Principles of Polymer Synthesis

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Lecture – 23
Design of Chemical Reactors (Contd.)

Welcome back to this NPTEL course on Principles of Polymer Synthesis. In the last class, we started talking about the design principle of chemical reactors. And we ended the class by talking about the general very simplified design equations of three of the reactors, batch reactors and then two kinds of flow reactors, one is continuous stirred tank reactor and another is plugged flow reactor. So, we will continue in the same again today. So, the topic of today is the continuation of the design of chemical reactors the principles.

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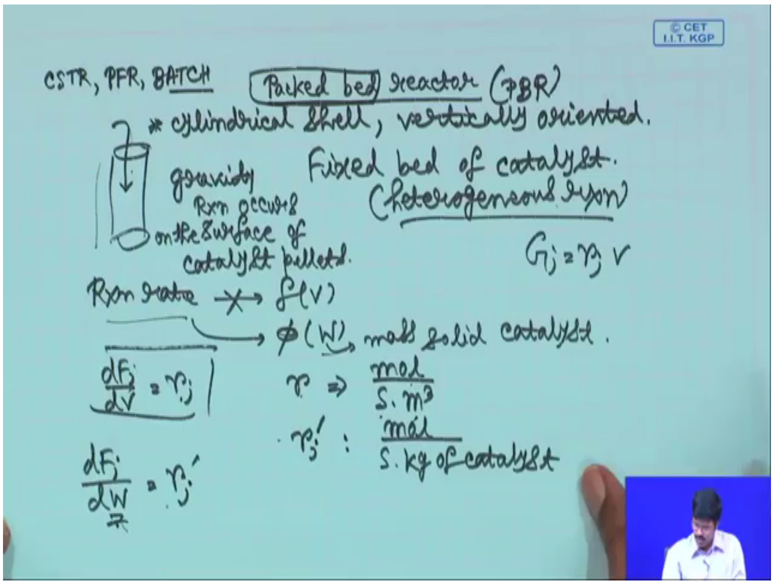

CSTR, PFR, BATCH

Packed bed reactor (PBR)

* cylindrical shell, vertically oriented.

gravity

Fixed bed of catalyst.

(heterogeneous rxn)

Rxn occurs on the surface of catalyst pellets.

$G_j = r_j V$

Rxn rate $\cancel{\rightarrow} f(V)$

$\rightarrow \phi(W)$, mass solid catalyst.

$\frac{dF_j}{dV} = r_j$

$r \Rightarrow \frac{mol}{s \cdot m^3}$

$r_j' : \frac{mol}{s \cdot kg\ of\ catalyst}$

$\frac{dF_j}{dW} = r_j'$

So, we have talked about design principle of CSTR, CSTR the plugged flow rector, the batch reactor. Today, we are going to talk about start talking about the design principle of packed bed reactor, we did not introduce this at all when we classified the reactors before, but now I am going to tell you this is also a kind of flow reactor other than your CSTR and PFR. So, packed bed reactor this is PBR. So, basically you have a cylindrical shell cylindrical shell which is vertically oriented. So, you have a vertically oriented shell and you are so you have a shell like this. And your flow is often driven by gravity and this is called a packed bed because there is a fixed bed of catalyst inside there is a fixed bed of catalyst inside.

So, the reaction occurs the catalyst will catalyze the reaction, the fixed bed of catalyst is there so that is why the name the packed bed. So, obviously, then this is a heterogeneous reaction unlike your homogeneous reaction for example, in CSTR if you have a liquid homogeneous reaction that you are doing you generally CSTR continuous stirred tank reactor. If you have a gas that you are gas reaction, if you are having a gas that you are doing a reaction say you are using ethylene, you are making a polymerization polyethylene then you can use a plugged flow reactor. Typically for gases you will use that flow react that that kind of flow reactor, and for liquids you use CSTR homogeneous.

