Mathematical Modelling and Simulation of Chemical Process
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Lecture 48
Dispersed Phase Modelling – Breakage Process

Hello everyone, in this class today, we are going to talk about the breakage phenomena. I hope all of you recall in the last class we are discussing about how breakage is an important physical phenomenon and how do we account for in the population balance equation or in the dispersed phase modelling.

So, during this breakage process, it leads to the formation of the daughter particles and these are generated or produced from the parent particle. And of course, there are three factors or three functions which based on which this breakage phenomenon is actually depend on. So, the three factors are one is the breakage frequency, one is the, this number of particles which is formed during the breakage, the other one is the, this daughter size distribution.

So, these three functions essentially describe the whole of the breakage process. And the loss of the parent particles during this breakage process is written down as a sink term or the loss of the particles from the number density function and the generation of the new particles of a different size of a smaller size, this is what we refer to as the daughter particles are in fact, the source term to the population balance equation.

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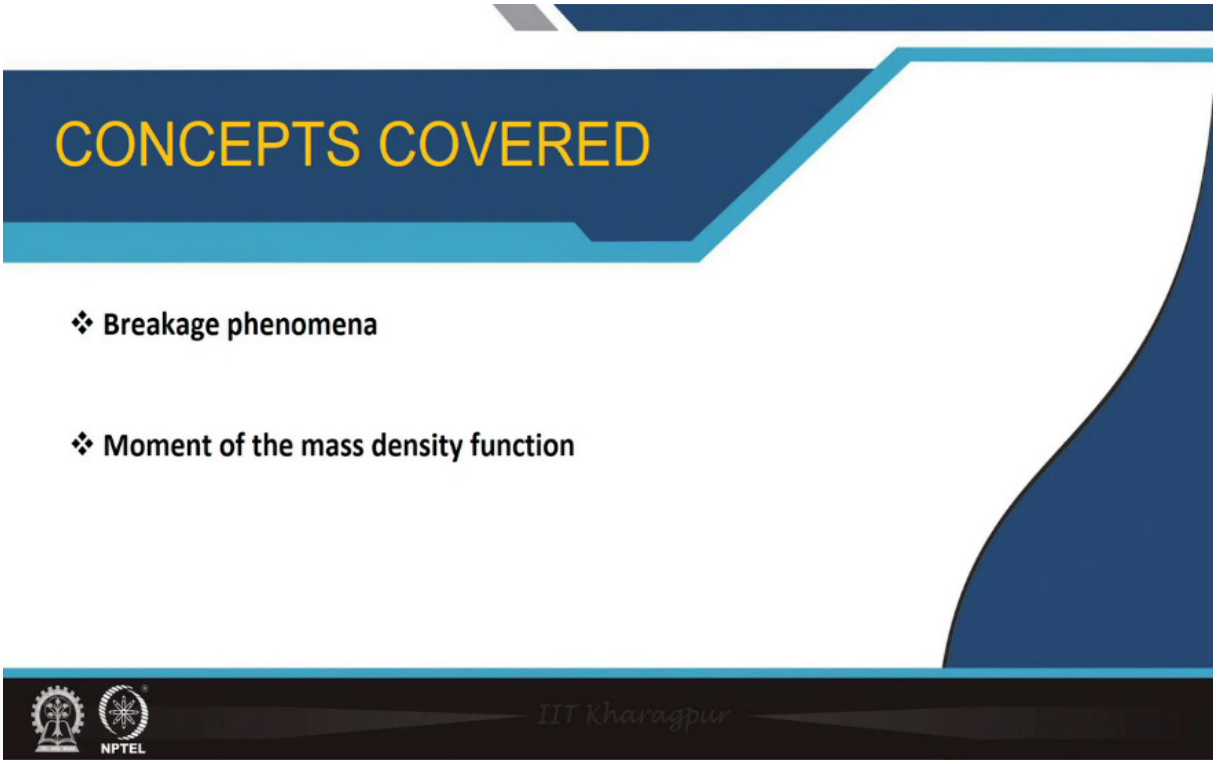

Now, typically the applications of these. So, in this class we are going to talk about the more details on the breakage phenomena and we also looking to the mass density function during this breakage process and we see that the mass density is actually conserved or the moment of the mass density function is actually conserved for the first order moment.

