Advanced Chemical Reaction Engineering

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Lecture - 32
Population Balance Modelling – II

We talk about population balance modelling today. You know the background to population balance of modelling is that we have in our process industry, where we have to deal with particulates. Good example is petroleum industry; some of you may have seen the cat cracking probably the most interesting example of solids moving between two environments. We have a catalytic reactor, the catalyst gets deactivated it is moved to a regenerator, where it is regenerated by burning of the coke and the solids are returned to the cat cracker by pneumatic convey.

So, our interest is to understand what happens to the particle. How the catalyst activity is distributed over the particles? So, means we need to now look at some detail about what is happening inside the equipment so, that is the motivation for looking at population balance modelling of course, and these applications are much wider. You can look at in economic system in ecology and so on. But we will by enlarge concentrate on chemical engineering kind of applications.

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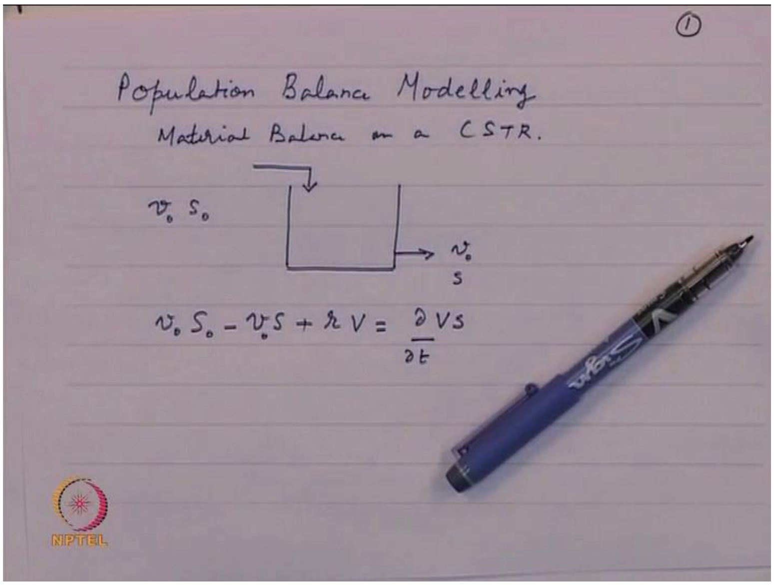

To do this we will look at a material balance something we are all very familiar material balance on a CSTR; something that we have learned for a very long time so, I will state this once again. So, the material balance for CSTR we have written for a very long time I written it once again; input, output, generation, accumulation. So, when you go from basic statements that we have done for a long time to population balance modelling.

We try and understand, what is meant by s naught? What is meant by s? What is meant by r? I have said this before and I say it once again whatever measurements we do, the measurements are based on some sampling. Sampling means what you take a large number of samples and you do an average sampling refers to an average.

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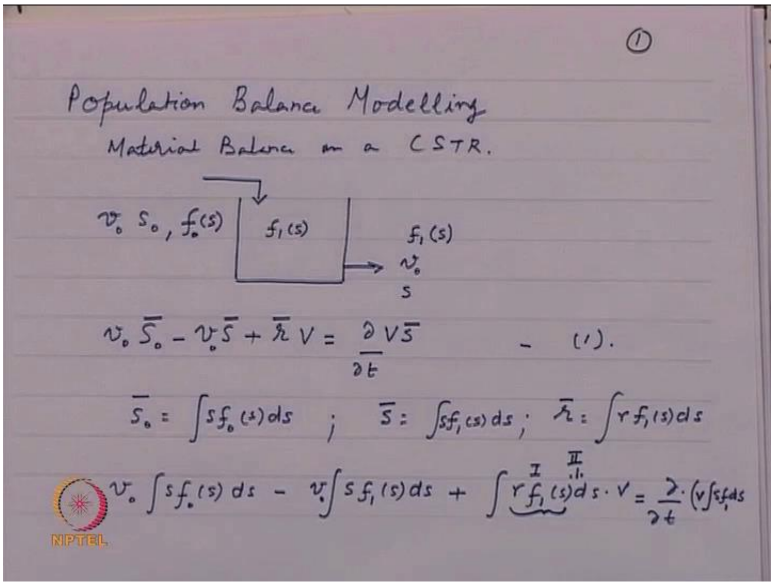

So, once again here we say that these samples s naught s and r are basically averages; moment we say it is an average if you say what is the average age of this class. Then, I should know how the age of the class is distributed and therefore, I can find the average of the class. So, any average refers to existence of what is called as a distribution of the property of interest. If the property of interest is s then, we should talk about distribution of property; I can say this distribution of this property is f naught the distribution of this property here is f 1.

What is the property of interest? The property of interest is s, in this case its concentration if it is a stirred tank where a chemical reaction is taking place we say its concentration. Now, if you go into a forest and if you want to say what is the age distribution of animals, and then clearly it refers to age; it could be any other property with some interest. Therefore, we say s naught is essentially a first moment of the distribution. So, average is the first moment of the distribution something that we have learned for a long time. So, s naught refers to first moment of the distribution of that property f naught at the inlet.

Similarly, s I say is the first moment of the distribution f 1. I will put s here and r is first moment r bar this s bar f 1 of s ds, we agree with this. So, all these are averages with respect to the distribution that exist. We recognize that, f 1 is the same as f 1 in the equipment that is the meaning of a stirred tank if I call this is equation one. Now, I can put this representation into equation one therefore, equation one looks like this integral s f naught of s ds integral v naught s f 1 of s ds. We have integral r f 1 of s ds times v equal to del by del t of v integral. What is s bar is here? Not enough space here.

Now, what I want to do now is. This term let me say this once again this term inside this term here I want to integrate by parts. So, I will multiply this by one; so, first function and this is the second function so, we integrate this by parts. So, I will quickly write down what it is then we will so, let me write the result and then we look at it once again.

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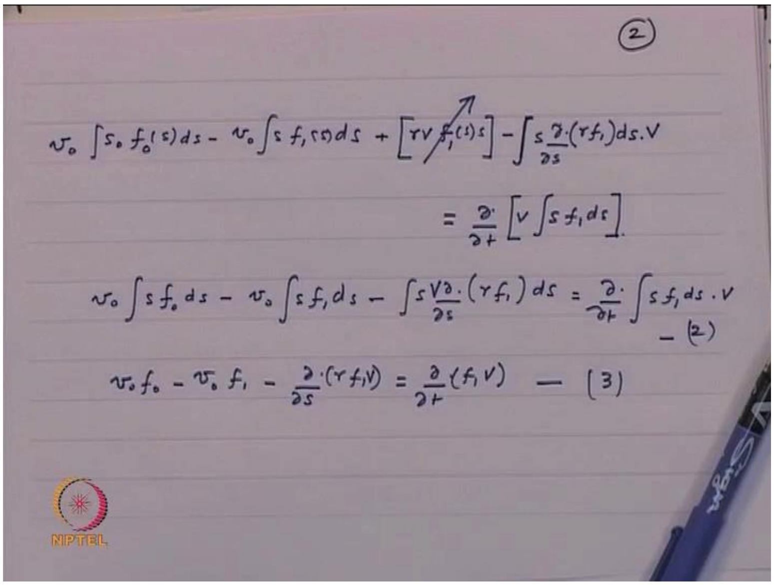

Integral s naught f naught s ds v naught integral s f 1 s ds second term then, I write the differentiation by integration parts r v f s minus so, integral s del by del s integral r f ds equal to on the right hand side del by del t within brackets v integral s f 1 ds. Have you got it? Please tell me have you got all the items properly done. First function into integral of the second its v is missing. So, we can write this as v naught let me just write this just sort of draw your attention to minus v naught s f 1 ds; I am deleting this term, which I will explain to you shortly why I am doing this integral s del by del s of r f 1 ds equal to del by del t integral s f 1 ds; I tend to figure the v frequently, I hope the v is here also I will put it here.

So, what I am saying is that this let me write this we will come back to in a minute. Now what we are saying is that these equations if I call this as equation three you call this as two; two is actually the first moment of three. So, what we are saying is that what we have been writing for a long time or material balance; equation three it looks like a more fundamental statement of the material balance that we have been writing for a long time. Now, the advantage of looking at three as the way of representing material balance is that now it gives us an insight into what happens inside the process.

So, it tells us how the distribution of property effects whatever is the process we are trying to understand. So, this is the most important point that it comes as a more fundamental statement of material balance having said this having said this anything that we write has to be proved through experiments. We need to validate whatever we say, material balance we have validated for a long time conservation of mass is known for a long time conservation of energy is known for a long time. But that this represents a description of material balance we have not proved yet.

So, as we go along perhaps in the next few lectures we will try to see how this way of trying to understand reality how it describes reality that we know. So, if it describes every reality that we know, there is reason to believe that this is probably an equally acceptable representation of material balance; something that we have to see as you go along now, when we look at literature the literature writes population balance in a slightly different way.