Now, for PBR packed bed reactor it is a heterogeneous reaction. Now, reactants enter from the top and they will flow through the catalyst bed. And of course, there will a concentration radiant and the reaction will occur on the catalyst on the surface of the catalyst pellets. So, reaction occurs on the surface of catalyst pellets. And the reaction rate you have seen the reaction rate is a function of volume for plugged flow reactors; allow me to show you the previous page here. So, reaction rate is a function of volume in the plugged flow reactor. Here the reaction rate basically is not a function of volume of the reactor, but it is a function of the mass of the solid catalyst the mass of the solid catalyst.

So, if you are looking at the mole balance equation it was dF j dV equals to r j for the plugged flow reactor, where your r the unit of r was moles per second meter cube. So, that was the unit because this is rate of generation per unit time per unit volume if you remember, your G j was equals to r j into V and so on and so forth.

So, now for catalytic reaction, because this is a catalytic reaction, you are defining another rate of generation where you are using basically the unit as moles per second per kg of catalyst instead of meter cube you have a kg they are of the weight rate. So, ultimately instead of this your design equation will become d F j d W equals to r j prime just to differentiate this r j with that in general when you are writing design equation you can just write r j, but overall then w is the weight of the catalyst. And that is why it depends not on the volume reaction rate actually depends on the weight of the catalyst.

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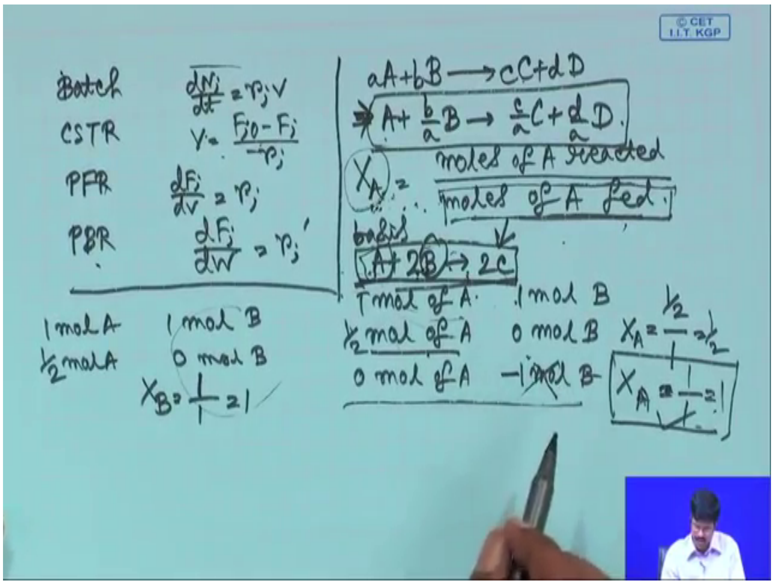

So, to summarize up to this part what we have is this thing, so you have the kind of reactor which is batch reactor, you have say CSTR, you have plugged flow reactor, and you have packed bed reactor. So, if you are doing the mole balance, the mole balance for the batch reactor is d N jd t equals to r j V uniformly start let us say. CSTR is V equals to F j 0 minus F j divided by minus r j. PFR is d F j dV equals to r j, and PBR is d F j d W equals to r j dot.

Now, one thing you have to keep in mind in actuality when you are doing the reactions, you have to look at the conversion. Here all these design equations, they do not contain the term conversion, you want a particular conversion, then you want a particular volume. Let us say if you are looking at the CSTR, CSTR is equal to flow rate in minus flow rate out divided by rate. Here we do not have the information of conversion in this particular form. So, ultimately then you have to mould your design equation in such a way that it will contain that information of conversion.

Now, again we will here a little bit away from chemical reactors at the moment. So, what is conversion. So, when we talk about conversion suppose a molecule A is reacting with another molecule B two different reactants and then it is producing say C plus D on the basis of which component you are going to calculate the conversion that is a question, whether on the basis of component A or on the basis of component B. So, to start with we will try to have a look at that particular question.

