have to look beyond that because mathematics is just a tool in this particular case in order to arrive at your goal which is to understand the chemical reactors. So, in the initial classes, it will more like what are the reactors, what different kinds of reactors that we are going to talk about. And then we are going to talk about what are the how do you design this different reactors.

Say you have a specific volume of the reactor, and you want to a particular conversion of a particular reaction say simple chemical reaction, then how do you relate the volume to that conversion. What volume you have to use to that conversion or what time, you have to use to achieve that specific conversion. And hopefully this will lay enough foundation for you to later on go on and tackle problems with polymers and chemical reactors because the foundation we will lay to some extent here although in a simplified way, but it is also mean to be introduction to chemical reactors.

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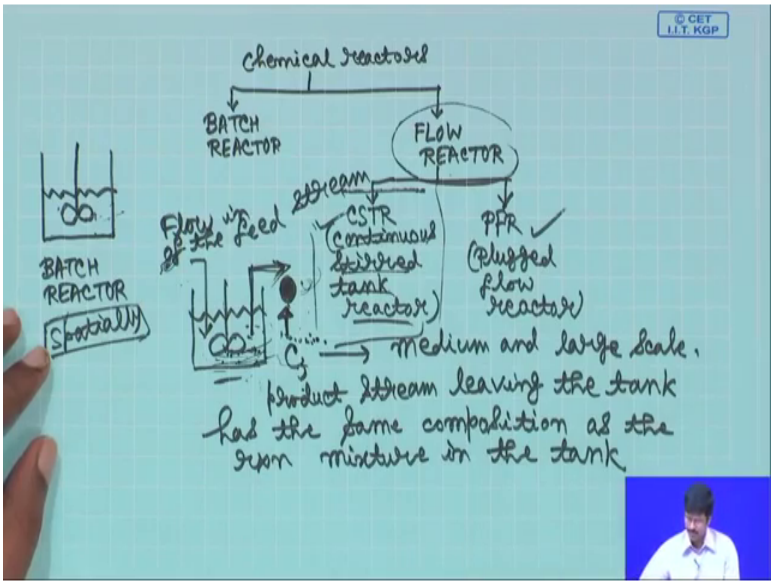

So, we will begin chemical reactors I mean in general there are different kinds of reactors. So, you can have say what you call as batch reactor and you can have flow reactor, I will tell you what some of those things actually mean. And under the purview of flow reactor we will talk about what you call as CSTR which is continuous stirred tank reactor, and then you can have say PFR which is your plugged flow reactor.

So, you might feel like some these things do not relate to the polymer at all when we go into some of the details of these the design principles by considering normal chemical reactions, but you must keep in your mind that these are the basics. So, in order to get around understand, you know what kinds of polymerizations can be done in what kinds of reactors which may not be covered in detail in this particular course except for one or two examples. Later on if you study those things, this is the groundwork for that. So, this is the very important in its own right to understand in general what the reactors mean and how to tackle the reactor problems.

So, what is a batch reactor. So, normally what you will do is say you are talking about a batch reactor or continuous stirred tank reactor, you will give this kind of symbol to that. So, let us say this is a stirrer, you can talk about mechanical stirrer, and this is a stirrer. This is your reaction mixture, and this is your container that are talking about. And something is coming in and something is going out or something may not be going out and so on and so forth.

Now, when you are looking at a batch reactor, basically this means here you have a container, so you are adding all your reaction feed reacting mixture feed into the material into the container, and then you are allowing the reaction to proceed as a function of time. So, nothing is being taken out as a function of time. So, for a specific amount of time, for a specific length of time, you do the reaction a particular conversion is achieved. So, conversion will be a function of time.

So, if you have a very well stirred reaction mixture then the concentration everywhere and the temperature everywhere will be the same as for as you know space is concerned. So, spatially your concentration and temperature they will remain the same, but as a function of time your concentration might change, and your conversion also will change because you are not taking out anything from the system, you just added and you are waiting. And after the end of the reaction, you take out your product. So, the composition changes as a function of time.

So, what you can do is that you can actually put all the components into your system in a batch reactor. So, this is called the batch reactor in the most simple term. So, you charge all the components as feed into your batch reactor. And what you do then you continue the polymerization for a specific length of time, so say 6 to 10 hours. And afterwards you take out the reactor mass and then you isolate your polymer by may be centrifugation and then you can do various verification processes and so on and so forth.