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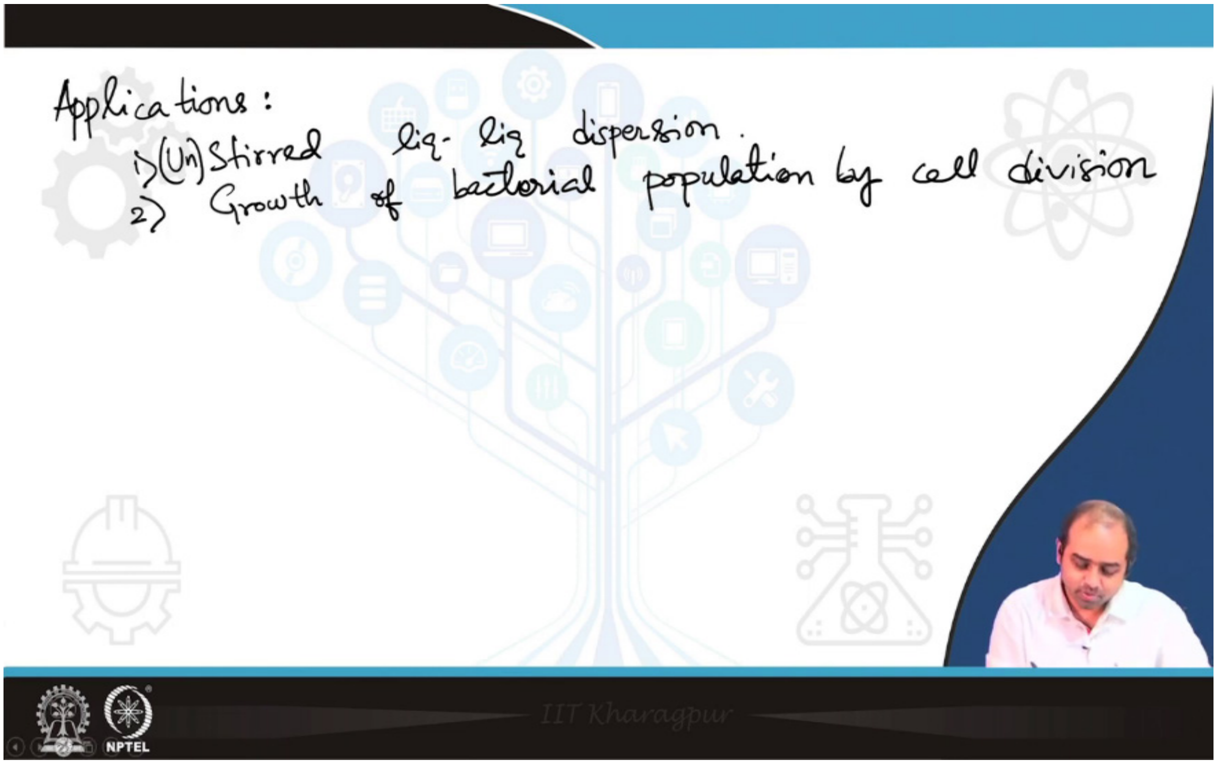

So, this in this first let us try to let me just list down some of the applications of the breakage phenomena. So, typically the applications that we the applications are this stirred or unstirred, liquid-liquid dispersion where you have one immiscible phase that produced. So, there is one dispersed phase and one continuous phase. Another example of the breakage is growth of bacterial population by cell division.

So, cell division or reproduction of the bacterial colony can also be represented as a sort of breakage process where it disintegrates into, I mean this fission, binary fission or whatever fission we talk about for the bacterial cell growth. It is essentially reproduction and leading to the formation of new particles of smaller size.

So, the mass overall mass that is introduced into the system by the substrates or the food et cetera is actually can be conserved hold together that can explain the formation of the new mass. Stirred liquid-liquid dispersion could be stirred, could be unstirred, is again when you have one dispersed phase and one continuous phase.

So, that dispersed phase is actually immiscible in the continuous phase. It could be dispersion of oil droplets in water or water droplets in oil. Similarly, it may be also fluid like air bubbles or bubbles of a particular gas in a liquid that is another application and the you have some mechanism at during this action of a shear or external forces, let us say ultrasound or some mechanical stirring, these particles can or whatever these dispersed phase molecules or droplets that we have can essentially break down and leading to the formation of new smaller sized particles.