So, let us say you are talking about this reactant. And as I told you it may at times appear as it is not a class of polymer at all, it is a class of simple chemical reactions and physical chemistry, but it is not true things are actually inter related. And we are talking about the basic principles, laying the foundation of the design of chemical reactor. And for that we have to start from the most basic level and that is what I am doing; just to make things much more easily understandable for you. So, just bear with me.

So, this the reaction let us say you are considering these particular reaction. So, A equals b by a B c by a C d by a D. So, if you are so the conversion based on A as the basis is equals to moles of A reacted divided by moles of A fed. So, for a batch, so if you are defining the conversion on the basis of A then it is this. What is the moles of A fed? So, for a batch system this moles of A fed is basically equal to the amount of A at time 0; to start with whatever amount of A is there that is the mole of a fed for batch system. For flow system, for example, CSTR or PFR or PBR, this moles of A fed is basically equal to the amount of a entering the reactor see this difference you have to keep in mind.

So, flow in so amount of A that is coming into the reactor that is the moles of A fed, but as such you are not feeding anything into the batch reactor everything is inside when you are starting the reaction, so basically that will be the moles at times 0, V equals to 0 that is the denominator then.

So, let us say you are talking about this particular reaction A plus 2 B equals to 2 C. So, for this the conversion you will define on the basis of A or on the basis of B. Let us say you define on the basis of A, then you start with 1 mole of A and 1 mole of B. So, now, when half a mole of A has reacted then you have half mole of A, and since one mole reacts with two moles, so basically half a mole actually already has reacted with one mole of B, so you basically now have 0 mole of B. So, what is the conversion at this point moles of a reacted which is half divided by total number of moles fed to start with that is half.

What happens when you go to 0 mole of A? So, another half mole has reacted, so basically another one mole of B has to react. So, this becomes minus 1 mole of B and your X A then will become, so moles of A reacted 1, moles of A starting is 1, so this is one. So, when you are talking about extent of conversion you have to look at you have to choose that particular reagent that particular chemical as the basis for which you can go to 100 percent conversion, because 100 percent conversion is the physical reality. So, when you coming to the equations you have choose that particular reactant as the basis for which your conversion could actually go to 100 percent.

So, if you look at that this taking the A as the basis does not work, because you cannot go to you cannot actually formulate a situation where your conversion is 100 percent because this is unrealistic situation. So, you have to take B as the basis. If you take B as the basis again you start with 1 mole of A and 1 mole of B then when it becomes half a mole of A you already have 0 mole of B and that actually tells you the conversion is full 1 mole has reacted divided by 1 mole you started with, so this is 1. So, basically in this particular situation you have to take B as the basis to calculate conversion and not A; otherwise you will be wrong.

And basically here your B is the limiting regent your B is in higher amount with respect to this unit more amount of B. So, B is your limiting regent. So, in whatever reaction you are tackling, when you are trying to find the conversion now you know this in this particular question is important because we are trying to put this conversion into the design equation then only we start to gain an understanding how much conversion for how much conversion, how much volume for example, here is required. So, in order to then calculate the conversion we have to find out what is the limiting regent with respect to that in this case B is limiting with respect to that you have to then define conversion. So, in this case for this particular reaction you define the conversion with respect to b and not with respect to A; otherwise, it will be wrong.

So, the next step then will be to express the other components. Now, you again go back to A, we will go back to this general expression and let us assume that A is the limiting regent because we are not putting what is small b what is small a and so on and so forth. So, if we have a conversion with respect to A, considering A is limiting regent which is not this example this is specific example then we have an expression of X A that we are getting. Now, what we have to also do is that the other components, components B, C, D all of these components the amount of those component you have to express in terms of that X A that is the extent of conversion. All of those components you have to express in terms of X A that becomes important when you are designing when you are trying to find out if you are using a particular reaction for a particular reactor. Then what kind of yield you can expect at what kind of time say if you are talking about batch reactor and what volume when you are talking about CSTR. So, things hopefully will become clear with time.

