Mathematical Modelling and Simulation of Chemical Engineering Process
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Lecture 54
Solution of the population balance equation

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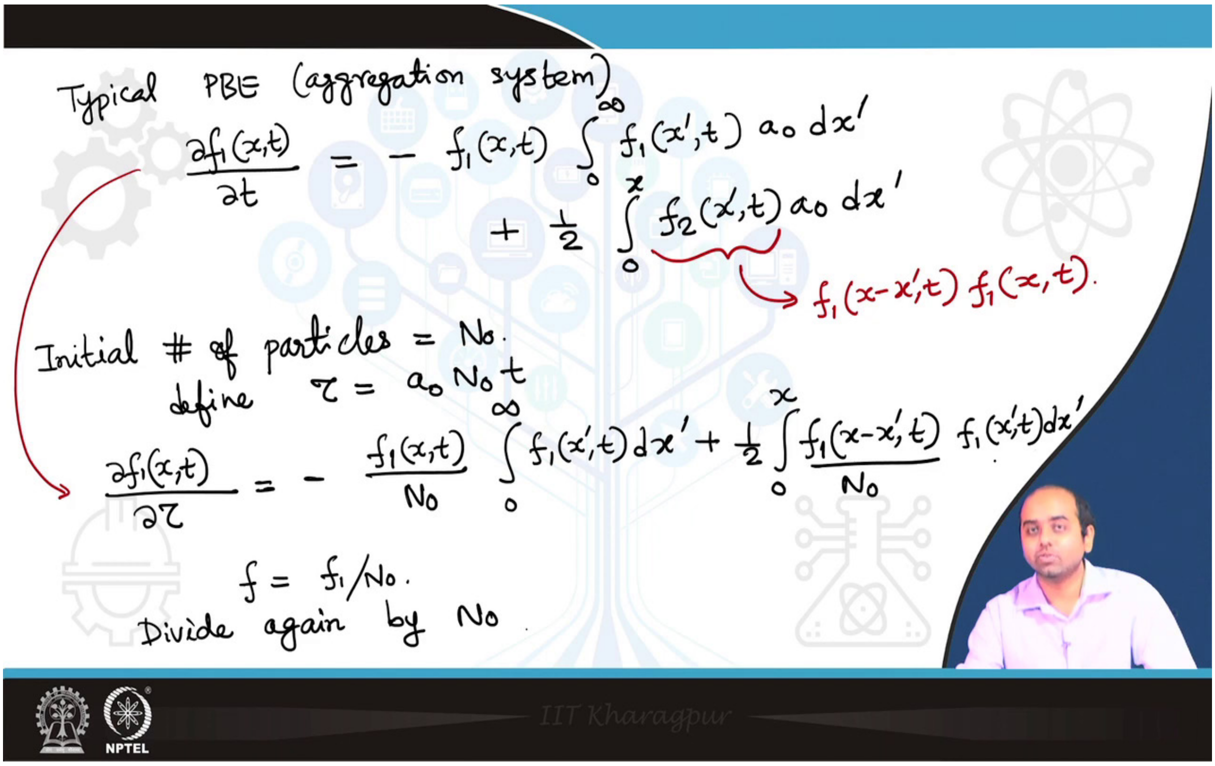

Hello everyone, in this class we are going to talk about the solution of the population balance equation. So, in the last few classes we have talked about, how does the, framework of the population balance equation for different scenarios, no growth, growth, with breakage, with aggregation process, but essentially, we see that the population balance equation is a partial non-linear integral differential equation. And in this class will talk about analytical technique by the use of Laplace transform. And in the next class we will talk about a numerical technique based on discretization.

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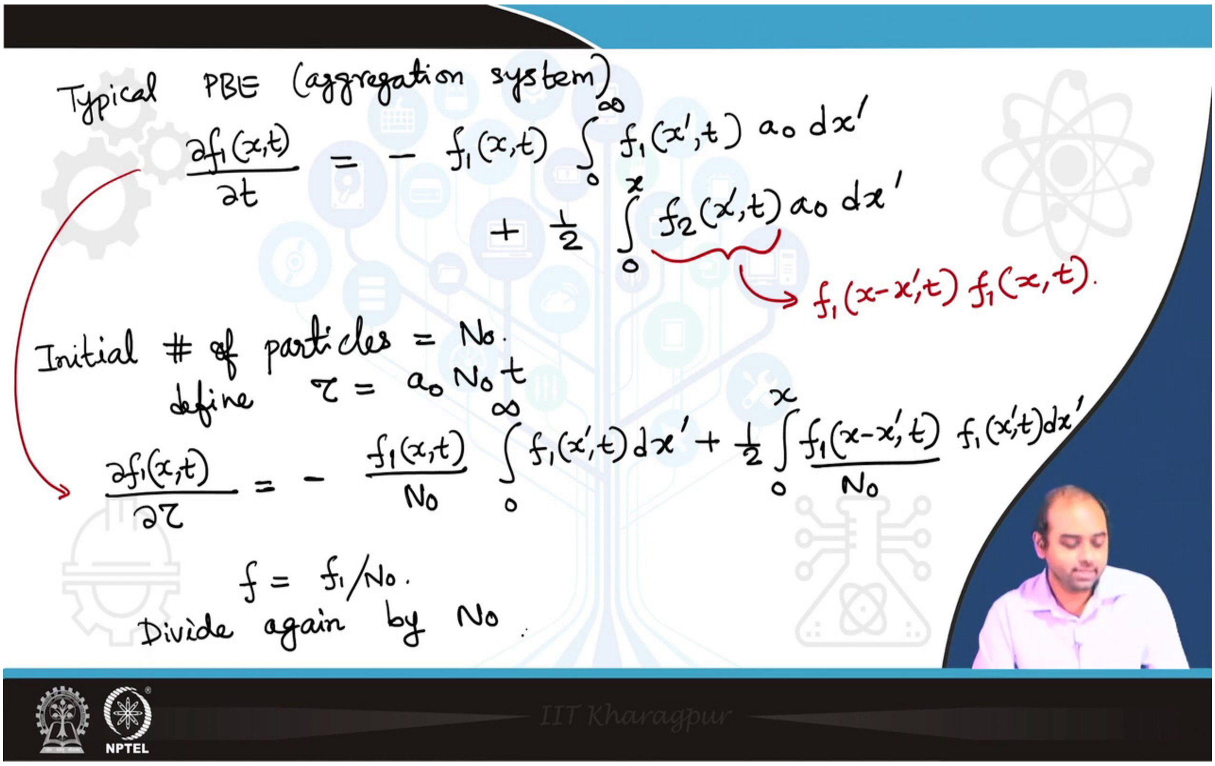