Now, what is the difference of this with a say continuous stirred tank reactor this is a kind of flow reactor. So, basically here what you have again you are putting the same symbol. So, you have something going in and continuously something is also being taken out. So, there is an inlet flow at a particular rate, and there is an flow through the outlet which is also at some rate which may or may not be equal to this rate.

So, what happens is that your reaction mixture is coming in and there is already a solution. So, reaction mixture gets immediately diluted. So, you start with some concentration here; and when you put it here the concentration becomes much reduced because it is diluted in the reaction mixture and that concentration is throughout the reaction mixture is stays the same. And if it is an isothermal system your temperature also stays the same as a function of time, it does not change. And whatever conversion you are having for a particular species if you have a mixture of species and so on and so forth that conversion also does not change with time.

So, as a function of time, what is also happening is that there is an outlet through which you are collecting out your product or whatever is flowing out from the system. So, the concentration that you are getting in the solution that you have taken out that concentration is same as the concentration everywhere inside and the conversion that you are seeing here, when you have taken out the solution that is the same conversion that is there everywhere in this reaction mixture that conversion does not change as a function of time.

And not only that the composition that you are seeing here, so let us say you may get the concentration of your reactant contradictor whatever in this outlet, whatever you have taken out, that concentration of the different species whether it is a reactant or whether it us a product that concentration or this different concentration of different species you are seeing here is basically the same in the reaction mixture all through.

So, if your jth component of the reaction mixture has a concentration C j that you have measured in the outlet that jth component has the concentration C j all throughout this reaction mixture and as a function of time that also does not change. So, the composition does not change as function of time something comes in something goes out. So, the composition does not change as a function of time. So, this is steady state situation you are talking about. And assumption under that condition only we will design the things which is different from your batch reactors say.

So, an plugged flow reactor we will talk about after. So, basically this is the batch reactor. So, batch to batch reaction may be one batch you put, the reaction is over you put another batch. So, typically this is you know the labor cost is higher, may be reactor cost is lower, but this is suitable for smaller scale reactions. You take one reaction mixture, you do the reaction, after that you put again and so on and so forth. But this is you know for big scale reaction you can it is suitable so something is going in something is coming out you can continuously go on this reactor may cost a lot, but the labor cost is much lower because this is automated process.

So, these are some of the general principles and typically you know for the flow for liquid phase flow reactions you are doing you are using the CSTR the continuously stirred tank reactor. So, reactants have been diluted immediately on entering the tank and rate of polymer reaction if you are looking at the rate of reaction, so this rate of reaction is the same throughout the reaction mixture; and that rate of reaction does not change. So, if you are doing a polymerization reaction, the rate of the polymerization is the same; as a function of time, it will not change. And it will be the same as the rate of polymerization when you are seeing outside for example.

So, the product stream, the product stream leaving the tank leaving the tank has the same composition as the reaction mixture in the tank. So, this is for medium and large-scale production, suitable for medium and large-scale production. So, this is for small-scale batch reactor. And the reactors are costly, lower level cost, all these things we have discussed because automated control. Now, so basically you have a flow in of the feed stream, these are some of the technical terms flow in of the feed stream into the reactor and flow out of the product stream out of the reactor for CSTR, PFR we will come to it after.

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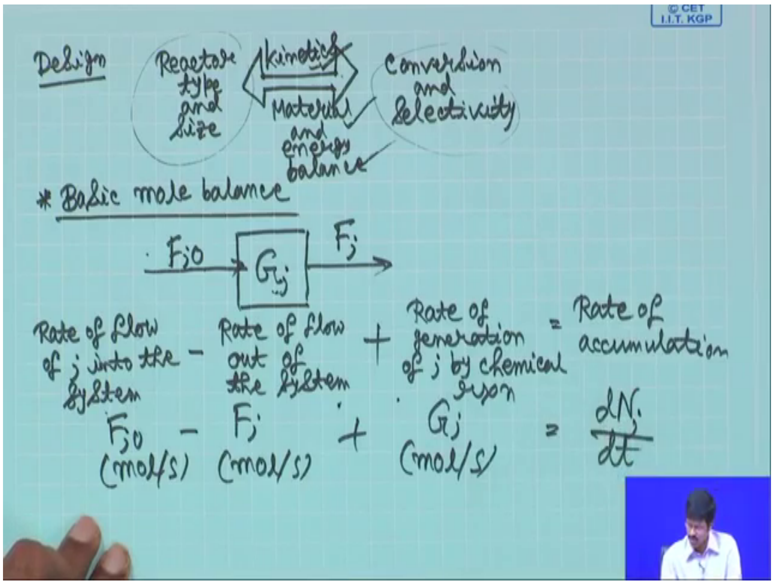