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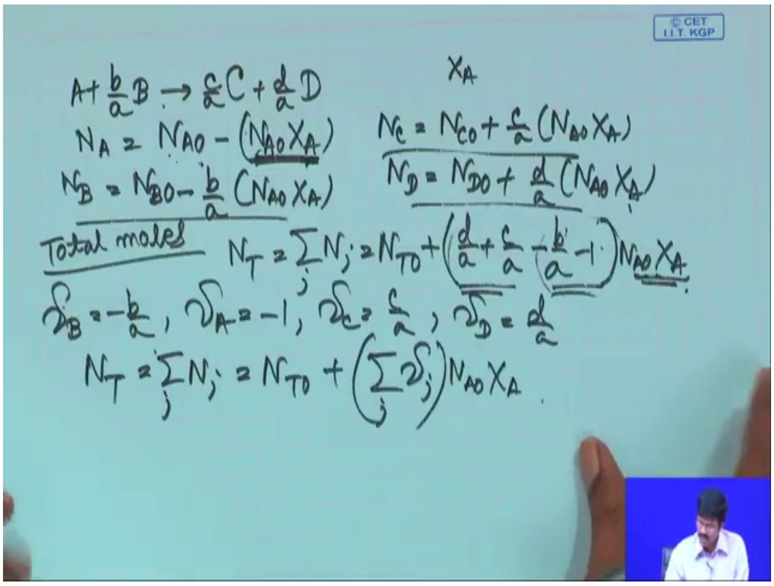

X_A

$$A + \frac{b}{a}B \rightarrow \frac{c}{a}C + \frac{d}{a}D$$

$$N_A = N_{A0} - (N_{A0}X_A)$$

$$N_B = N_{B0} - \frac{b}{a}(N_{A0}X_A)$$

$$N_C = N_{C0} + \frac{c}{a}(N_{A0}X_A)$$

$$N_D = N_{D0} + \frac{d}{a}(N_{A0}X_A)$$

Total moles $N_T = \sum_j N_j = N_{T0} + \left(\frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1\right)N_{A0}X_A$

$$\nu_B = -\frac{b}{a},\ \nu_A = -1,\ \nu_C = \frac{c}{a},\ \nu_D = \frac{d}{a}$$

$$N_T = \sum_j N_j = N_{T0} + \left(\sum_j \nu_j\right)N_{A0}X_A$$

So, now, the next step is to express other components in terms of X A that is the conversion with respect to A. So, in terms of X A, we are trying to express this thing. So, let us say you are again taking this general reaction, this is your general reaction. Now, if you are looking at the moles of A at time t that is equals to the moles of A at time 0 that is moles of A that is fade minus this term, this is the moles of A that has been consumed. Similarly, you can also find out, so I am trying to find out the amount of all the other species in terms of the conversion, which is X A which will be extremely useful afterwards. So, this is N B 0 minus b by a into N A 0 X A same way your N c will be N c 0 plus c by a into N A 0 X A and N D will be N D 0 plus d by a into N A 0 X A. So, this something for a if you are looking at for example, a batch reactor or if you are looking at for example, a CSTR then this things will be useful after.

So, from here then the total moles whatever is the total moles total moles of all the species at time t total moles at time t is N T equals to sum of j all the species N j equals to total moles to start with total moles fade plus d by a plus c by a minus b by a minus 1. So, these all are one the coefficient say for the reaction into N A 0 into X A. So, this is the total moles at time at t. So, this is the total moles of product formed this into this and this is the total moles of reactants consumed total moles of reactant consumed is b by a into N A 0 X A plus N A 0 X A consumed. So, this is subtract.