Now, this let us write down the equation and take it from there. So, these are typical aggregation, I mean this typical, sorry, this typical populates, typical PBE equation. Let us say in the aggregation system, looks like this, the h minus term, you can clearly understand that this is your writing an aggregation system, constant aggregation frequency plus half, zero to x prime f2, this is the aggregating pair.

And this is something we can write by the approximation and this is nothing but f1 x minus x time. So, this is like on the right hand side there are some integral terms. So, this is the integral differential equation, integral differential equation that is what we call.

Now, let us define the initial number of particles as N0, and we also define a timescale tau, define tau as a 0 N0 t this is something I can do, a0 is the aggregating frequency and then 0 is the total initial number of total particles and t is the time. So, instead of writing t, I will write everything in terms of tau. So, if I do from just a small algebraic step, so, from here I can write as df1 x comma t, essentially, I divide everything by N naught and a naught.

So, if I do that, I will be getting this as d tau and which is equal to minus f1 x comma t by N naught, a naught will go over there is a constant, we have chosen this to be aggregating frequency as constant and rest of the things will remain as it is. This is the first term on the hand side and this is the second term half by N naught, let us say, then we have multiplied with f1x, this is not x, this is x prime. Now, we divide again by N naught, so, we see that f is f1 by N naught. So, we divide again by N naught.

So, what will happen, so, the left-hand side from f1 it will convert to f and the hand side everything will convert to f. Let us just recall this equation. So, the left-hand side if I divide by f naught, so, this will be f, right hand side already, the first time is given by f naught second time if I now divided by another N naught it will be f, and the last term, this of the second term will again be divided by N naught, so, that will be again f.

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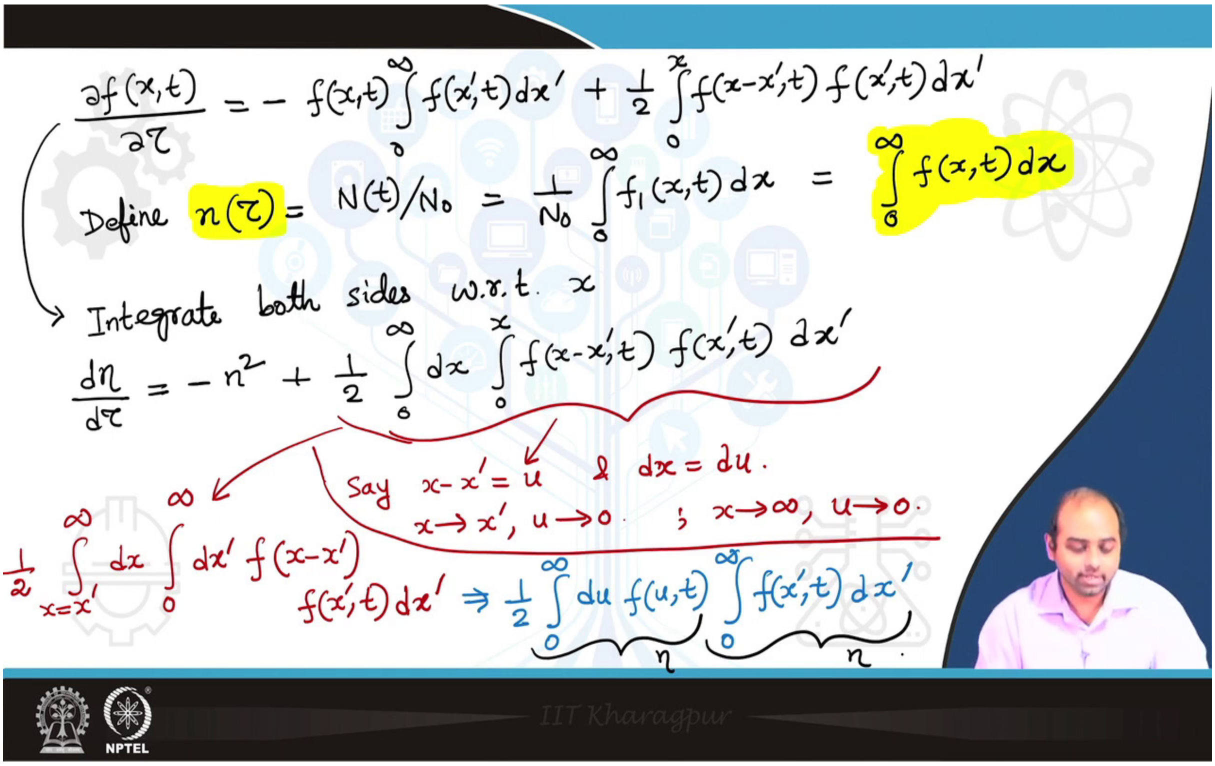