So, when you are talking about design of chemical reactors, you really talking about something like this. Let me draw something like this, reactor type and size. What kind of reactor you are going to use, are you going to use CSTR continuous stirred tank reactor or you are going to use PFR plugged flow reactor or you are going to use batch reactor? That you have to decide. What has to be the size of reactor that also you have to decide.

And you have to also keep in mind the kinetics of your reaction, you have to also keep in mind what you call as material an energy balance for simplicity we would not be talking about energy balance in this particular course on the material balance.

So, then you get what you call as conversion and selectivity. So, you want selectivity in your production of your chemical reaction as well as you want high conversion. So, in order to achieve that you have to talk about what kind of reactor you are going to use, what is the size of it, and these things kinetics material balance energy balance these things are going to determine your result. So, you design you have talked about all these things.

So, let us start with what you call as basic mole balance. So, about all these kind of reactors there will be what you call as basic mole balance equation, and I will tell you what it is in a while. So, this is your reactor, something is going in, something is coming out in general. So, F j 0, basically F j 0 is the rate of flow of j component j or species j into the system rate of flow of j you may have several components into the system. Something is coming out for that particular species, let say F j is the rate of flow out. So, rate of flow out. So, it could be mole per second amount per second, mole per second. And G j is basically let us say the rate of generation of whatever species of that particular species say species j rate of the generation. If the j is the reactant then the rate of generation this will be a negative component.

So, if you consider these things will so flow in and flow out at the rate of generation. So, rate of flow of j into the system minus rate of flow of j out of the system plus rate of generation of j by chemical reaction which happen in your reactor this is equal to rate of accumulation of j. So, just pause to think about it. So, basically something is going in. So, rate of flow inside minus rate of flow outside, so that subtraction gives you what is inside now. Now, so that is the rate of accumulation how much it is accumulating something going in minus that is something is going out plus if something is being generated then that will be the rate of accumulation everything is rate here. So, this is also rate of accumulation equal to rate of accumulation. So, this is then F j 0, this part is F j 0, this is in moles per second. This is in moles per second minus F j which is again in moles per second plus G j it could be in moles per second rate of generation of j equal to rate of accumulation as a function of time, it will accumulate.

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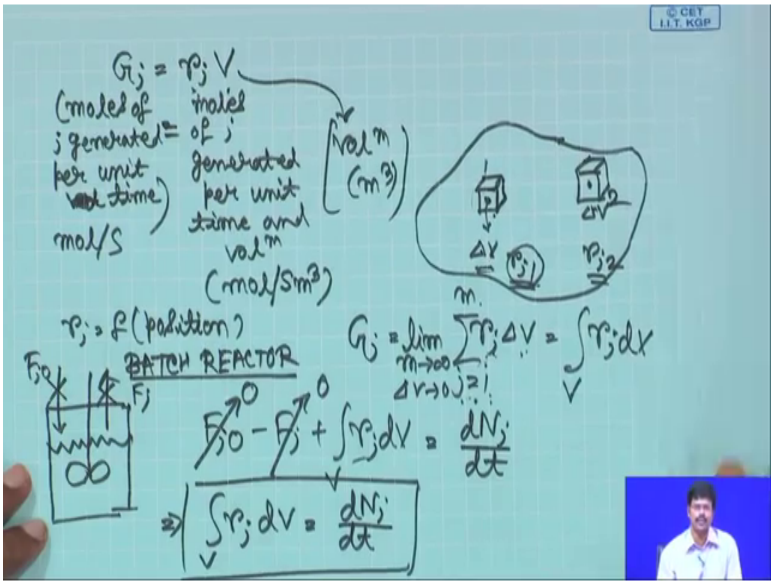

Now, if the system is uniform throughout the entire volume, then what will happen then your G j the rate of accumulation is nothing but the rate of the reaction into total volume. So, let us say this G j is moles this G j is moles of j generated species j generate per unit time. This is not that difficult actually. If you follow the logic am trying to make it as simple as possible, but not too much simple that is unwarranted. So, this is moles of j generated per unit time that is mole per second that is equal to r j which is moles of j generated per unit time and volume. So, that will be moles per second meter cube at the bottom into V is equal sign into V, V is the volume in meter cube. So, the units are also matching.