So, your Stoichiometric coefficient of B is minus b by a, of A is 1 minus 1, of C is c by a, and the Stoichiometric coefficient of D is d by a. So, these are nothing but Stoichiometric coefficients. So, in general then your N T will b equal to sum of our N j will be equal to N T 0 plus sum of our j means all the Stoichiometric coefficients you add up into N A 0 X A.

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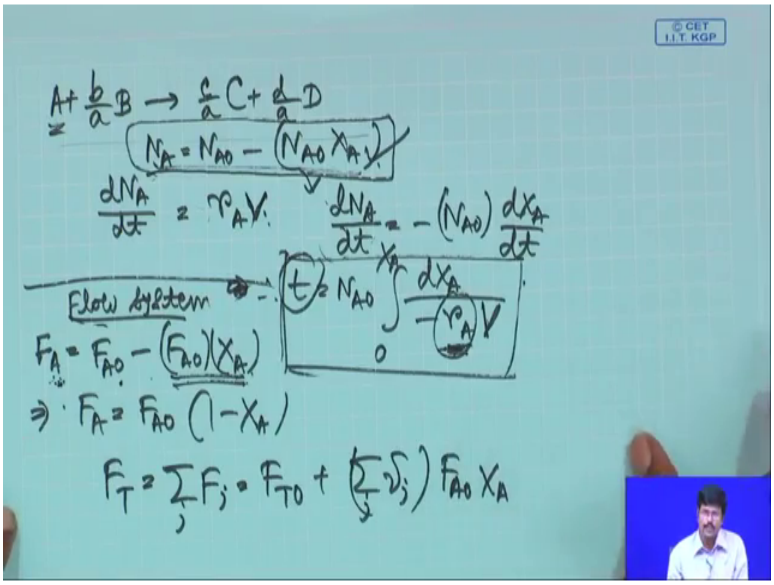

$$A + \frac{b}{a}B \rightarrow \frac{c}{a}C + \frac{d}{a}D$$

$$\boxed{N_A = N_{A0} - (N_{A0}X_A)}$$

$$\frac{dN_A}{dt} = r_A V \qquad \frac{dN_A}{dt} = -(N_{A0})\frac{dX_A}{dt}$$

Flow system

$$\boxed{t = N_{A0}\int_0^{X_A}\frac{dX_A}{-r_A V}}$$

$$F_A = F_{A0} - (F_{A0})(X_A)$$

$$\Rightarrow F_A = F_{A0}(1 - X_A)$$

$$F_T = \sum_j F_j = F_{T0} + \left(\sum_j \nu_j\right) F_{A0} X_A$$

Now, what will be the batch reactor design equation in terms of conversion? So, if you are looking at this particular reaction, for this particular reaction let us say the conversion is X A. So, then in terms of conversion what is the batch reactor design equation. . So, let us say you are saying the conversion is in terms of A, A is the basis. So, you are defining the conversion in terms of A for this particular reaction. Then your N A at anytime whatever amount of species is there is N A 0 minus N A 0 this will only be told N A 0 into X A. Now, the batch reactor design equation is nothing but d N A dt equals to r A V well we talked about that rate of accumulation is equals to rate of the reaction because nothing is going in nothing is coming out.

So, you might as well ask the question then how long you want to leave the reactants in the batch reactor in order to get a certain amount of conversion that is the question that is related to the same question in which you are trying to formulate your design equation with respect to the conversion. So, if you now differentiate this with t as a function of t I mean with respect to t that is the right word, so d N A d t. So, this is constant that goes, so that will be equal to minus N A 0 into d X A d t. So, ultimately if you into d X A dt that will become. So, d N A dt is r A V. So, if just replace that and if you integrate after your t the time N A 0 0 to X A into d X A minus r A V. So, this is the design equation.

So, if you want to have a conversion of X A for this particular reaction, and your rate of reaction is r A, rate of reaction with respect to say if you are looking at A, the disappearance of A if it is r A, and this is the total volume of the reactant then the time taken for this conversion is this. So, in terms of the design equation, you know then why it is useful to formulate the design equation in terms of the conversion.