So, I will be getting df x comma t by d tau is equal to minus f x comma t 0 to infinity f x prime comma t dx prime, this is the first term, a single term. And the second source term will be converted to like this f all no f1 now, just algebraic steps we are doing. Now, let us define n, small n as a function of tau, small n is the fraction of the number of particles at any time t with respect to the initial number of particles, and how do we get this. So, this is like 1 by n naught of integration of 0 to infinity of the number density function. And we know that f1 divided by n naught is f. So, this is nothing but the integration of f, 0 to infinity.

So, this is defined as eta and I will put this in the highlight, this eta is equal to this quantity. So, what we are trying to do from this equation is that we try to integrate both sides, integrate both sides with respect to x, you can understand that we are trying to bring the things in terms of n tau, or the small n or eta or whatever you think of, that is like the fraction of the number of particles.

So, if I integrate both sides, since left hand side is a derivative with respect to tau, so, this will become like d eta, I mean d eta by d tau. Second one will become minus eta square, where eta is a function of time, this will be minus n square and this one is something we have to see what can be done, is like we are integrating.

Now, in this part, there are some tricky things needs to be done here, now this part or this part of the equation. Let us look carefully and see that if we say that x minus x prime is defined as u and this also means that dx is equal to du. So, as x tends to x bar, this u will be tending to 0, is not it, and also as x tends to infinity, u will tend to 0. So, for the first term or the first term this, part of the equation, what we are going to write, I mean instead of writing I mean this part of the equation, where this from 0 to infinity and this integration is essentially over dx.

So, this d, I mean this integration is converted to, instead of from 0 to infinity, I can write it from x prime to infinity. And the second one, instead of from 0 to x, I can interchange the limits and I can write that x prime instead of from 0 to x, this is from 0 to infinity again, x prime. This is a change of the limits which I try to do here, then we have x, this outer integral has the limits of x from 0 to infinity, and the inside integral has the limits from 0 to x.

Now, instead of writing the internal integral from 0 to x, so, where essentially, we are saying that x prime is up to x, I take the outer limit as a starting from x prime, and set the internal limit instead of x to infinity. So, this will cover the entire range. So, the x prime is now changed from, it range instead of from 0 to x, I change it from 0 to infinity and the outside integral instead of from 0 to infinity I started from x prime, considering that this x prime starts from 0, is not it because there is also an internal integral.

So, this is the limit change that I make in this integration or this term of this integration. And now, with this substitution that we described here, I can write this as, this integration term whatever we discussed as half of integration of du, is not it, dx conversion known as du and x is equal to x prime can be written down as 0 to infinity. And then the internal limit x minus x prime can be written down as f of u comma t, and then I have the another integration from 0 to infinity this is f of x prime whatever the remaining terms are there. So, this entire thing suggests nothing but half n square, is not, this is the first. So, this is one part which represents n. So, this is n and this is also n, this is half n square.

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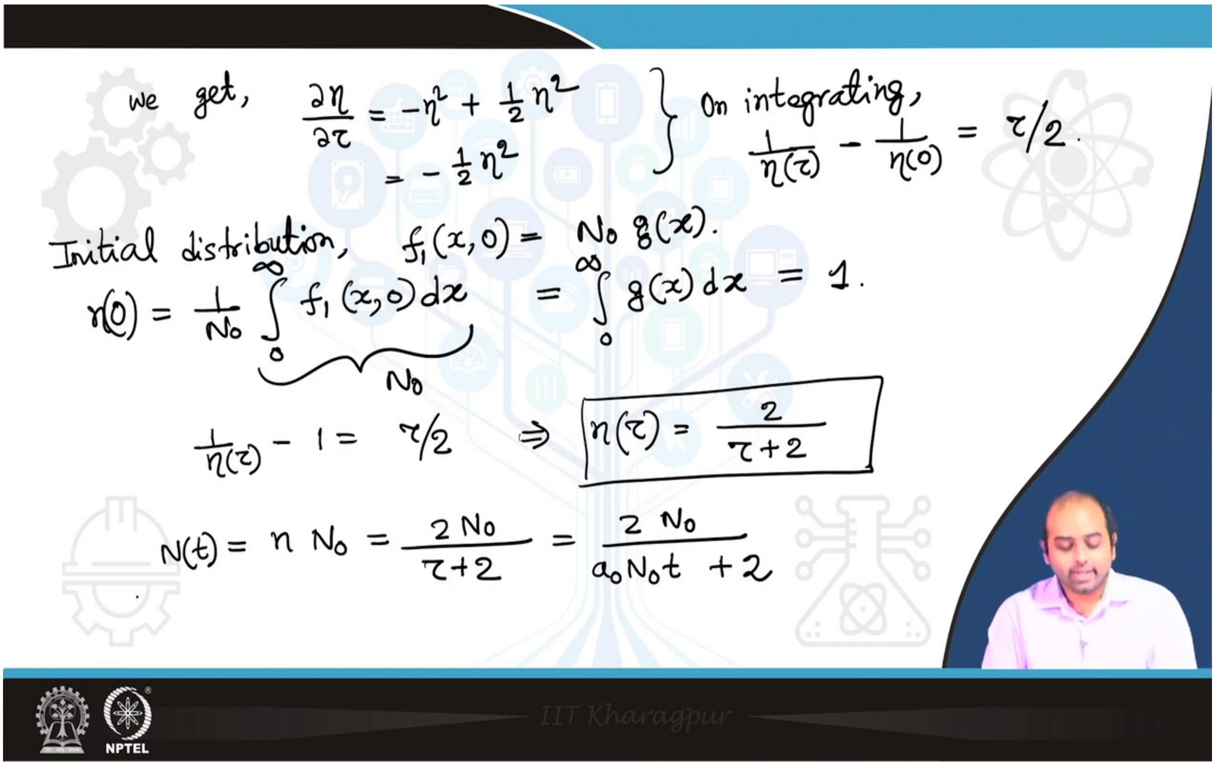