Now, what can happen is that this rate that you are talking about. So, this is rate of generation j by chemical reaction, it has this component r j that you are talking about. This r j it could be a function of position because we are saying uniform throughout. If it is not uniform throughout, then what will happen is that at different points, this r j that is rate of generation per unit time and volume that will change at the different points. Then how do you modify this particular equation? Now, how it can change at different points, suppose your temperature is varying at different points, local hotspots are generated then this rate of generation may change. And not only that suppose the concentration of the species is varying at different points, because it is not stirred uniformly, then also the rate of generation per unit time per unit volume will vary. So, in that case, this r j is not constant throughout V.

So, what you can do is that you can take your sample, and you can create this kind of areas around this. So, this volume this volume is delta V around the point at which the rate is r j 1 say the point is one point is one. You start with a point where the point you designate as 1, and there the rate is r j 1 that is rate of generation per unit time and volume. And let us consider a small volume element delta V around that. So, in that volume, this r j 1 is constant in this small volume.

Similarly, if you take another point, which is point 2, there the rate is r j 2. So, you can also construct a small volume around that delta V in which this r j 2 is constant. So, likewise in this small volume all these volumes you have to add in order to get the overall generation. So, ultimately your G j will be r j into delta V, because r j into V you have talked about, so that is r j into delta V. So, in this small volume r j is constant. So, you can write r j into delta V. What is this j, this j varies from 1 to m, where your limit m tends to infinity, delta V tends to 0.

So, infinite number of such points if you are talking about, so j equals to 1 to m, so it goes from 1 to infinity. So, infinite number of points, so infinite number of r j values correspondingly to the j point and infinite so your delta V is very, very close to 0, because the rate otherwise will changes as you go away from this particular point. And then you just add data; basically it is nothing but integral over the whole volume r j dV. So, d j equals to r j into V, but if the composition is not uniform let us say a temperature is not uniform then your moles of generation moles of j generation per unit volume and unit time will change from point to point. And then you have to actually integrate over the whole volume this r j could be some function of this, and then because r j may not be independent of volume. So, r j will b some function of V. If you know the functional form then you can integrate and this becomes your overall expression.

So, now if you are looking at the batch reactor, now you are prepared to design reactors. So, if you are looking at a batch reactor, what will be the design equation of these batch reactor. So, this is how I will draw the batch reactor. So, you have a stirrer, you have some reaction mixture something going in something coming out. Now, nothing is going in and nothing is coming out, because we have put everything together. So, there is no you know rate of flow that is only valid for flow reactors. So, this rate of flow of j into the system, this is 0. Rate of flow of j out of the system that is also 0, because nothing is coming out as the reaction is progressing, only these two terms remain.

So, your F j 0 that is not happening F j is also not happening nothing is coming out. So, this equation is F j 0 minus F j plus integral V r j d V that is rate of generation, so that will be equal to rate of accumulation d N j dt as a function of time. Now, this is zero and this is zero, so your design equation becomes integral V r j dV. With time it will become clearer because we will go step-by-step to deconstruct this particular systems and try to correlate with how may be with normal chemical reactions it is related and probably with polymerization processes also then you can relate after. So, this is then the design equation of the batch reactor.