So, if you do not have stirring then there should be some other means of breaking up these particles as I say ultrasound, it can be some sort of other mechanical action, but if you have a stirring that means stirring itself acts as a external force that helps in further breaking up of these droplets or the dispersed phase or the emulsion particles or whatever. So, consider now, let us look into some more analysis the details of this breakage thing.

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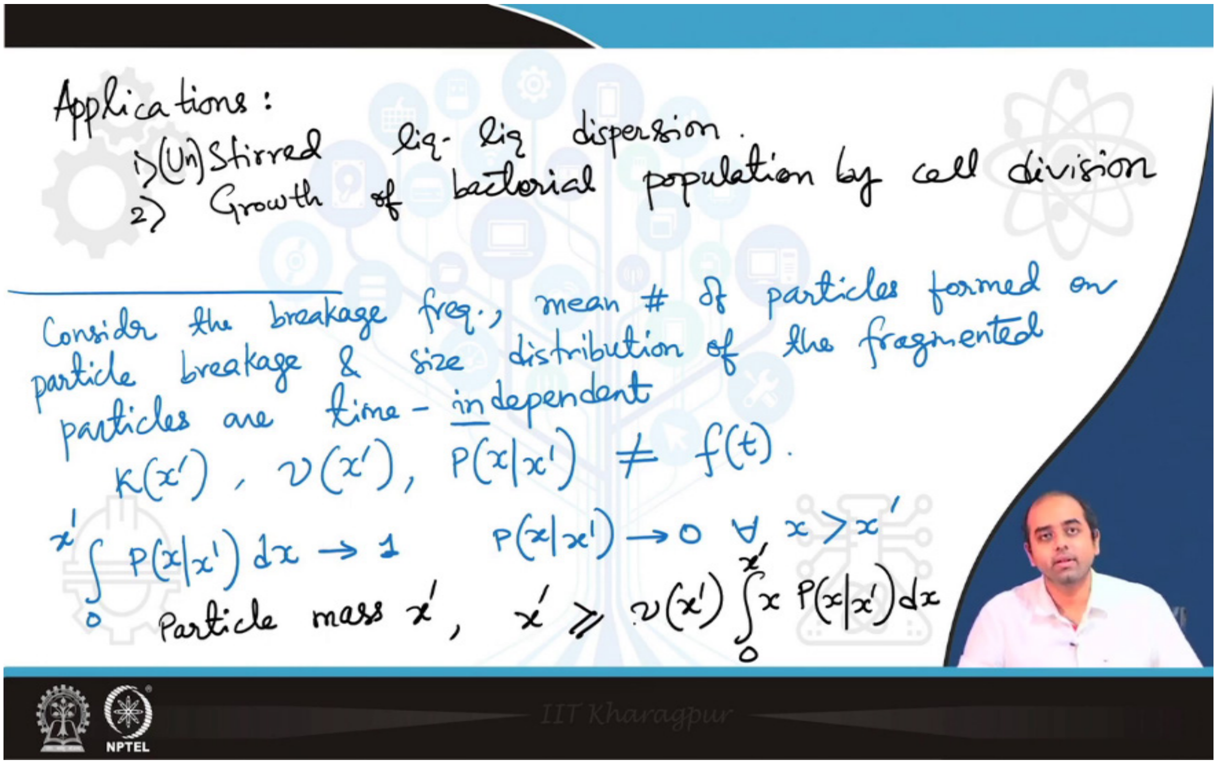

So, consider if you consider that the breakage frequency then these mean number of particles formed on particle breakage and the size distribution after fragmented particles are the broken up particles, are time independent. So, these functions the particle frequency is only a function of the internal coordinate not time, number of particles formed are only function of the internal coordinate P x x prime all these are not function of time anymore.

So, of course, then if we have this integration of the probability distribution function of the daughter size particles, 0 to x bar. this will be equal to 1, P x x prime will be equal to 0 for x this thing and if we consider that the particle mass is consider that this x prime is nothing but the particle mass, then we also have this inequality. This needs to be satisfied. So, the utility hood will hold if there is no loss of the particles during the process.