So, now we get as minus eta square plus half this n square and this is equal to minus half n square. So, on integrating, this I get 1 minus of course, this depends on tau minus 1 minus is equal to tau by 2. So, let us say that the initial distribution f1, in terms of f1 is possibly something that we will be known, as something like N0, g of x. So, small n 0 is 1 by N0 integration, now f1 when x term integrating both sides, x 0, dx 0 to infinity. And this quantity is nothing but our x 0. So, this will ultimately lead to integration of 0 to infinity, g of x dx and this is equal to 1.

So, this also satisfies that g of x dx or this is also sort of the distribution function essentially over the limit 0 to infinity will lead to 1. So, N0 is essentially 1, if we think of this type of distribution, initial distribution, so, we get 1 minus n tau minus 1 is equal to tau y 2 and this will lead to the conclusion then and n tau is equal to 2 by tau plus 2. So, this is the solution of n tau.

But this does not solve this f1 yet, because n tau is nothing but integration of f1. So, we do not know what essentially is. So, N t is something that we can say, N t is something we can say as, this n into N naught. So, I can write as 2N naught by tau plus 2. So, and even I can replace tau as this a naught, n naught t plus 2. So, this is N t or change of the particles, total number of particles with respect to time is something that I know, and this can be done. But n t or n, small n whatever it is, that is like the integration of f1 over 0 to infinity, but we do not know what is the f1, this does not help me to find out what is f1.

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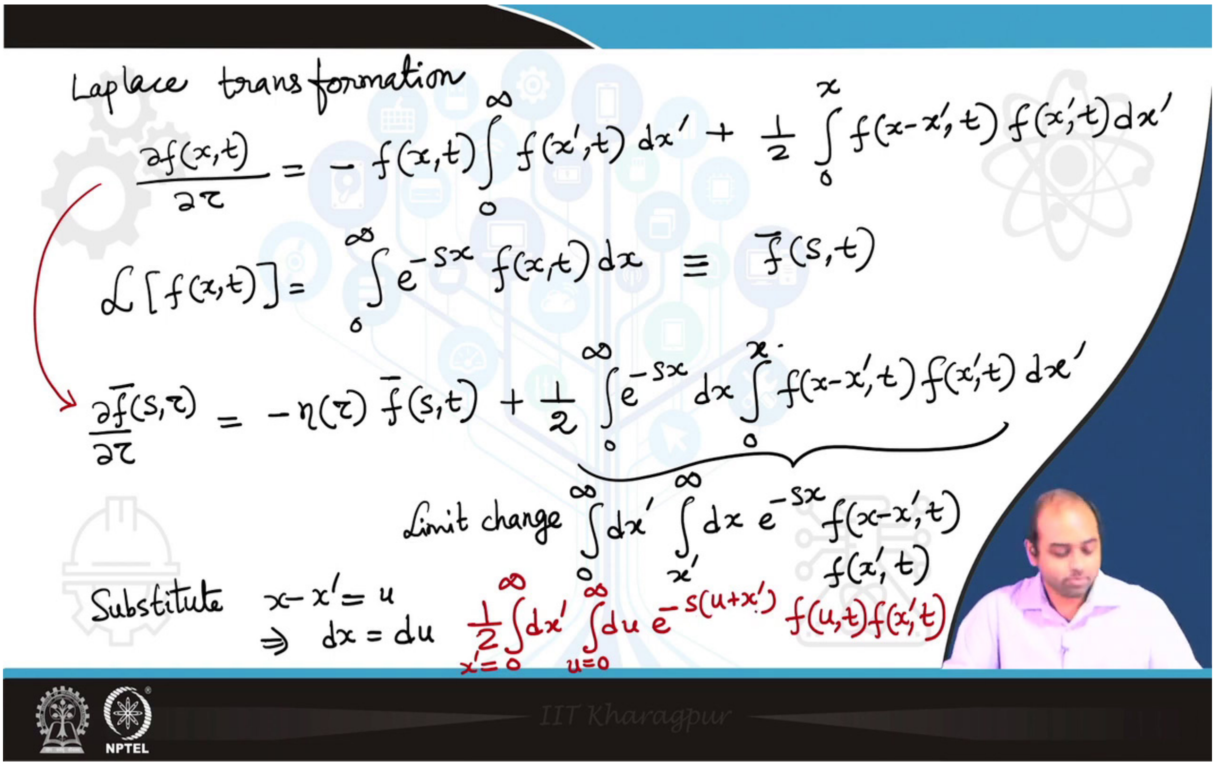