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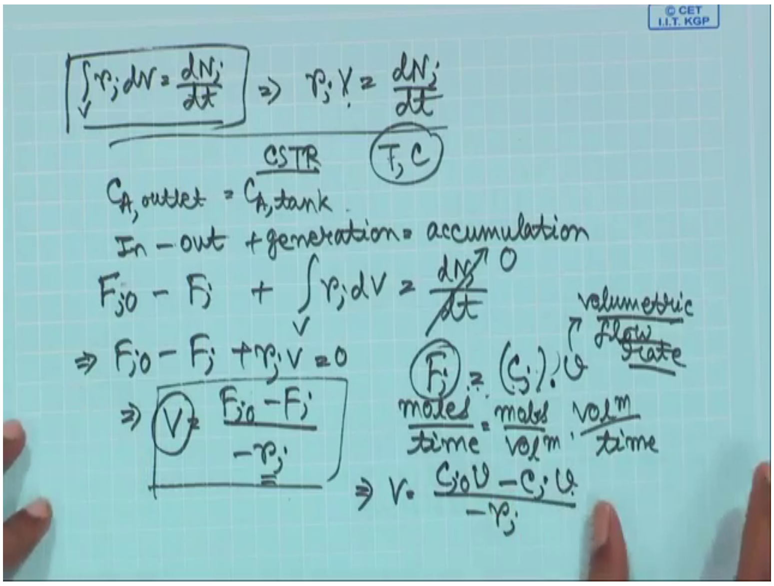

So, design equation is this r j dV equals to d N j dt. If you have a perfect mixing, so what will happen is that the batch reactor, then the temperature, concentration and the reaction rate will be constant throughout your reaction mixture as a function of space. You see when you are having a batch reactor, everything is there as a function of time concentration is changing; as a function of time, a temperature might change; as a function of time, there your reaction rate also will change. But we are only considering specially that means, at different point of the reaction mixture at a particular time. If you are mixing it very well enough then the temperature is constant all throughout at a particular time.

Temperature composition is also constant; reaction rate is also constant. So, then what will happen is that your this expression this becomes equal to r j V equals to d N j dt, then you can take out this integral because you know if r j does not vary with different points means point to point then this is the equation. If it varies then you have the integral. So, this becomes a design equation; so if you come to continuous stirred tank reactor, this is basically an open system, you are continuously adding reactants, and you are removing the products which also will contain some unreacted reactants and so on and so forth.

So, temperature and concentration they are constant specially as well as with time we are considering only isothermal situation; there could be adiabatic situations we do not go in to that kind of complexity. So, the concentration of any other species, it could be reacting species, it could be product species at outlet is equals to concentration of that in the tank which are steady state situation we are talking about. So, this is a steady state situation, and the reaction rate does not change with time. And reaction rate is also spatially constant point to point everywhere it is constant.

So, basically mole balance equation so in a abbreviated way you can say in minus out plus generation equals to accumulation. So, this is the rate at which the component j is entering, this is the rate at which it is going out. And this is the generation rate r j d V. And there is no accumulation, continuously stirred tank reactor things going in things coming out there is no accumulation that why the concentration is not changing of all the species whether it is reactant or a product inside the reactor it is not changing. And also whatever outward stream is there it has the same composition as the reaction mixture composition. So, this particular equation so d N j dt, so this is 0.

So, then you will have F j 0 minus F j and now let us say if it is uniformly stirred then it becomes r j v like this here equals to 0, then ultimately you will get v equals to F j 0 minus F j divided by minus r j . So, basically this is the rate at which the j is generated as a per unit time per unit volume. So, if it is j is being taken up then this will continue minus sign and so on and so forth inside that minus sign will be there, but this is the general term whether it is a reactant or a product and so on and so forth.

Now, this volume basically is the reactor volume that is required to reduce the entering flow rate of the species from F j 0 to the outgoing flow rate F j. So, F j is basically lower than F j 0. So, the flow rate will be reduced as it passes through the volume. Now, this F j is basically the unit is mole per time whether it is through inlet inward stream or outward stream, so that is equal to your concentration of that particular species whether it if it is F j 0 then it is C j 0 and so on and so forth this into small v. Where v is the volumetric flow rate, v is the volumetric flow rate, which is nothing but volume per unit time and concentration you know is moles per unit volume. So, you see the units match.

So, F j the rate of flow in or out, you can equal to so if it is rate of flow in that is equal to the concentration in the of the particular species in the flow in. Means in the stream that is flow in the concentration of that particular species into the volumetric flow rate which is say volume per second, say this much ml per second or meter cube per second. So, if you just replace that here your v becomes equal to C j 0 v minus C j v, let us assume that the volumetric flow rate in is equal to volumetric flow rate out minus r j. So, this is the design equation.