Now, what happens in case of a flow system, this was a batch system. So, if you are looking at the flow system this is in general true for all say for example, CSTR or PBR or PFR. So, if you are looking at the flow system then you can write down the equation the same way instead of N a equals to this, you can write down F A equal to F A 0 minus F A 0 into X A. So, this is the molar flow rate of A leaving the reactor molar flow rate because moles per second, molar flow rate of a leaving the reactor this is the molar flow rate of A fed into the reactor minus this into X A just analogous to this X.

So, this is basically the molar rate of consumption of A. So, this becomes to then equals to F A is equals to F A 0 into 1 minus X A. So, in general then just the same way as we treated this thing, so you can now see already that this is for the batch reaction the particular treatment was for the batch reaction. For the flow reaction, this will be replaced by the flow. The same way if you treat this you will get the general relationship which is total flow is this F T 0 plus sum of a j nu j into F A 0 into X A.

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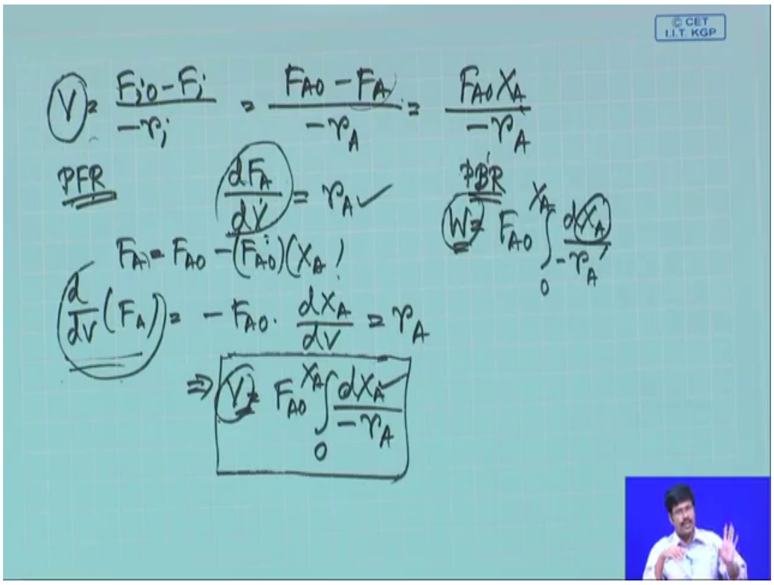

$$\boxed{V} = \frac{F_{j0} - F_j}{-r_j} = \frac{F_{A0} - F_A}{-r_A} = \frac{F_{A0} X_A}{-r_A}$$

PFR

$$\frac{dF_A}{dV} = r_A \checkmark$$

PBR

$$W = F_{A0} \int_0^{X_A} \frac{dX_A}{-r_A}$$

$$F_A = F_{A0} - (F_{A0})(X_A)$$

$$\frac{d}{dV}(F_A) = -F_{A0} \cdot \frac{dX_A}{dV} = r_A$$

$$\Rightarrow \boxed{V = F_{A0} \int_0^{X_A} \frac{dX_A}{-r_A}}$$

So, if you are writing the mole balance then for CSTR, the mole balance for CSTR is nothing but F j 0 minus f j divided by minus r j the general mole balance that we had derived that is equal to F j 0 is nothing but F A 0 for the species A minus F A divided by minus r A. So, the V, so if you now replace F A with this particular expression, so if you replace that, so ultimately your v becomes equals to F A 0 into X A divided by minus r A. So, this is the ideal CSTR design equation steady state situation in terms of your conversion.

So, this volume is the CSTR volume required to achieve a conversion of X A. Again to recall CSTR is your flow reactor one of the kinds of flow reactors that is your continuously stirred tank reactor. So, this is the expression then. And what is the expression for PFR - plugged flow reactor for example, again you can derive this for yourself. This is the general design equation for plugged flow reactor; if it is packed bed, it will be d F A d W. Now, if it is plugged flow this is d F A d v, so that is equal to r A.