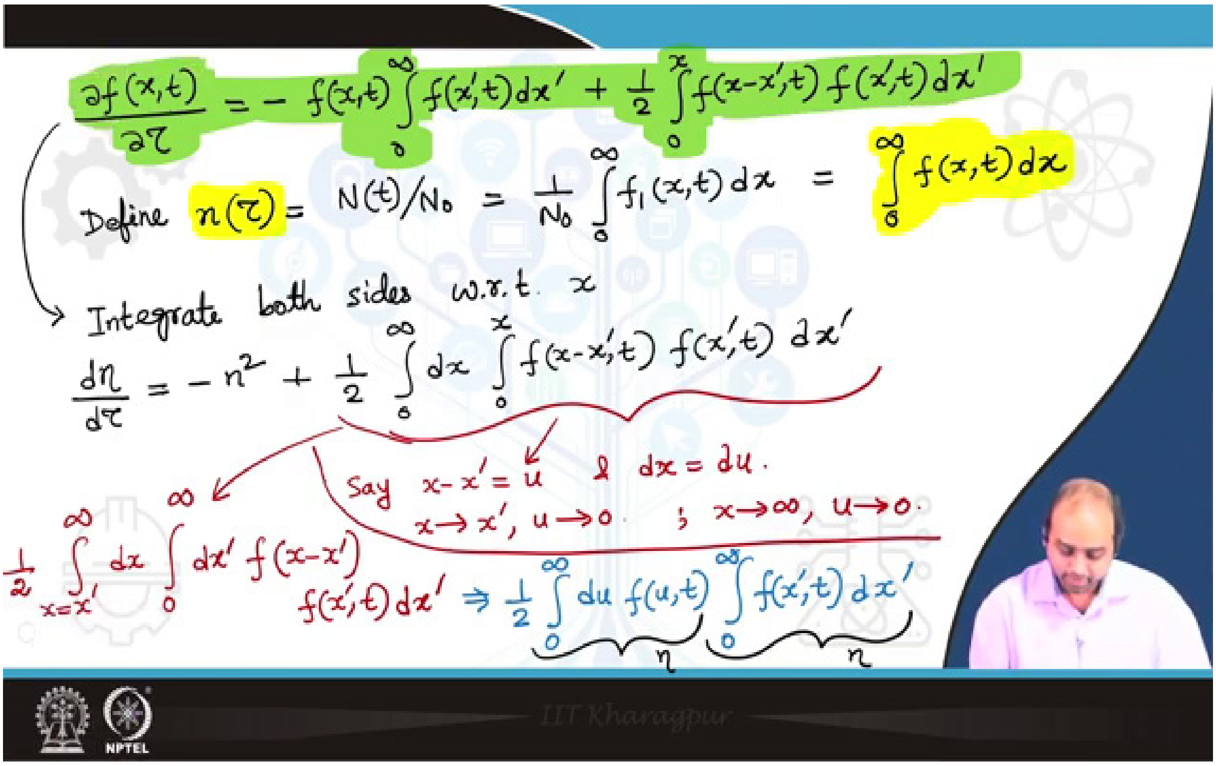

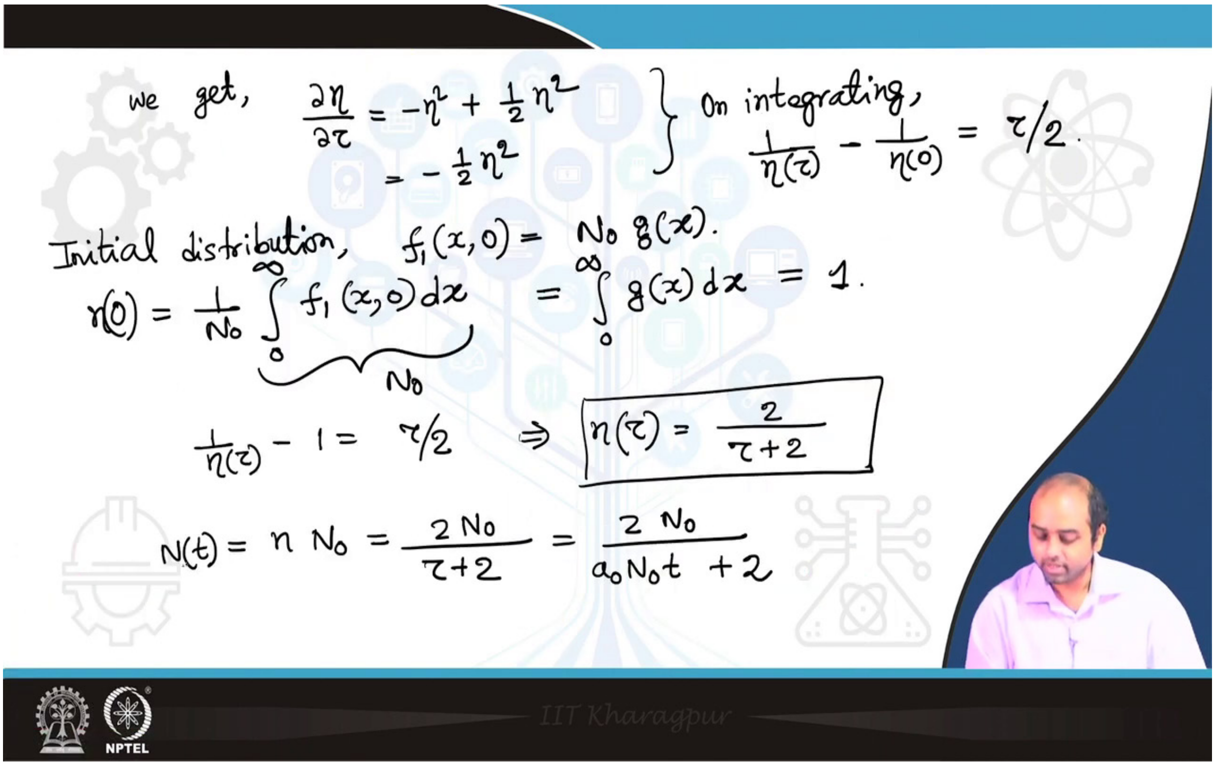

So, to find out what is f1, we need to do. I mean the next step we need to work out in this problem is to do a Laplace transformation and which is the starting equation. So, the equation where we removed all the subscript one, so, this is the equation. So, this is the equation, the top equation that you see here, this is the starting equation for the Laplace transform from here we will apply the Laplace transform, over this equation we will try to apply the Laplace transform. And at some point, of time or at the end, we will try to utilize the information that we got for, the integration of this quantity of this f1.

So, let us write down that partial PBE population balance equation in terms of f not f1, this was the equation. So, if your motive or the final conclusion is to have an understanding of variation on the total number of particles with respect to time, then whatever we have done just before here is sufficient. I mean this gives you that how N t is essentially changing with respect to time, is inverse of the time and based on the initial distribution you can find out all everything.

So, this is for the case of when we try to find out the total number of the particles with respect to time how it is changing, but to find the particle size distribution, we take this extra step and kindly follow this carefully. This was the starting equation; we are doing for the Laplace transform. So, this Laplace operator, we define over F is equal to, this is the classical definition of the Laplace transform e to the power minus s and then x, x is, this S is the Laplace variable this is the, this, what we called exponential function is the cardinal to the Laplace transform, which we have started on the beginning of this course, sometime, long back. And this is we define as f bar in terms of the Laplace variable s. So, we are applying the Laplace transform over the x domain not our time domain, in this case.