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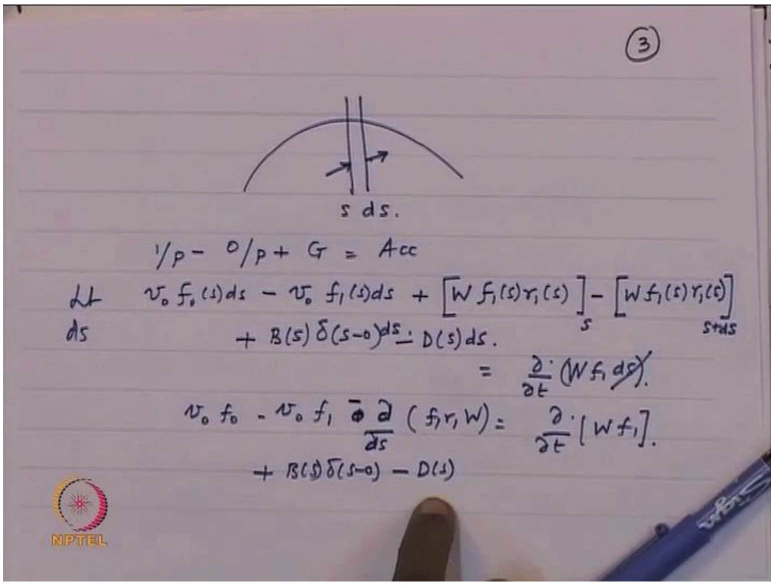

What they do is this, I mean if you look at any of the literature they will look at a material balance this is s, this is ds; they will write convective flows in convective flows out. What is input, output, generation and accumulation, like what we have written let us do that once again. Let us see how our friends who write this equal to accumulation. So, our input how do you represent input to a distribution if flow is v naught if f is the distribution of interest, then we say its v naught time f naught of s ds. So, this is the connective flow into the element of interest.

Now, similarly what is the output? Output is v naught times f 1 of s ds; this is the convective flow outside the interval this is an important. But how do you represent convective flows into a distribution if v naught is the flow v naught f naught ds is input v v 1 v naught f naught f 1 ds is the output. Now, generations they would represent like this if I say w is the sometimes I write w sometimes v so, its meaning is a same this is minus. So, they would write equal to accumulation. What we are saying whenever we write material balance in the way of friends in population balance they would write like this.

So, we take in the limit as ds tends to zero this becomes v naught f naught minus v naught f 1 this becomes d by ds or del by del s; I have to write them in del s f 1 r 1 w into del by del t I should say w here w f 1; the meaning of w and v w is often used because we are talking about catalyst sometimes v is used sometimes w is used so, both have the same kind of meaning. So, when we want to write our material balance using the same kind of approach that people do in population balance you can do this way or you can do it the way I have shown you earlier both ways are equivalent.

Now, suppose for example, we have a forest in which animals are born and animals can also die. On other words in this forest environment there can be birth and there can be death. How do you take into account birth and death? Birth means what birth means it takes place at a; that means, it is called zero; age birth means it is zero age; that means, the property belongs to s equal to zero. If a property belongs to s equal to zero we represent it by a delta function; you would have learned this in control theory it is not new to you.

Now, if there is death will be some function of s times ds I have to put it is here, I forgot to put ds here therefore, this equation will have plus delta of s minus 0 minus of d of s. So, this will how the population balance will look like if there is birth and death, this is with all of us. So, we talked about convective flow convective flow out a reaction that brings about a change in the property plus there can be birth, if it is a catalytic reactor if there is birth of catalyst activity it could be it may not be or death; that means, activity get degenerated for some reason.

So, the statement of population balance is input, output, reactive generation this birth, this death. Now with this background we want to solve a problem. So, let us take one problem of commercial interest the problem of commercial interest is what happens in the cat cracking.

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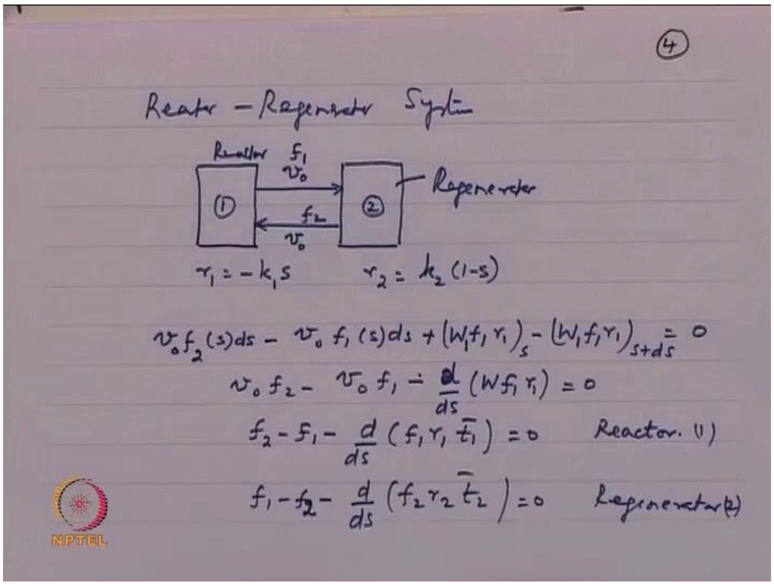

So, reactor regenerator system of the cat cracking industry, but it can be the any other industry. So, I am just looking it cat cracking as an example, but there could be many others. So, what is the problem we want to solve? We want to understand this is reactor one; this is reactor two and material is flowing between the two. So, in the reactor we expect that our catalyst is undergoing some kind of deactivation. In the reactor, we expect our catalyst undergoes some kind of deactivation normally due to coking in cat cracking it is all due to coking.

So, in the regenerator what we do is that we restore the activity we restore the activity. How is it done? In the process, they actually have hot gas going up and then they burn of the coke it is burnt and then it continuously it is restored and then broad back into it. So, this is what it is coming in and its going out I can put this as v naught showing that this whole process is operating at steady state. So, we are now not looking at the dynamics we can look at dynamics as well for the moment we are looking at steady state. Now, we want to write the material balance at steady state. What do we say? Our material balance, let us write the material balance just for the sake of completeness it is I will call this as f 2 I will call this is f 1.

So, the distribution of catalytic activity that is coming out of the regenerator f 2 going out of the reactor is f 1 at steady state. So, let me simplify this by taking the limits it become v naught f 2 minus v naught f 1 minus d by ds; I will write d by ds times w I will put w 1 because w 1 f 1 r 1 equal to 0. I will divide throughout by v naught it becomes f 2 minus of f 1 minus d by ds of f 1 r 1 t 1 bar equal to 0. Now, this is for reactor we can do the same thing for the regenerator. So, this is the reactor this is the regenerator so, we do not write this again. But I will simply write it is d by ds of f 2 r 2 t 2 bar equal to 0, this is the regenerator.

Now, I ask you now that if we can solve this differential equation it should be able to tell us how the two reactors interact with each other. Therefore, it should be able to tell us how we should run this process to get what we want. So, all answers that are required from the point of view of running this cat cracking should come out of solving this differential equation. So, let us see how to solve this and see what kind of results it gives us. Let me see what I have done to solve, I have got this 1 and 2; what I do is that add 1 and 2.

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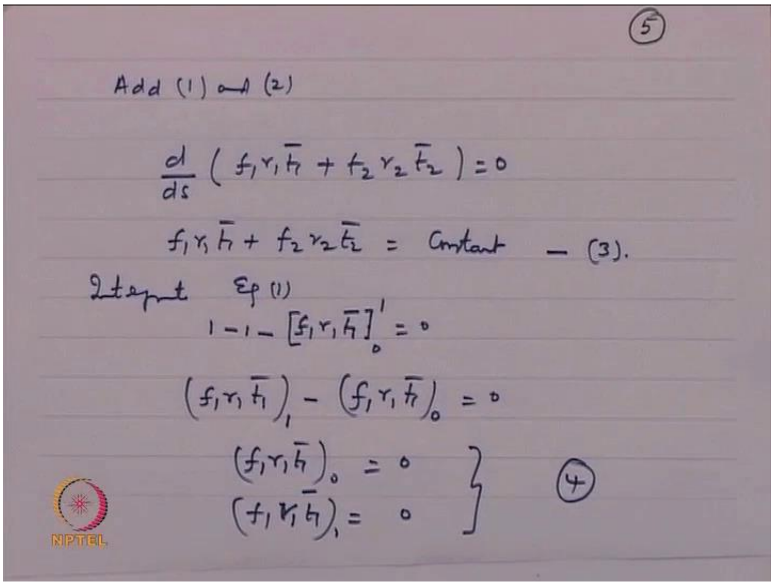

Let us add 1 and 2, so what do we get d by ds of f 1 r 1 t 1 bar plus f 2 r 2 t 2 bar equal to 0. Now, I want to integrate this, let me integrate this f 1 r 1 t 1 bar plus f 2 r 2 t 2 bar equal to some constant of integration. How do I generate some conditions on f 1 and f 2 so, that I can determine this constant time integration? What do we do? Let us look at equation one, what is it that we know suppose a integrate equation one between what are the limits of s; s is let us say its catalyst activity that it will go from 0 to 1. So, if I integrate equation 1 between 0 and 1 what is integral f 2 d f 2 ds by definition all distributions will integrate to 1 integral is 1.

So, let us integrate equation one and see what it tells us integrate so, I will call this as equation three for the moment; integrate equation one we get 1 minus 1 minus f 1 r 1 t 1 bar then, what is it between 0 and 1 equal to 0. Integrating equation 1 so, integral f 2 d f 2 ds is 1 integral f 1 ds is 1 and minus f 1 r 1 t 1 bar between 0 and 1. So, it gives us f 1 r 1 t 1 bar at 0 at 1 minus f 1 r 1 t 1 bar at 1 at 0 equal to 0. What do we know about f 1 r 1 t 1 bar and f 1 r 1 at 0 and 1 at r 1 at 0 at 0? Now, what is this function f 1 is it a bounded function at 0.