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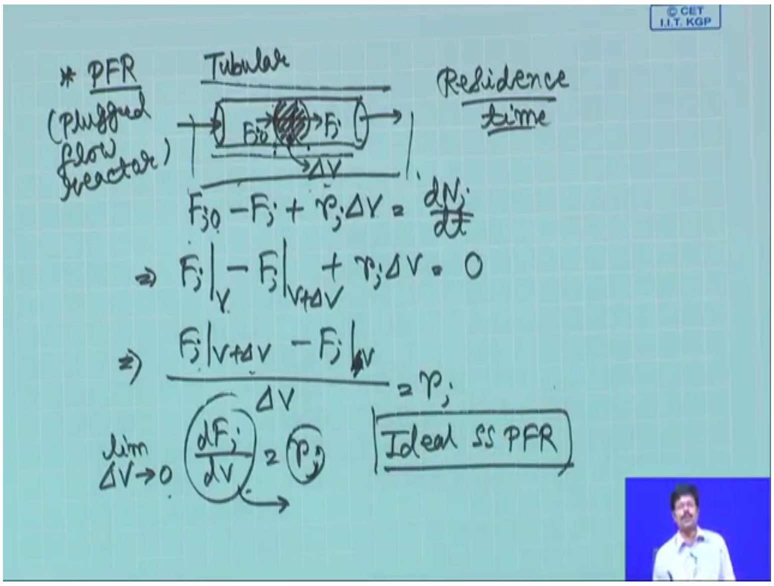

So, finally, in the concluding part of this particular lecture, what we will do is we will conclude by talking about the design equation for plugged flow reactor. We did not yet tell you what is plugged flow reactor. So, this is basically your plugged flow reactor is basically a tubular reactor, and it is a cylindrical pipe which has opening on both ends cylindrical pipe. And there will be steady movement of material down the length of this reactor something comes in, something goes out. And there will be no radial variation of temperature concentration of the reaction rate radial variation means variation in this direction, but in this with a length things can vary, but in this direction there is no variation of temperature concentration or reaction rate. In all the components of the same time, they reside in the particular chamber for the same time which is called a residence time of course, residence time of all the components residence time of all the components is basically the same.

So, now, let us consider a small volume element inside here. So, the differential volume being delta v, and it is flowing through the material is flowing through this. Now, of course, the composition is varying through the flow path, but it does not change along the radial direction. So, what about the mole balance equation for this. If you just look at this particular element for that mole balance equation is F j 0, so here it is entering F j 0, here it is going out F j from this particular volume. So, F j 0 minus F j in minus out plus rate of formation over the volume delta v small volume element and this is the rate of accumulation. So, nothing accumulates. So, this will be 0.

So, basically you are talking about the value of flow at V flow in I mean am just taking out the zero because the F j in general I am putting here at the point where it is entering here at the point value v and this is V, and this is V plus delta V. So, this volume is delta V. So, V minus what is coming out at volume V plus delta V which is on this side plus r j into delta V equal to 0, because there is no accumulation. So, then F j V plus delta V minus F j V divided by sorry delta V divided by delta V. So, V plus delta V minus so this will be v sorry by delta V equals to r j.

So, if you take it in a differential form limit at which delta v tends to 0 that will be equal to d F j dV equals to r j. So, this is your ideal again this are all steady state condition we are talking about that your composition does not vary along the radial direction. The same way the steady state condition CSTR tells you that the concentration reaction at composition does not vary with time throughout the reaction mixture. So, this is your ideal. So, this is your design equation for ideal steady state plugged flow reactor. So, this is called plugged flow reactor. So, you can see that the degree of completion of the reaction which is given by this r j that is only affected by the volume of the PFR.

So, what we will do is we will stop here because our time is up. And in the next class, we will continue with talking about the design equations. Again we will see that there is some mathematics involved, but again as I told you, you should look beyond that you have to try and understand. Once you understand the equation by a physical meaning then the complexity of the equation is greatly reduced, and always try to correlate how I can use this in design, when you come to particular chemical reactions, we will see step-by-step, how you can design the chemical reactor for that in a good way so that ultimately it will be a general thing that you can use for normal chemical reactions, you can make your own way of calculating these things, and tackle the problem.

So, until the next class then thank you and goodbye.