So, everything we are converting. So, with this transformation, I can convert this equation as df bar, d tau f bar is in terms of s and tau, eta tau, f bar, s comma t, s half of. So, to apply this Laplace transform essentially put an integration of e to the power, when with this cardinal. So, this leads to this form now that we are having because already there is one integration term present here, and half of 0 to infinity, e to the power this cardinal we write dx and the remaining terms. So, here also we try to do the similar change of limits and these variables.

So, here we try to do a limit change, so, we do the limit change as 0 to infinity, dx prime and here we do it from x prime to infinity and if you look carefully, you already said this these two remains the same and the entire region is covered with this even though with this limit change.

Next, we do this substitution same as we did it before, this x minus x prime as u, so, this means, we have dx is equal to du, so, with this limit change and with this change of the substitution, this integral now looks like 0 to infinity, this is for x prime and this is for u is going to 0 to infinity, du. Next, we have e to the power minus s and u plus x prime and then we have f of u t and f of x prime, these are the two quantities that we have. And if you follow carefully if I break this s, u and I mean this need to be per u plus x prime will be broken down into s u and then x prime.

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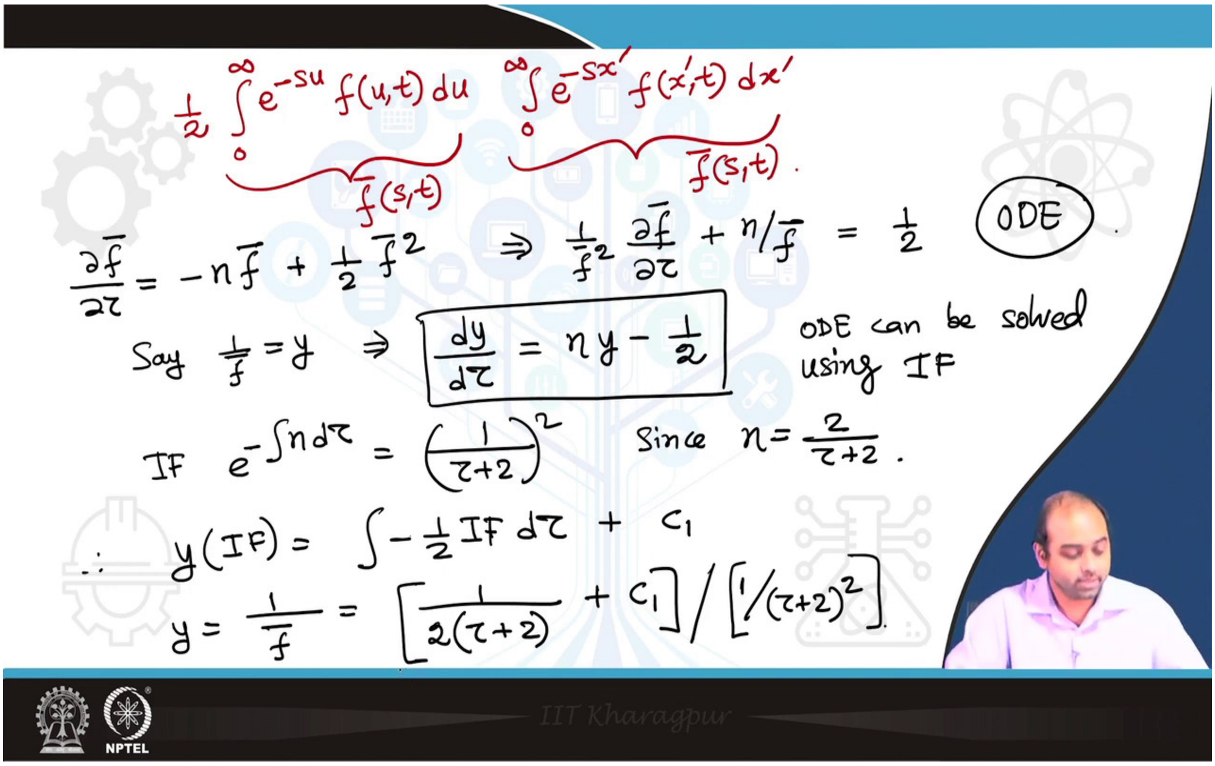