And F A again for all flow reactors in general we have already shown you this thing. So, F A is nothing but F A 0 minus F A 0 into x A. So, here d d V of F A will give you minus F A 0 into d X A d V, so which is nothing but r A. So, and then if you integrate after what you will get is that V equals to F A 0 integral 0 to X A d X A divided by minus r A, you cannot avoid this kind of calculations so in your designing chemical reactors. So, it is better that you introduced now to it, if you are planning to take further courses on chemical reactors after in a more detailed way, so this is important.

So, this is the design equation of PFR in terms of the conversion for the PBR you can derive for yourself for PBR that is the plugged that is the packed bed reactor that will be w equals to F A 0 similar to this 0 to X A d X A divided by minus r A dot, so that will be w, and here it is V. Because the conversion depends on V volume for the plugged flow reactor, but conversion depends on the weight of the catalyst for the packed bed reactor, so that is that.

So, what we have done now is to derive the design equations until now to derive the design equations in terms of the conversion, and we also gave you a concept of how to calculate the conversion. So, whatever reaction you are talking about, when you are looking at the conversion you should look at the limiting regent. With respect to that we have to calculate the conversion because if a is reacting with b you can have two kinds of conversion that you can define one is with respect to a that is amount of a consumed divided by amount of a that you started with if it is the batch reactor. Or it is the amount of a consumed divided by amount of a fade in case of a flow reactor or you could do the same for your a regent b, but in one of them the calculation will be wrong because one of them will be basically the limiting regent.

So, if one of them is the limiting regent, you will use that particular regent on as the basis of calculating the conversion; otherwise the calculation will be wrong. And then we showed you to simple calculations how the design equations will ultimately reduce to an equation your general design equation. So, it will ultimately reduce to equation in which you have the term of conversion. So, with respect to conversion, you can correlate the volume of the reactor or say volume of the reactor when you are talking about a say for example, the flow reactor say CSTR, your continuous stirred tank reactor or volume of the reactor say if you are talking about another kind of flow reactors say plugged flow reactor. You can relate to weight of the catalyst when you are talking about packed bed reactor or you can relate the conversion to the time when you are talking about batch reactor everything is inside. So, as a function of time your conversion will evolve.

And as I told you your conversion does not change as a function of time when your say for example, talking about CSTR. Whatever conversion you are getting whatever species you have say when you are talking about species A, if this A is basically a reactant that you are feeding then there is a flow rate in for that reactant and then there is a flow rate out because all the A is not reactant let us say. And then there is a particular conversion this conversion does not change as function of time; this conversion does not change in an ideal steady state CSTR as a function of space that means, everywhere conversion will be the same. Now, if A is your product, so they are starting stream does not contain A. So, in that case, your starting stream, so F A 0 that means, the molar flow in of A is 0. So, accordingly you put your mole balance in general there will be some molar flow rate in and there will be some molar flow rate out.

So, now let us see how this particular thing could be useful for us. So, what we would have done here. So, this equation is important let us start with say CSTR. So, your volume is related to conversion, so for this kind of this amount of conversion you want take this volume. So, let me ask the simple question what is the volume of CSTR required to achieve this specific conversion of X A.