Now, we would not write a differential equation on an unbounded function. So, we will assume for the moment that f 1 is a bounded function therefore; f 1 r 1 t 1 bar is 0 because r 1 is 0. What do we saying r 1 is 0 at s equal to 0. Since, f 1 we are writing it differential equation on f 1 if it is unbounded we would not have written so, for the moment let us assume that f 1 is a bounded function. We do not know we should come back and find out whether it is correct or wrong. Assuming that, f 1 is the bounded function therefore; f 1 r 1 t 1 bar is 0. Therefore, this gives us the result is f 1 r 1 t 1 bar at 0 is 0, f 1 r 1 t 1 bar at 1 is 0. Now, we can do this same thing with equation two repeat; let us repeat what we have done with equation two.

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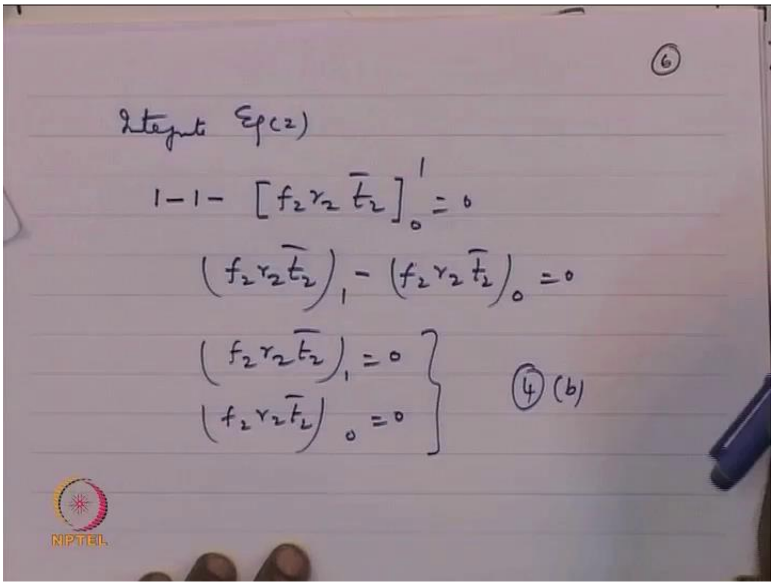

So, integrate equation two. So, we go through the same process so, see becomes 1 minus 1 minus f 2 r 2 t 2 bar 0 to 1 equal to 0. Therefore, f 2 r 2 t 2 bar at 1 minus f 2 r 2 t 2 bar at 0 is 0. Now r 2 if you look at the function r 2 you find that as s equal to 1 r 2 goes to 0 at s equal to 1 r 2 goes to 0 therefore, we will have f 2 r 2 t 2 bar at 1 is 0. Therefore, f 2 r 2 t 2 bar at 0 is also 0. So, this is I will also call this is 4, 4 b and 4 a. So, we have now to find the constant of integration in equation three. What is the constant of equation integration equation three? What is the value of the constant? It is zero. The constant of integration in view of what we have done so, far is zero. So, let me substitute this.

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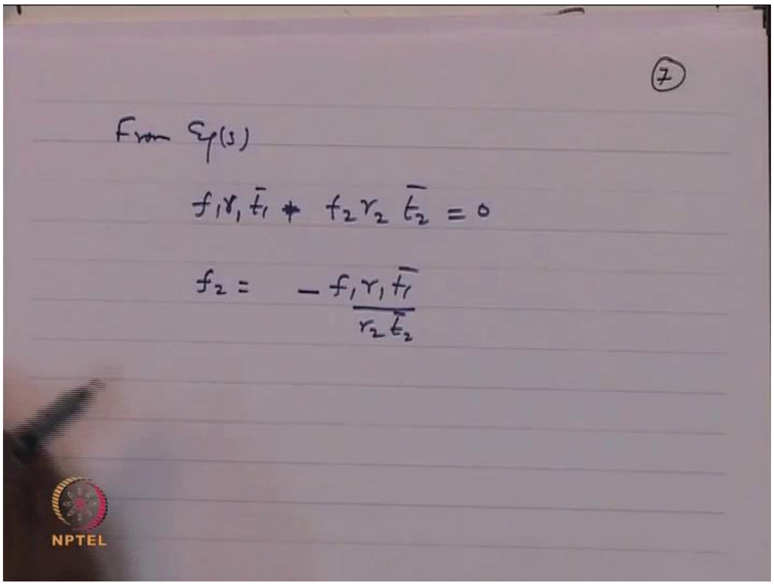

So, we get from equation three from equation three f 1 r 1 t 1 bar plus f 2 r 2 t 2 bar equal to 0 therefore, f 2 equal to f 1 r 1 t 1 bar divided by r 2 t 2 bar with the minus sign. Now, things are much easier our equation one, which describes reactor this is our equation one. So, if we just recall here our equation 1 is this. Now, we got f 2 in terms of f 1 you already got f 2 therefore, we can substitute for f 2 in equation 1 and then solve this problem.

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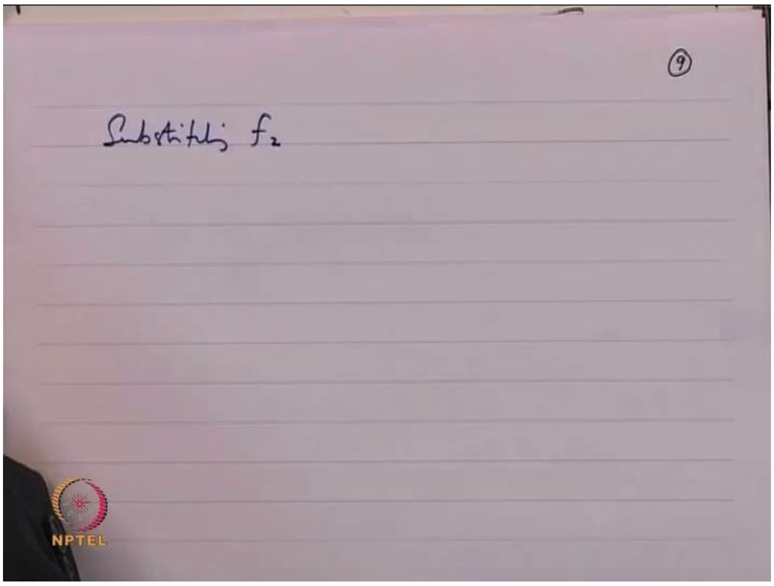

Let us substitute f 2 so substituting f 2 from where so, let me put some equation numbers here so that fine.

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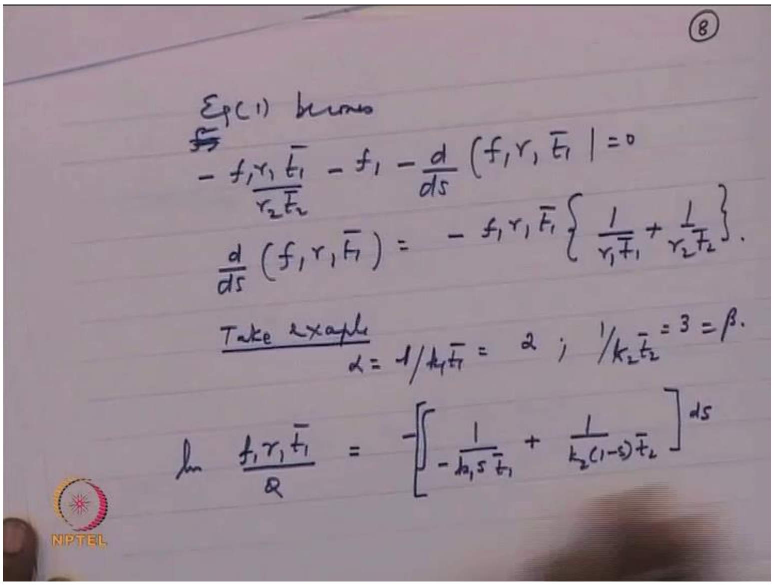

I am substituting in equation one therefore, minus f 1 r 1 t 1 bar by r 2 t t 2 bar. I am just substituting in equation minus of f 1 minus d by ds of f 1 r 1 t 1 bar equal to 0. So, this is how equation one becomes so, equation one becomes this. So, let me simplify it a little further let me see what I have done when I simplify it a little further it looks like this; d by ds of f 1 r 1 t 1 bar equal to minus f 1 r 1 t 1 bar within brackets 1 by r 1 t 1 bar plus 1 by r 2 t 2 bar. So, this is how our equation looks like; if I ask you what is the solution to this equation what will be the solution to this equation we can integrate this directly f 1 r 1 t 1 bar f 1 r 1 t 1 bar.

So, it should be possibility integrate the answer; that means, we have solution to the problem. Now, there is a constant of integration here which also will have to be determined. So, to do this we will take examples; now we take an example because take one example just to illustrate how the answers look like. Let us say I have taken 1 by k 1 t 1 bar as 2 and 1 divided by k 2 t 2 bar equal to 3, is what just to solve this problem for the case of 1 by in the nomenclature in literature, this is called as alpha; this is called as beta. So, to solve this problem to illustrate I will take an alpha as 2 m beta as 3 so, that you know we get nice numbers. let us now integrate this so, I want to integrate this.

So, what is the integral of may be I can write it here itself so, integral is f 1 r 1 t 1 bar divided by I have taken constant of integration as Q, l n equal to integral with the minus sign 1 by k 1 s t 1 bar with the minus sign plus 1 by k 2 integral I have done and ds minus I have taken the minus sign here this minus sign is here r 1, I put as minus k 1 s t 1 bar r 2 I have put it as k 2 1 minus of s. Can you help me integrate this so, I will write the integral here at now I will write the integral in the next page.