So, let us write it out explicitly, so, this term would be looking like half 0 to infinity, e to the power minus s u, f u comma t du and then there is another term 0 to infinity, where we have e to the power minus x prime s x prime f of x comma t, I am sorry x prime dx prime. So, this means, this is nothing but f bar, s comma t and this is also another F bar Laplace transform of s comma t. So, the final equation looks like the Laplace transform equation df bar d tau is equal to minus nf bar plus half f bar square. So, if this equation is like 1 by f square d, I am sorry, f bar square df. So, this is now algebra, we try to solve this, differential equation is equal to half, this is an ODE.

And you know that this sort of ODE, let us say we do this one more transformation say I write 1 by f bar as y. So, I can get as dy d tau is equal to ny minus half, this is something I will be getting and this is a classical ODE that can be solved with the help of the integrating factor, this ODE can be solved using integrating factor.

So, what is the integrating factor in this case? The integrating factor is minus n d tau which is equal to 1 by tau plus 2 whole squares. Since, we know n is equal to 2 by tau plus 2. So, therefore, we have y multiplied with the integrating factor is equal to integration of minus half integrating factor, d tau plus c1. So, ultimately this looks like y which is equal to 1 by f bar in this if you work out you will be getting 1 by 2 tau plus 2, plus c1 whole divided by 1 by tau plus 2 square. So, this is the solution of f bar or the Laplace domain thing.

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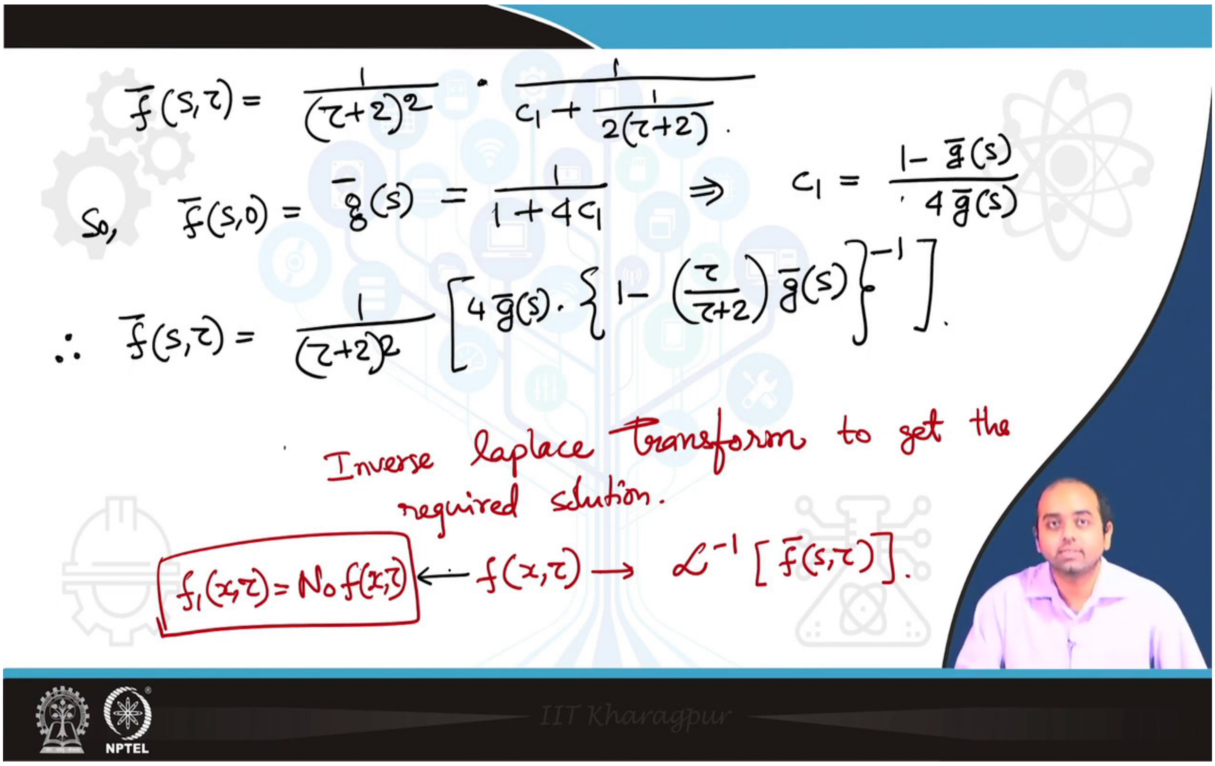