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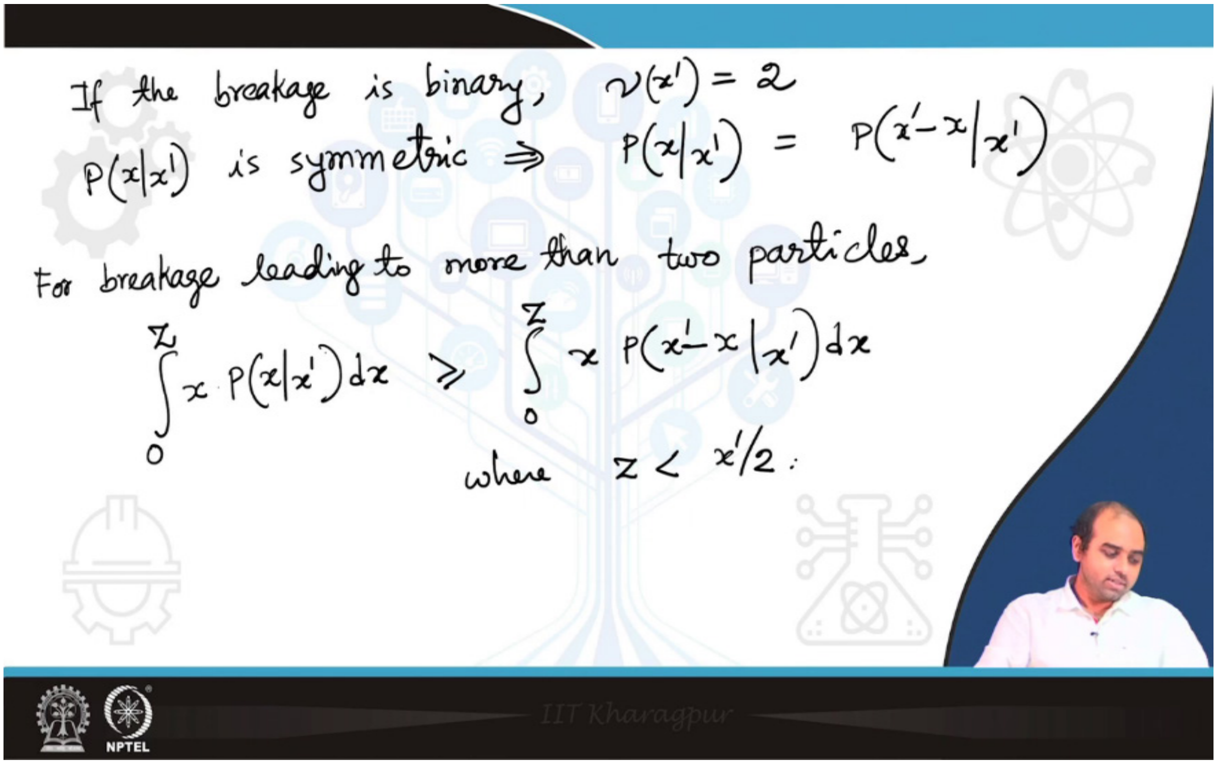

Further if the breakage is binary, if the breakage is binary. For example, cell division. So, this nu is equal to 2. So, there are two particles which are forming on breakage of the parent particle. So, then in that case this daughter size distribution is symmetric. So, by symmetric we mean that P x x prime is equal to P x prime minus x of x prime.

So, because the probability density distribution function is like the number density function of the different particles that are formed with this breakage and the breakage is always binary then there would be the particles that are forming would be almost not almost would be actually identical in nature, is not it? So, if the original mass of the particle is x prime, then if it is breaking up into two particles, then these two particles would actually constitute the total mass of the parent particle.

So, ultimately over the range of 0 to infinity, you will be getting always two size, I mean they are the size distributions of these particles in this entire domain. There will be some part of the I mean there will be some region of the daughter particles which has the same distribution as the other half, because these two has to be same to constitute the parent particle. So, if there is some part of the particle and there should be another complementary part and these two would be equal.

So, always if let us say 1 size of the particle is 0.1 then another would be 0.9. So, in the other way around if there is 1.9 particle which is forming the other one has to be 0.1. So, there has to be symmetric. If we from breaking up a particle you can get I mean the two size of the particles one of the size can be anywhere from 0 to let us say anywhere from 0 to 0.9 or close to 1. If I am talking about in a percent or a fraction sense, then there would be another particle would be always 1 minus of the x.