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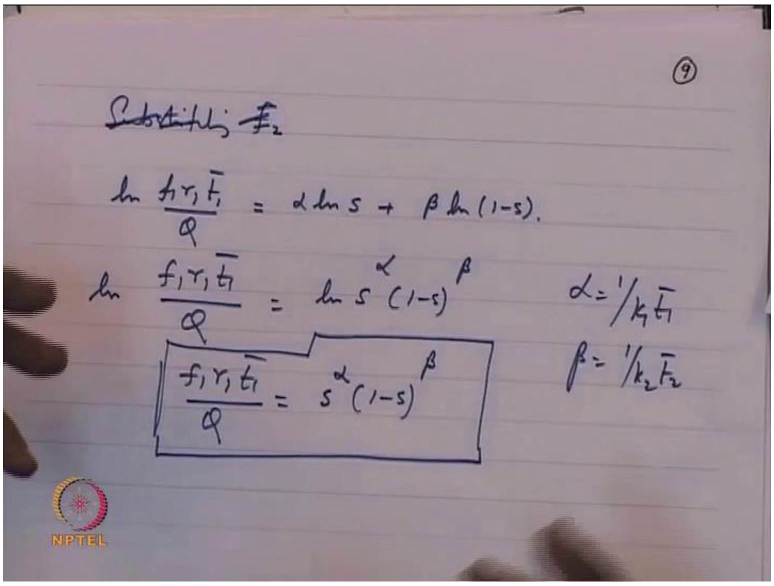

I am writing the integral l n f 1 r 1 t 1 bar by Q equal to l n alpha s plus beta l n 1 minus of s integral; I am just writing I am just writing this integral write it here itself. So, I am just integrating here itself l n f 1 r 1 t 1 bar divided by Q equal to alpha l n s plus beta l n 1 minus of s. So, this becomes f 1 r 1 t 1 bar divided by q is l n of this is l n here l n here s to the power of alpha 1 minus of s to the power of beta. Therefore, f 1 r 1 t 1 bar divided by Q is s to the power of alpha 1 minus of s to the power of beta so, this is our solution. So, let us just go back and then look at our original problem. So, we started with this that they are reactor there is a regenerator and the reaction is the deactivation is given by a first order function and the regeneration is also given by a first order function.

They transfer between them at a certain known mass flow so, that steady state is maintained and that gives us this kind of relationship that the function f 1 is related to alpha and beta in this form. What are alpha and beta? Alpha is 1 by k 1 t 1 bar; beta is 1 by k 2 t 2 bar. So, k 1 and k 2 are rate functions determined by some chemical kinetics; t

1 bar and t 2 bar are operating variables, how we operate the processes. So, this k 1 k 1 t r alpha and beta essentially tells you how the process will be run by you. So, if you know alpha and beta you know how to run the process.

So, we can make appropriate choices of alpha and beta and appropriate it run the plant to the extent you want to achieve. So, essentially it gives you a handle on how to run the plant so, that is the important thing, which means you are able to tell how alpha and beta determine the distributions of f 1 and f 2. So, if you want to operate the plant in your own way it will tell you, what is the f 1 and f 2? Let us just quickly put alpha equal to 2 and beta equal to 3 and see what kind of numbers you got.

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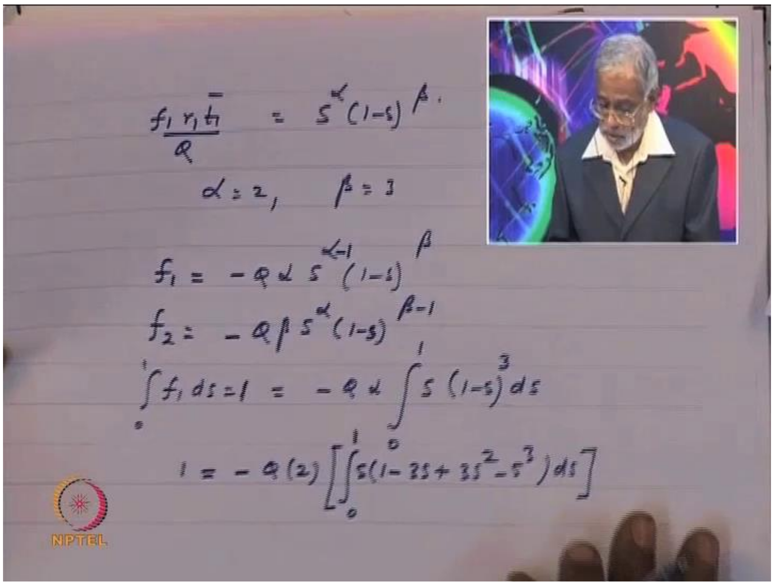

So, f 1 r 1 t 1 bar divided by Q equal to s to the power of alpha 1 minus s to the power of beta; alpha equal to 2 and beta equal to 3. Now, I want to find out what is Q? We still do not know what is Q, how do you find Q, how I have found Q; I will say see so, what I do is let me put f 1 this will be what f 1 equal to Q alpha s to the power of 1 minus s to the power with the minus sign. I have just substituted for r 1 t 1 bar this is r 1 is what k 1 s so, this becomes 1 by alpha i will just put all that together. What is f 2? Minus of Q beta times s to the power of alpha 1 minus of s to the power of beta minus 1. What is f 1 and f 2 alpha minus 1? Now, suppose I want to find out Q what will I do?

You simply say integral f 1 ds are 1. So, that will define so if you do integral f 1 ds is 1 so, integral f 1 ds equal to 1 0 to 1. So, that is equal to what minus of Q alpha integral s to the power of alpha is 2 s and then beta is 3 0 to 1. So, this should give us the value of Q. So, let us integrate now and find the value of Q? So, 1 equal to minus of Q and then alpha is 2; let me integrate s times 1 minus of 3 s plus 3 s squared minus of s cube ds, this I have to integrate 0 to 1. So, I have done it properly I hope let us go through this integration quickly.

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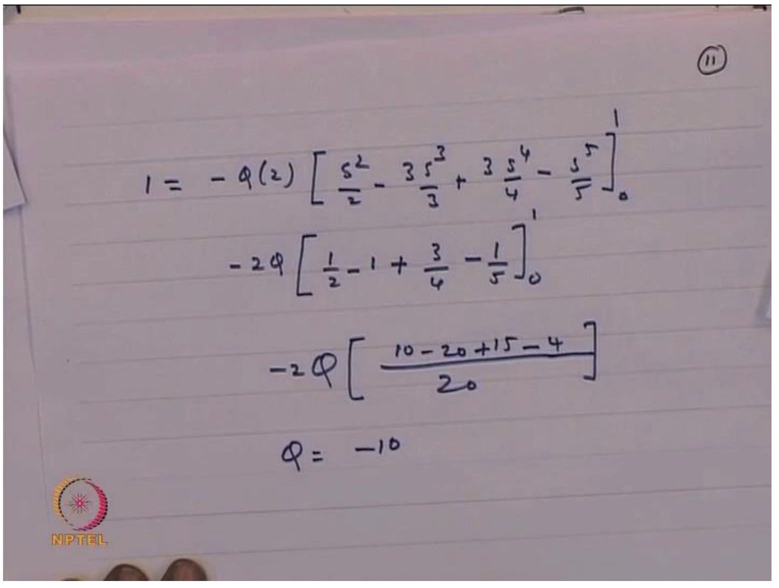

So, I will get 1 equal to minus of Q times 2 within brackets so it is s squared by 2 minus of 3 s cube by 3 plus 3 s to the power of 4 by 4 minus of s to the power of 5 by 5, I am just integrating it. So, I will get minus of twice Q 0 to 1 this is 1 by 2 and this is what 1 plus 3 by 4 minus of 1 by 5 0 to 1. So, it is minus of 2 Q so, I will take 20 common denominator is 10 minus of 20 plus 15 minus 4. So, what is Q? That is equal to minus 10.

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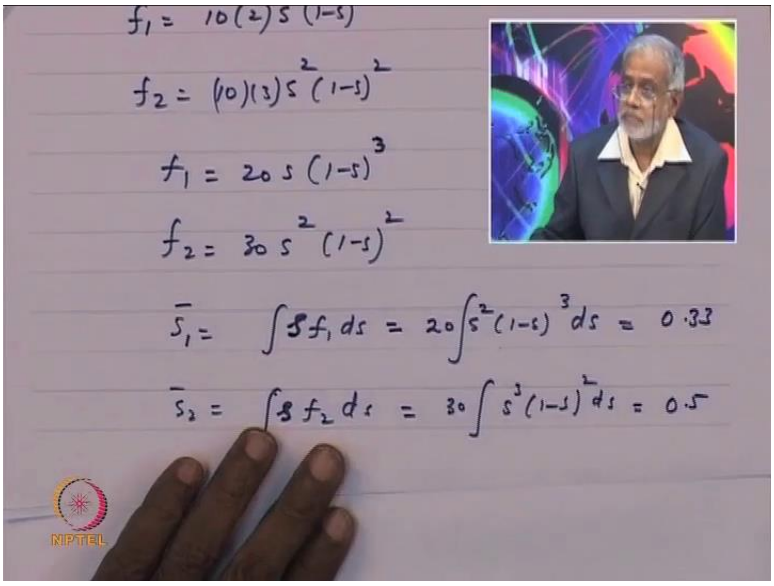

So, now we will be able to write our answers fully where what are Q and f 1 and f 2; I would have written somewhere here it is here it is. So, value of f 1 is what f 1 equal to Q is minus 10 alpha is 2 s to the power of 2 minus 1 1 minus of s to the power of 3 f 2 is 10 3 s to the power of 2 1 minus of s to the power of 2. So, that become f 1 is 20 s times 1 minus of s cubed and f 2 is 30 s squared into 1 minus of s whole square. So, to just looking back at what we have done is that is the first order problem in which reaction deactivates the catalyst by a first order process and the regeneration also is a first order process k 1 and k 2 or constants, which describes the process kinetics.