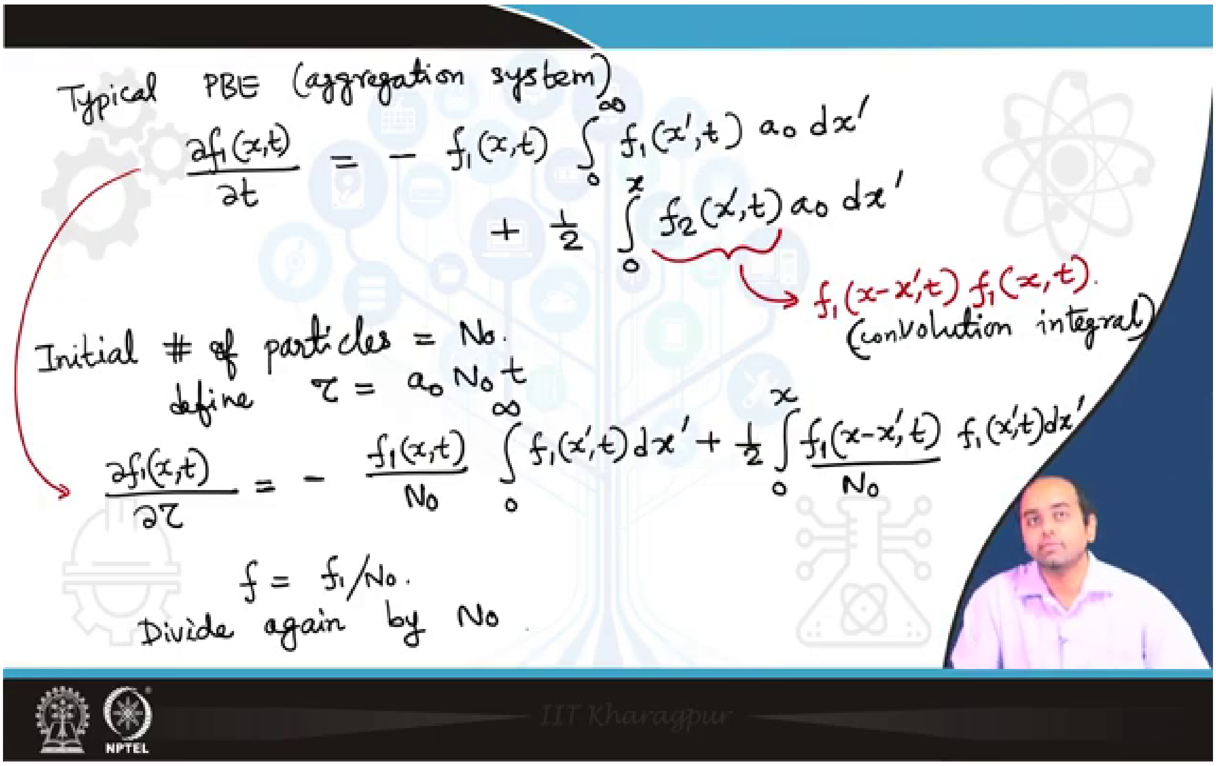

So, let us write it down more explicitly in terms of f. So, f is s comma tau, so, I just inverted. So, I get tau plus 2 whole square, multiplied by 1 by c1 plus, this is what I get as f bar. Now, what about the boundary condition that also is transformed in the Laplace domain, essential that needs to be worked out in the Laplace domain. So, depending on this condition, this is 1 plus 4c1, if I put this tau is equal to 2, I will get this quantity, is not it?

So, this can represent therefore, C1 as 1 minus s prime by 4g s. So, therefore, this one now becomes a complete solution in terms of g bar s. So, you can do inverse Laplace transform, this f you can do inverse Laplace transform, we are not going to do it in this class, but what is the technique, inverse Laplace transform can be done for this case, numerically also you can do, to get the required solution. So, this f x comma tau is nothing but the Laplace inverse of f bar and this, from this f we can also work out what is our f1. Because there is the f1 is f1 x comma tau is equal to N naught times f, is not it?

So, like this we can attain the number density function, the solution or to the number density function with the help of a Laplace transform and before that we tried to do that integration technique and find out the total number of, this number, I mean, total number of particles present in the system by integrating this everything out.

So, this is a way or perhaps analytical treatment and how we can solve the partial, sorry the population balance equation under some certain conditions. I mean some simplified conditions, when this convolution integral. I mean essentially when we have this integration of f2 or the pair aggregating, number distribution from that point, it is actually a convolution integral. So, if you look back, so, this is essentially a convolution integral and this is the convolution integral, convolution integral, which is something we tried to handle herein and then found out a specific solution in this case.

So, I hope all of you understood and once again this is another example of the application of Laplace transform in this case. So, I hope all of you understood that how the population balance equation can be handled. And how Laplace transform comes in so, handy in this case of the situations.

So, in the next class, we are going to talk about that numerical solution of the population balance equation, using the method of discretization of this PDE equation. Thank you. I hope all of you, found this quite useful. And once again, thank you for your attention. See you in the next class.