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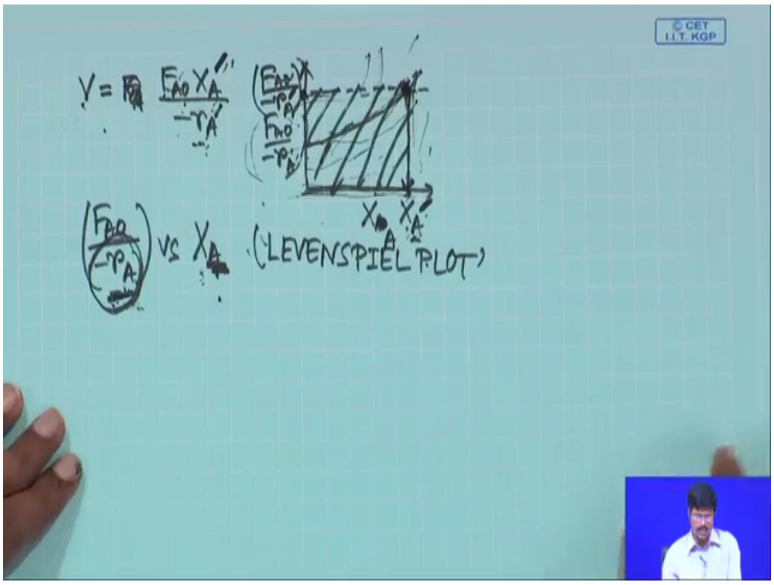

So, let me write down this particular equation again v equals to F A v equals to F A 0 into X A divide by minus r A. So, what is the volume of CSTR necessary in order to have a specific conversion of X A. So, what you will do in order to find that out. If you plot F A 0 by minus r A as a function of X A, so you will get this kind of plot as a function of X lets say or X A. So, am just putting it as X A dash. So, at a specific X A value of X A dash what is the value of V. So, let us say on this particular curve this is the point at which you have conversion of X A dash.

Then if you are completing this particular rectangle here if you let us say you complete this particular rectangular here then what is the value of F A 0 minus r A at X A prime or X A dot that value is this value. So, at this point, the conversion is X A prime; and at this point the value of this plot this thing this value is this. So, here it is F A 0 by say minus r A prime F A 0 is constant, and your rate of the reaction may vary with conversion. So, then let us say I am putting minus r A prime here. So, this F A 0 by minus r A this will take specific value of F A 0 by minus r A prime at a conversion of X A prime.

So, this parallelogram, so ultimately this not parallelogram excuse me wrong choice of word this rectangle that you have if you take the area of this rectangle that will be this length into this length this length into this length, so that is this F A 0 into X A prime divided by minus r A prime in this case. So, at a particular conversion if you are looking at particular conversion, you plot so the idea then to summarize this here.

The idea is if you plot F A 0 by minus r A versus X A conversion this is called this kind of processes are called Levenspiel plot. So, if you plot this then the area of the rectangle with a base X A and with a height F A 0 minus r A will give you the volume of the CSTR necessary for that specific conversion X A. So, if you are targeting a conversion of X A prime, then you take the area of the rectangle with the base X A prime and the height F A 0 by minus r A prime because F A 0 by minus r A prime is the value of F A 0 by minus r A at a specific conversion of X A.

Remember F A 0 does not change molar flow rate in does not change. However, the rate of the reaction of a whatever, so rate of generation of A or whatever destruction of A depends on whether it is reactant or product that may vary with conversion. So, that is why you have the graph that is going like this, it is not a horizontal line like this. So, it is changing. So, this ratio changes with conversion. So, you construct the speller that that rectangle and the area of that rectangle will give you the volume

So, finally, what I will do is let us say before I complete this particular class I will try to impress upon you this particular fact that as I told you r A this values this can vary with conversion. So, in order to construct this particular plot that means, for every X A to get the corresponding value of this or in other ways to know the nature of this function how it is going up like that or which way it is going up it is going up like this or it is going up like this, you need to have the rate of the reaction, you have to express that you have to know the rate of the reaction in the functional form as a function of the conversion. Once you know that only then you can for all the values of X A different values of X A you will know this particular value. Because F A 0 you know and if you know the value of r A, if you know the r A as a function of X A, then you can plot this particular graph and you know this value.

So, in the next class, we will start with developing this concept little bit more because the time is up for this class. So, we will talk about we will keep talking about the chemical reactors then in general, and we will start with this particular concept again.

Till then thank you and goodbye.