Then, when you go through the population balance it tells you what the function f 1 is and what the function of f 2 is. Now, if I ask you what is the mean value of f 1; what is the mean value of f 2 how will you find out? So, mean value of s 1 is integral s f 1 ds and mean value of s 2 is integral s f 2 ds. You have this is s see the mean value of a property is the first moment of the distribution our property is what catalytic activity and the distribution of that activity is given by f 1 in the reactor f 2 in the regenerator. Therefore, the mean value of catalytic activity in the reactor is s time f 1 ds; mean value in the regenerator is s time f 2 ds.

So, let us quickly do this and get a feel for what these number is s 1 20 times s square 1 minus cubed integral ds this is 30 integral s cube 1 minus of s whole square ds. So, you can do this integration yourself it is not a very big thing I have done this and then what I get is that mean value here is 0.33 mean value here is 0.5. You can do this as no point in spending time on this. Now, what we are saying is that reactor operates a 0.3 regenerated operates a 0.5 and what is the driving force 0.5 to 0.3. Now you can operate at 0.1 and 0.9. See the choice, what is the choice in which you will operate will be determined by what you think is appropriate for your economics whatever that economics may be.

This is an example, which says that it appropriate 0.5 and 0.33 various choices depend upon choice of alpha and beta catalytic activity. In this case in the cat cracker the property of interest is activity of the catalyst. How much coke is present on the catalyst? More the coke less is the activity. So, to what extent you will regenerate so, that you have a highly active catalyst in the reactor because the cost of regeneration and the you know the benefit of having a higher activity is what you have to balance in your process.

Now, I deleted this term r times v times f 1 s; I said that you know it is I mean our friends in population balance do not write it, but if you look now you can now you know what is f 1. Now you do this look at this value r times f 1 times s between 0 and 1 does not go to zero. What is the value of f 1 at s equal to 0 for the function that we have what about the other f 2 s equal to 1 also zero. So, you find that this this actually disappears at both ends do you recognize this we deleted this term.

I said we will come back and tell you why we are deleting this term our friends in population balance understood this that is why they deleted it. But it is not so obvious therefore; I have done this to show you that this term actually disappears. So, every example that we do we should ask this question and if it does not disappear, which means we have not understood the process fully. I mean we have to understand little bit more than you will realize that it actually disappears. So, there would be instances where it does not obvious.

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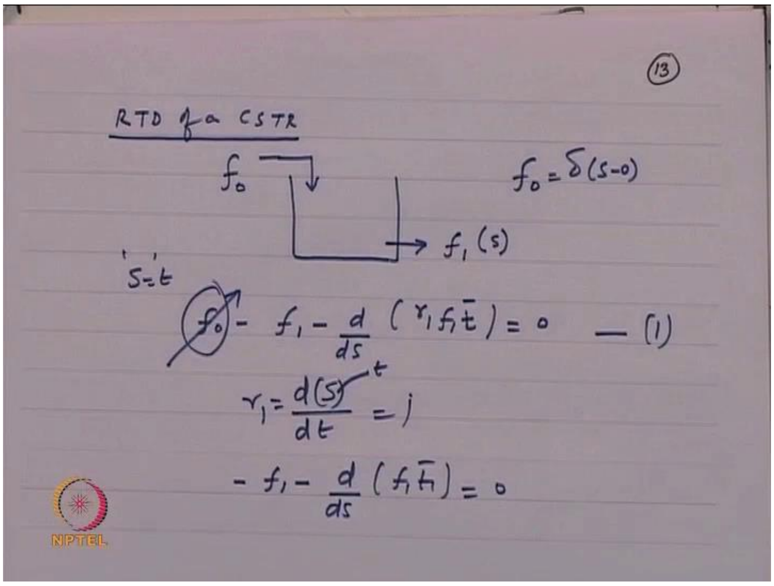

Let us take one more example an example for which all of you know the answer R T D of a CSTR. So, we want to apply population balance to understand what is the R T D of a CSTR we know the answers, but still we want to apply this so, what is our system our system is this. So, what is going in fluid elements, some fluid elements fluid is coming in and fluid is going out. If you want to find out what is our property s; what is this property s, what is the meaning that we attached to this property s time of residence in the equipment. What is our population balance? Let me write population balance we will not derive it this time because you have done this before.

Why are you putting equal to zero on the right hand side because now process is running at steady state. We want to find out the residence time distribution of our fluid elements when the process is running at steady state. Now, what meaning do we attached to this f naught, what is f naught? F naught is the time of residence of fluid elements at the inlet in the equipment. On other words how much time fluid elements at the inlet has spent in your equipment, what the answer is zero. On other words, the age of every one of you is the same, which means the age of every element which is entering is the same what is that age zero.

Therefore, f naught is a delta function at 0. What is f naught? f naught by definition by is this a delta function at zero, because no element has entered the equipment. Therefore, every element has a time of residence in the equipment, which is zero. Now, this equation I will call this equation one; I want to solve this equation. For solving this equation there are two things that we should know one, how do we solve a problem in which there is an unbounded function; there is an unbounded function, f naught is an unbounded function and our understanding out equation theory of this differential equation will tell us that whenever there is an unbounded function you must get rid of that term.

That is the way to solve the problem you must get rid of that term then only you can solve the problem that is one. Second is that what is this r 1 what is this term r, what is r? Yes, which means what we have a property s we have a property s and we want to know the time rate of change of this property or d by dt of this term d by dt of s itself refers to t in this case time of residence. So, we are actually looking at were s is s itself is t. So, we are looking at d by dt of t itself or it is equal to 1. What we are saying is the property of interest is s, what is that property time rate of change in the equipment time rate of change in the equipment; that means, s refers to the property t; therefore, d by dt of t is 1.

So, from the point of view of trying to determine the time of residence in the equipment the function r in the population balance is r is 1. Therefore in this equation one, we said that we should knock out this term. So, what our friends in mathematics tell us is that get rid of this term. Solve the homogeneous problem first, solve the homogeneous problem first what is the solution to this homogeneous problem r is 1; we have f 1 minus of d by ds of f 1 t 1 bar equal to 0.

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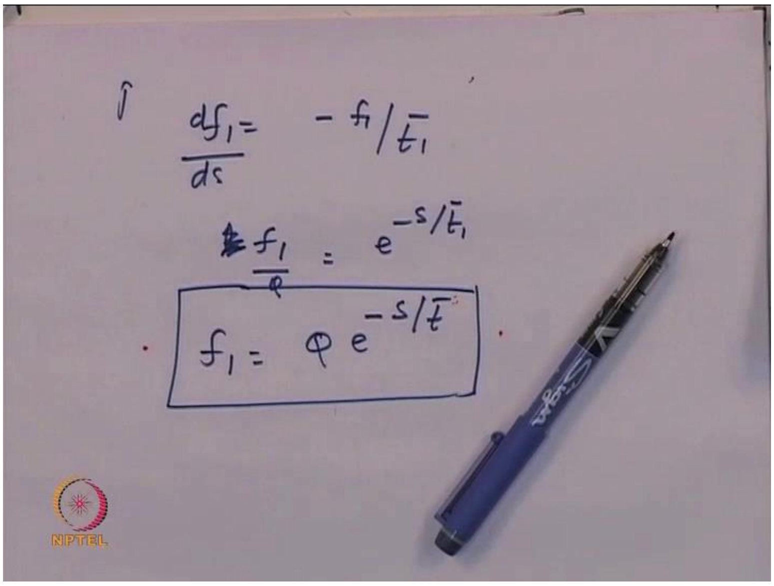

So, what is the solution to the homogeneous problem, what is the solution shall write the solution so, f 1 is, I will write like this df 1 ds equal to minus of f 1 divided by t 1 bar therefore, solution is f l n of f 1 l n l n f 1 by Q equal to e to the power of minus s by t 1 bar. So, this is the solution f 1 equal to Q times e raise to the power of minus of s by t bar. This is the solution to the homogeneous problem. Now, what our friends tell us is that since you have knocked out this term f naught. What you should do is to generate a boundary condition at t equal to 0 at s equal to 0 in this case. So, we must generate a boundary condition at s equal to 0; so, that we can determine the value of Q.

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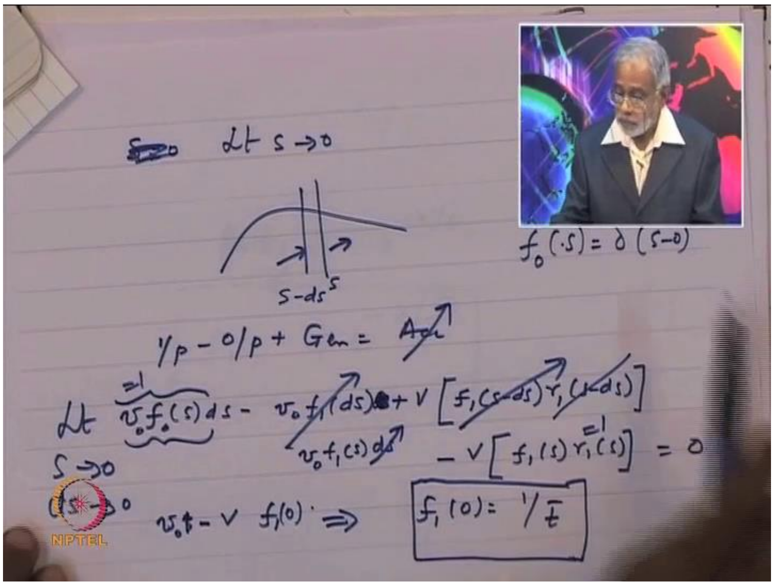

On other words, we must learn to write our material balance at s tending to zero. So, s tend we must write our material balance as limit as s tends to zero. What we want to determine to determine the where are we anyway to determine the constant of integration we should here it is I wrote it here. So, to determine the concept of integration you will find you will have to generate a boundary condition s tending to zero. So, let us try to do this you have s minus of ds and s we want to write our material balance between s minus of s ds and s inputs and outputs. So, input minus of output plus generation equal to zero accumulation.

So, let us write all the convective flows and then generations. What is the convective flow? f naught so we have v naught f naught of s ds input and then v naught I just me let me write it this down and there will be come back to in a minute input output plus generation v times f 1 s minus ds r 1 s minus of ds; this is at s minus ds then we have v times f 1 of s r 1 of s equal to 0. Convective flow and then this is because of we are assuming we are postulating r 1 is 1; it is a reaction term, in this case the rate function takes the value of 1. Now, we want to take the limit as s tends to 0 ds tend to 0.

This is the basic approach clear to you whenever you have an unbounded function, you must get rid of that unbounded function that is the first process. Then, try and look for a way of generating the boundary condition by writing the appropriate balances in this case material balance. Now, limit is s tends to 0 ds tends to 0 f is d ds I have written ds already f is ds. Now, what happens to this term ds tends to 0 this goes off. Now, what happens to this term is there any material that belongs to s less than zero. There is no material, which belongs to s less than zero; so, s minus ds must disappear.

Now, this term what is this term this is v naught delta of s ds, where delta function f naught is a delta function; f naught is a delta function. So, we know that the delta function this is actually equal to 1 by definition by definition delta function it is infinity and then it is zero everywhere therefore, the integral is one what we are saying. This first term is 1 y is it 1 because delta function is 0 everywhere it is infinity at s equal to 0 and the area is 1 that is a definition. Therefore, first term becomes 1 then this term disappears minus of f 1 0 r 1 so, f v naught v naught so, that we get f 1 at 0 equal to 1 by t bar.

What we have done we have simply generated a boundary condition at s equal to 0. Because in population balance you will find this approach you will use again and again;

this is the most important point in population balance how to generate an appropriate boundary condition to solve your problem, something that you have to do again and again. Therefore, it is good to understand what has been written and why some terms have been knocked out let me go through this again. Input what is this v naught f naught of s ds, what is it mean this means what is the convective input to this interval from this term.

That means, what is the convective input that is entering this if this interval the convective input is always v naught and f naught f s ds similarly convective output. The generation term comes from generation at s minus of s, which contributes to s generation of s at s which goes on. So, it is the difference which contributes to the interval in population balance the generation terms are always written like this for which you have already given a proof you have done that already. So, what is generated at s minus of s minus what is this difference will contribute to the interval.

Now, when you look at each term we find the some terms do not contribute at all. For example, here as limit s tends to 0 s minus ds it cannot contribute to because s minus s does not exist because s less than 0 have no meaning. Therefore, we have deleted this term. So, the first term is v naught this is not there and it comes to f 1 of 0 equal to 1 by t bar r 1 r 1 is 1, which we prove that d by dt for the case of residence time we said r 1 is 1 So, this this the r 1 becomes 1 because this is equal to 1. The second term this 1 because this 1 v naught of f 1 as ds 0 see f see this term; what is the second term v naught ds f 1 s s ds goes to 0 first term also ds, but this is the delta function.

See the first term v naught f naught of s ds why is it 1 it is because f naught of s ds it is f naught is a delta function therefore, that integral is one while the second term f 1 is a continuous function f 1 is a continuous function. Therefore, f 1 ds is 0 because ds tends to 0. So, this is the most important part of population balance is to be able to write this material balance and knock out terms that are appropriately not relevant to your process.

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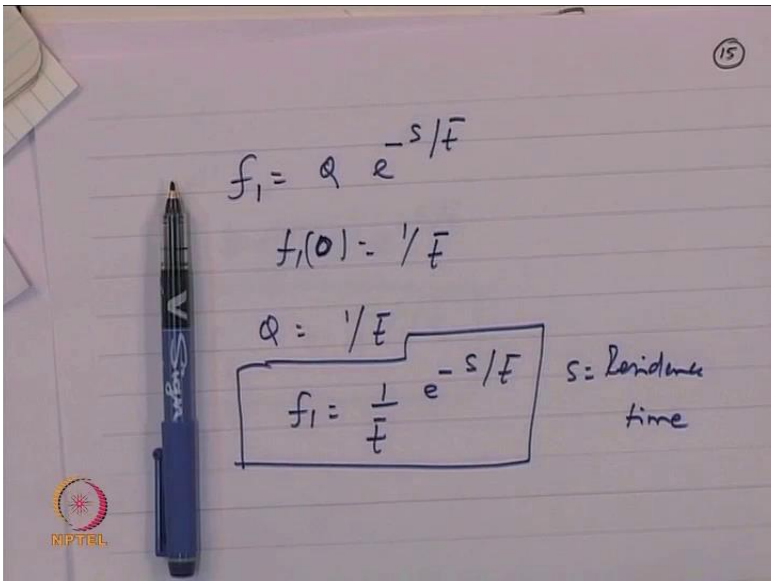

Now, let us look at our homogenous solution our homogenous solution say is f 1 equal to Q times e to the power of minus of s by t bar, where f 1 0 we say it is 1 by t bar so, f 1 0 is 1 by t bar. So, what is Q so, Q equal to 1 by t bar. Therefore, f 1 equal to 1 by t bar e to the power of minus of s by t bar and what is s, s is residence time s by definition is residence time; s is the property of our interest and that property is residence time. So, let us go through the whole thing once again what we have said? What we have said is that we have we want to find out what is the R T D of a stirred tank.

We said fluid elements that is entering the equipment these are material that has not entered the equipment. Therefore, all of them belong to the same property that they have not entered the equipment therefore, s equal to 0 all the elements at f naught belong s equal to 0 because they belong to s equal to 0 it is described mathematically by a delta function at s equal to 0. The second thing we said is that we wrote the population balance and we said that this function r, what is this function r this function r refers to time rate of change of property of interest, time rate of change of property of interest.

That means, property of interest is s in this case time rate time. Therefore, s equal to t is the meaning that we must attach to this r. Therefore, the time rate of change of is d by dt of s where s equal to t therefore, r is 1. So, the interesting point that I would like to draw your attention is that population balance is really able to understand the physics and try and capture from your reality, what is the function that we would use to describe that reality.

The moment, you do that this techniques becomes very powerful; that means, you must understand the physics of the problem. Then, if you do not understand then we do not know what meaning to attach to this function r lets go further. Let us take one more example, which is little bit more involved, but I think we should spent some time on that the example.

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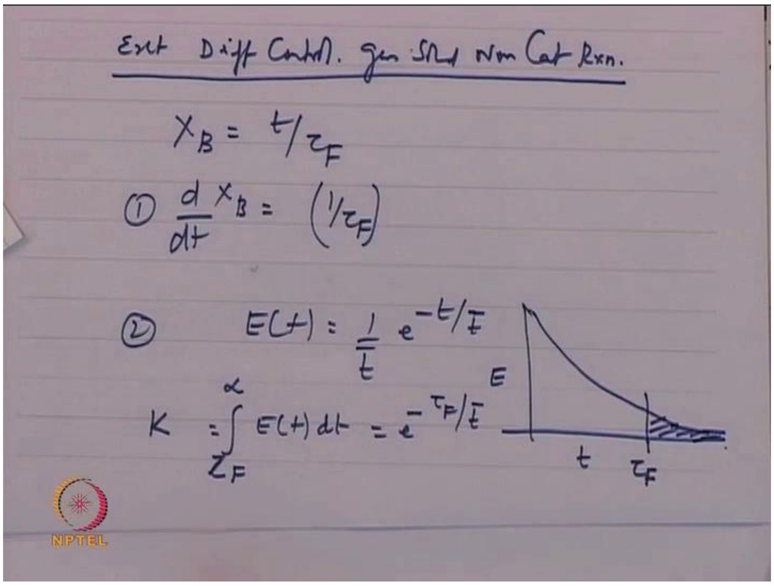

Now, I take is the example here is the case of external diffusion control gas solid non-catalytic reaction. This is the example I am taking, what is the example? The example is you have equipment into which this particular reaction is taking place, where it is external diffusion control. We have done this in our class we have said that in such cases the extent of reaction of the particle is given by this. We have done this; that means, if you take a single particle and expose it to an environment of constant gas composition, it will react as per this form we have done this in class no point doing it again.

Now, if I say now that what is d by dt of X B what will you say d by dt of X B is 1 upon 1 upon tau f, which mean that this rate function r seen in this context is with the minus sign it is not a minus plus sign only 1 by tau f. Now, let us take this one example second example let us say we look at R T D of a stirred tank t bar e to the power of minus t by t bar. Now, let us say this looks like this it looks like this and say this is suppose I say this is tau f this is E function. What is this area? We can calculate correct area is simply you have to integrate E function between tau f to infinity. So, let me do that tau f to infinity E t dt. What will it be I call this K you can be easily shown this becomes equal to E to the power of minus of tau f by t bar it is no point in wasting time what do we said now.

If you look at the E function for a stirred tank and we look at the fraction that belongs to time of residence greater than tau f that becomes equal to e to the power of minus tau f by t bar. This comes from simple integration is nothing to waste time. Now, I ask you in a process which is governed by this R T D function E t what is the fraction of material, which belongs to greater than tau f you will say it is given by e to the power of minus tau f by t bar, which means what this material which spends time greater than t f is completely consumed completely reacted because it is spending time greater than tau f.

So, a material which is completely reacted suppose I say I call it white it is a white particle, why is it white it is completely reacted it is a white particle some people say it is completely reacted it is a black particle it does not matter. What it is? It is a particle whose property is described by a delta function. You understand it is a property is described by a delta function because the value is a 0 or 1 since everybody having the same age you know that kind of.

On other words whenever you have a chemical reaction where the rate function is 0 order 1 by tau f it is 0 order then the problem is that in a stirred tank; there is a certain fraction of material which is completely black or completely white, whichever way you want to look at it; that means, that fraction of material to describe in population balance term it is a delta function. Therefore, whenever you have a property whose functionality is a delta function, which is it is in unbounded function in population balance when it appears you will have to appropriately deal with it.

Because you cannot deal with unbounded functions in a differential equation this the problem we want to deal with now. Because this we will encounter again and again not simply in chemical engineering in many such cases; unbounded functions appear and it has to be appropriately dealt with.

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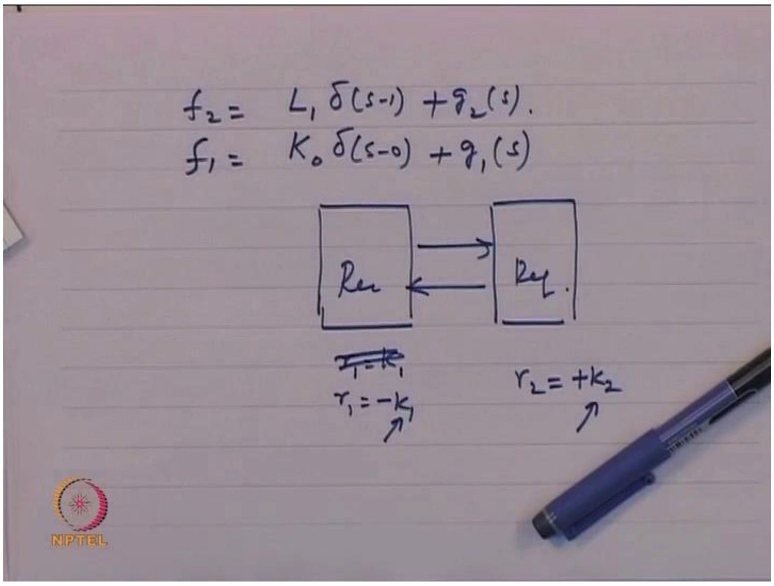

So, what we are saying now our distribution function which is f. It can have a discontinuous part what is meant by this because this fraction of material it is either completely black or completely white. We do not know, what it is and then there is a continuous function; it is continuous we understand what I am saying you can have situations like this. You have a chemical reactor regenerator going between these two, where r 1 is minus k 1 r 2 is plus k 2 this is the reactor this is regenerator. What is meant by minus k 1? It is zero order what is meant by plus k 2 it is again zero order.

So, instances where f 1 and f 2 it is I will call this as s minus 1 plus g 2. These possibilities are distinct so, how do you deal with situations, where you have such kind of discontinuities in your distribution. This is quiet common its very common in you knows theoretical physics they sort of handle very well. We have such a problem and we want to see how to handle these kinds of discontinuities in our problem. So, I will do state this once again.

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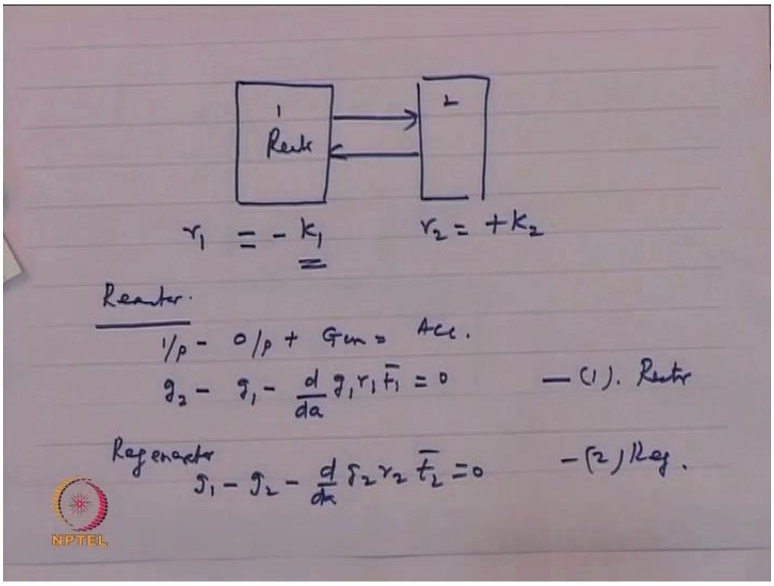

So, you have you have a reactor; we have a regenerator; this is given by r 1 equal to minus k 1; r 2 equal to plus k 2. Now, because of the fact that this is zero order zero order means what this material get completely consumed and there is a fraction finite fraction, which belongs to completely black when a black means it is completely consumed. In the regenerator, there is a finite fraction which is completely regenerated which is white; that means, it is white black means completely consumed; white means completely regenerated, these possibilities exist.

Here is a reactor regenerated system in which you have in the reactor because of the reaction that is taking place the material gets completely deactivated its fully coked deposition is such is completely deactivated and the possibility that in the regenerator because of the reaction it can be completely regenerated. So, complete deactivation means activity is zero; it belongs to delta s equal to zero it is a delta function at s equal to zero. Only for zero order this happens only for zero order, because if you look at a first order process first order process is what x equal to E to the power minus k t infinite time it takes.

So, this only in situations where the time of complete consumption is finite, which is the case with external diffusion we have done that in class. All these problems of non-catalytic gas solid reaction we have shown that the time required for complete consumption is finite. We know how to calculate this because we know the rate constant diffusion coefficients and so on. So, in situations where the time required for complete consumption is finite you will find that in stirred tank kind of R T D s there is a finite fraction, which belongs to completely black or completely white. We should be able to deal with this kind of discontinuities in the population balance.

So, this is the illustration that we are trying to do for which we said whenever we have this kind of problem we get rid of it and solve the homogeneous problem. To the homogenous problem, we generate the appropriate boundary conditions and solve to get all our answers so; we will try to do that now. So, I will write let us write the generation so, let me do it for a reactor first help me recognize that we will not worry about this we will only worry about the continuous. We will come back to it as you go along input minus of output plus generation equal to accumulation.

So, continuous one is what g 2 I will say this is 1 this is 2 this is so, g 2 minus of g 1 minus of d by ds or d a g 1 r 1 t 1 bar equal to 0 this is for the reactor. Now, let us write same thing for the regenerator g 1 minus of g 2 minus of d by da of g 2 r 2 t 2 bar equal to zero. This is for regenerator. Now, we have done this for the case of first order process and we could integrate and solve the problem the reason is that in the first order process the time required for complete consumption is infinity there were no discontinuity no unboundedness and all that there was no great problems solving.

Now, we know that these problems exist because our functions are zero order and therefore, these problems exists therefore, we should recognize that these functions have discontinuity, where are the discontinuities in the reactor it will be at s equal to 0 in the regenerator it will be s equal to 1; we know that why in the reactor complete consumption can take place therefore, it can be completely get coked and therefore, the activity can become zero. Therefore, we know the discontinuity occurs at s equal to 0 at reactor; s equal to 1 in regenerator we know all that. So, with this knowledge let us go through this and see how to generate the boundary condition at the appropriate location.

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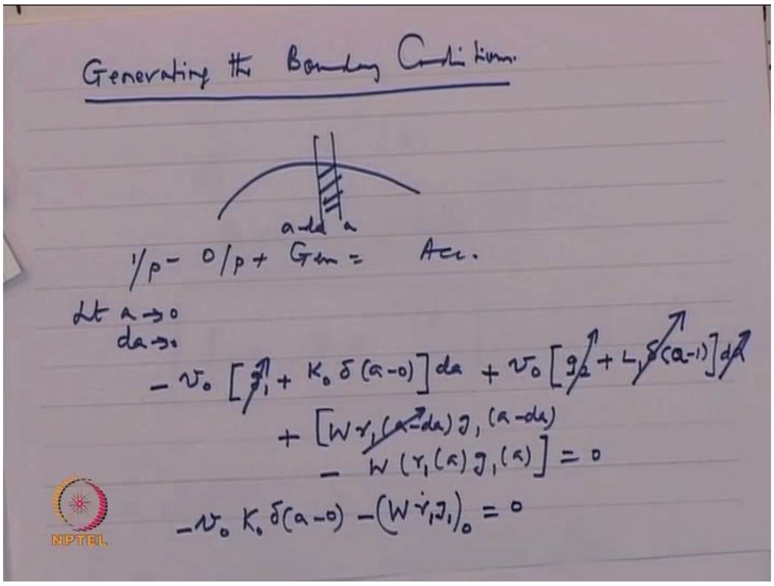

So, this problem now is generating the boundary conditions. Once again what do we write input minus of output plus generation equal to accumulation limit as a tends to 0 da tends this is 1. So, we write it between a minus a minus ds a minus da and a. So, let me write convective v naught where are we multiplied by g 1 plus k naught delta of a minus of 0 da; input do you agree with this why have you written this. We know this see based on the understanding of the physics of the problem; we know that the discontinuity occurs at a equal to 0; that is why this is the continuous part this is the discontinuous part we have taken both into account.

Now, input output v naught g 2 plus l we can write delta of s minus of 1 da, but this problem is it 1 so, it will disappear anyway. So, now, plus generation W r 1 a minus of d a g 1 a minus of d a minus w r at a g 1 at a equal to 0. Please look at it this no need to rush this term by term please understand; we are writing a material balance we want to write this material balance in the reactor that is why we are what is happening. Input, output, generation, accumulation so, this should be between s and a, see we have taken an element we have taken an element and we are writing inputs and outputs for this element.

So, we are writing a material balance so, how much is the input going in how much is the input coming out and reaction terms have to be written and whether we have written it correctly. We said that is convective flow we said convective flow and then there is reaction term. So, this is input this is output what we shall do; now let us go further now. Now, what are the terms that will disappear what are the terms that will disappear g 1? Now, this this happens only at a equal to 1 therefore, we are taking limit as a tends to 0 da tends to 0.

So, this term disappears and da tends to 0 this is the continuous function this term will disappear this is the continuous function this will disappear. Then, there is no material that belongs to a less than 0. So, this will disappear. So, what is left minus v naught k naught delta of a minus 0 minus w r I will put r 1 r 1 g 1 at 0 equal to 0.

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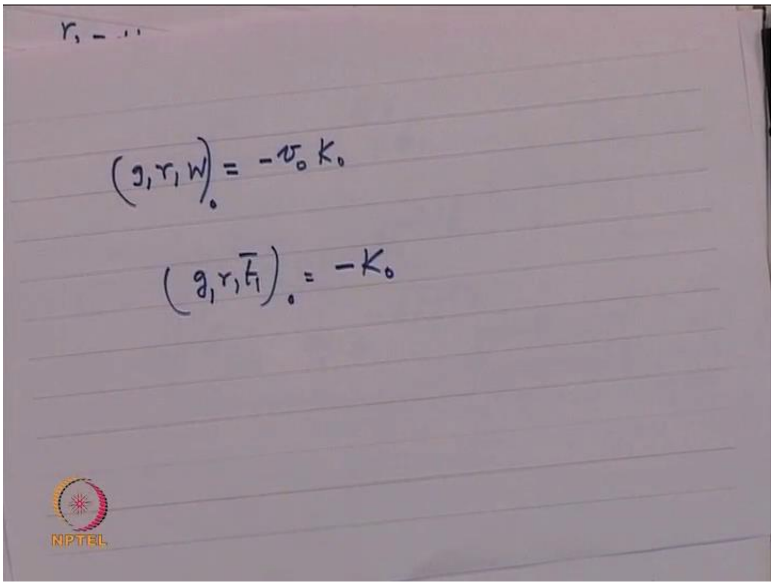

Can we simplify this please? Can we simplify what we get? g 1 r 1 W equal to v naught and this ds the ds this is da so, this holds goes to 1 therefore, it becomes simply k 0 with the minus sign. Let us do it once again out input output generation equal to 0. Now, we knocked out this term g 1 da because its continuous term g 2 da its continuous we knocked out there is no material belonging to a less than 0 g 1 g 2 are continuous discontinuity as an a equal to 0, for which we are separately representing see we said please recall we said the following.

We said function f 2 has the continuous part and a discontinuous part. There is a continuous part this is a discontinuous part. Now, we are writing the material balance input term output term and this is the generation term. Now, what we are saying is that g 2 d a g 2 being a continuous function g 2 d a goes to 0 because limit has d a tends to 0 so, this term disappears. This delta of a minus 1 discontinuity occurs at a equal to 1, but we are talking about a tending to 0 therefore, this term will disappear.

Therefore, the term there is no material that belongs to a less than 0 therefore; this term r 1 a d minus g 1 will disappear. So, what is left behind is only this and k 0 time delta a minus 0 da is 1 by definition. So, this gives us where are we here we are. So, our boundary condition says that g 1 r 1 at 0 equal to this or g 1 r 1 t 1 bar at 0 is minus k 0. We have got one boundary condition; now let us generate one more.

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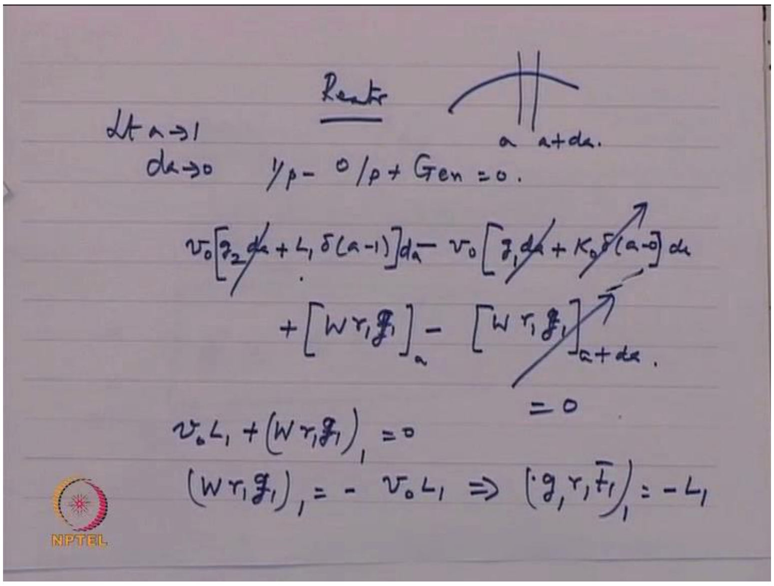

Now, we are going to do limit at a tends to 1 da tends to 0; once again input output generation equal to 0, which one we are writing for reactor we are writing for reactor. I should say that we are writing for reactor we will do for regenerator also we will do for regenerator also. We will finish reactor at a equal to 0 we have done a equal to 1; we will do similarly we will do for regenerator. So, this is for reactor please I should have said this. Now input is what input will be v naught g 2 da plus L 1 delta of a minus 1.

So, this is input output is what v naught integral g 1 da plus k 0 delta a minus of 0 da is there da is here plus W r 1 f 1 will take between a and a plus d a so, at a minus w r 1 a plus d a equal to 0 input output generation. Once again limit we have done limit a tends to 1 da tends to 0 whenever da tends to 0 all the continuous terms will go away and since there is no material belonging to a greater than one this will go away so, and then we are talking about material balance around a equal to 1 therefore, delta h this disappears what we are saying.

Therefore, we have v naught L 1 because and then the other term is plus W r 1 f 1 at 1 equal to 0. So, in the limit what does it become W r 1 f 1 at 1 equal to minus of v 0 L 1 therefore, it becomes I put g this is not f g about that this is g. So, this becomes g 1 r 1 t 1 bar at 1 equal to minus of L 1 what we have said.

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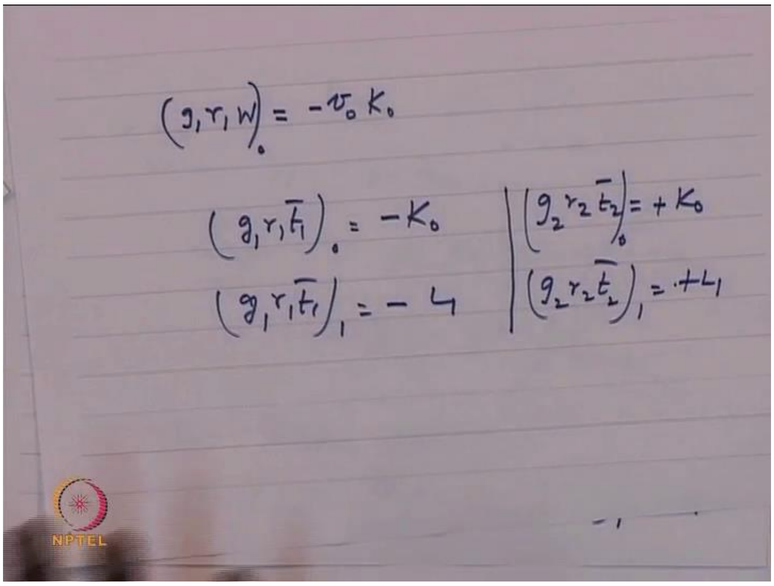

So, this I will put this condition here therefore, g 1 r 1 t 1 bar at 1 is minus of L 1. We can actually show this we will do it when we meet next time we have run out of time today. So, this become plus k 0 at 0 we will show this when we meet next time may be tomorrow to plus L 1. We will show this tomorrow what we have done is we are looking at an example of the population balance distributions having discontinuities and whenever there is a discontinuity; we said that we must generate appropriate boundary conditions to take care of discontinuous else we cannot solve the population balance equations.

We have generated those conditions now; basically we have got those conditions in front of us therefore, we will be able to solve the differential equations and find out those distributions and how those distributions are affected by choice of the process variable, which is k 1 t 1 bar k 2 t 2 bar or in our nomenclature alphas and beta we will finish that when we meet next time I will stop that here.