So, it is like the summing up the mass of that particle should be equal to the parent size of the particle. So, this has to satisfy if the breakage is binary, this we can easily understand from the binary breakage process, but if the breakage involves. So, for breakage involving more than two particles, not involving, leading to more than two particles then this inequality has to be satisfied, 0 to let us say this z.

So, this inequality suggests that the number of particles up to the size up to this size, half of the parent size particle, in that limit would always be greater than the particle size distribution that we are seeing for the case of x prime minus x. So, in the case of this equality, these two would be equal.

So, particles that are disintegrated into two particles all the size range from 0 to 0.5, I mean if I am talking about a unit fraction, all the size range from 0 to 0.5 would be same as the number of particles from 0.5 to 1 because then only this would conserve and this would tell us that the overall mass balance is satisfied.

But if there are more number of if, there are particles or more than I mean if there are more than two particles or these breakage average number of particles form by more than two, in that case this equality will not hold and then we will end up with this inequality. So, whatever fraction of the particles we are thinking of is forming the other complementary fraction would be always less than this because there are some intermediate range of the particles which could also form. So, please think about it this leading to the inequality that how it is established.

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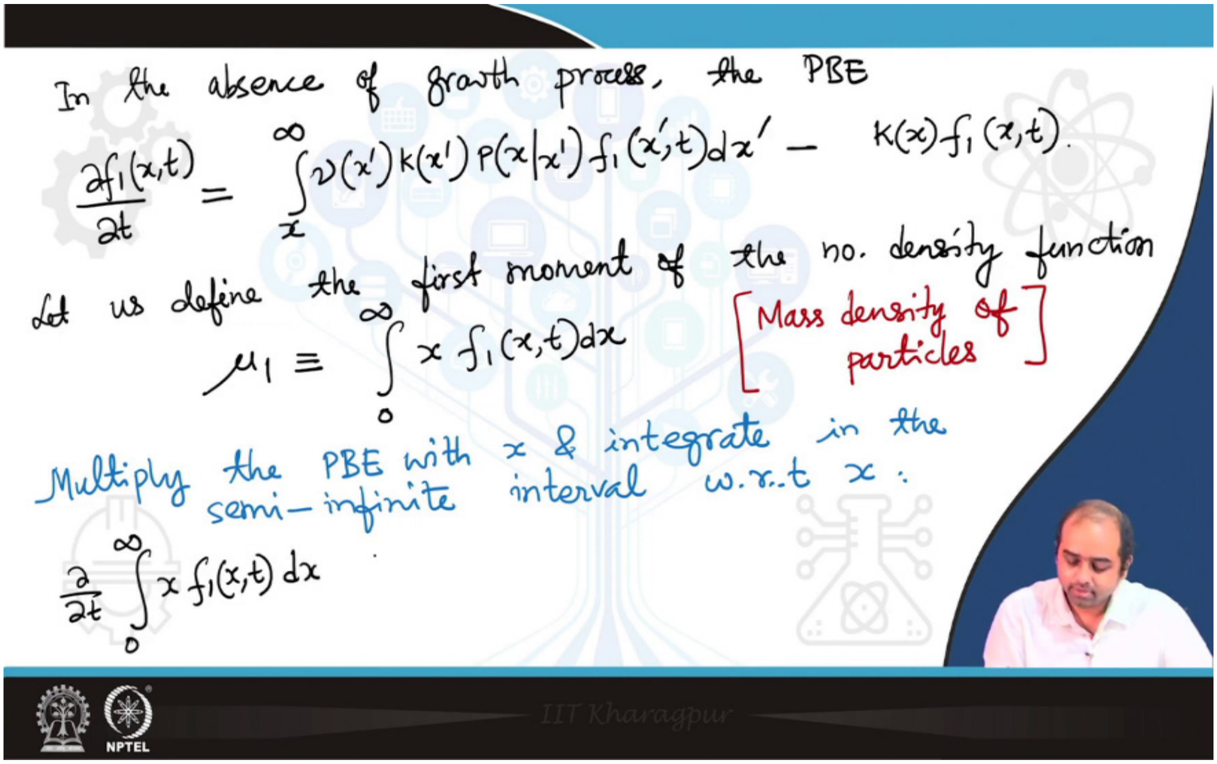

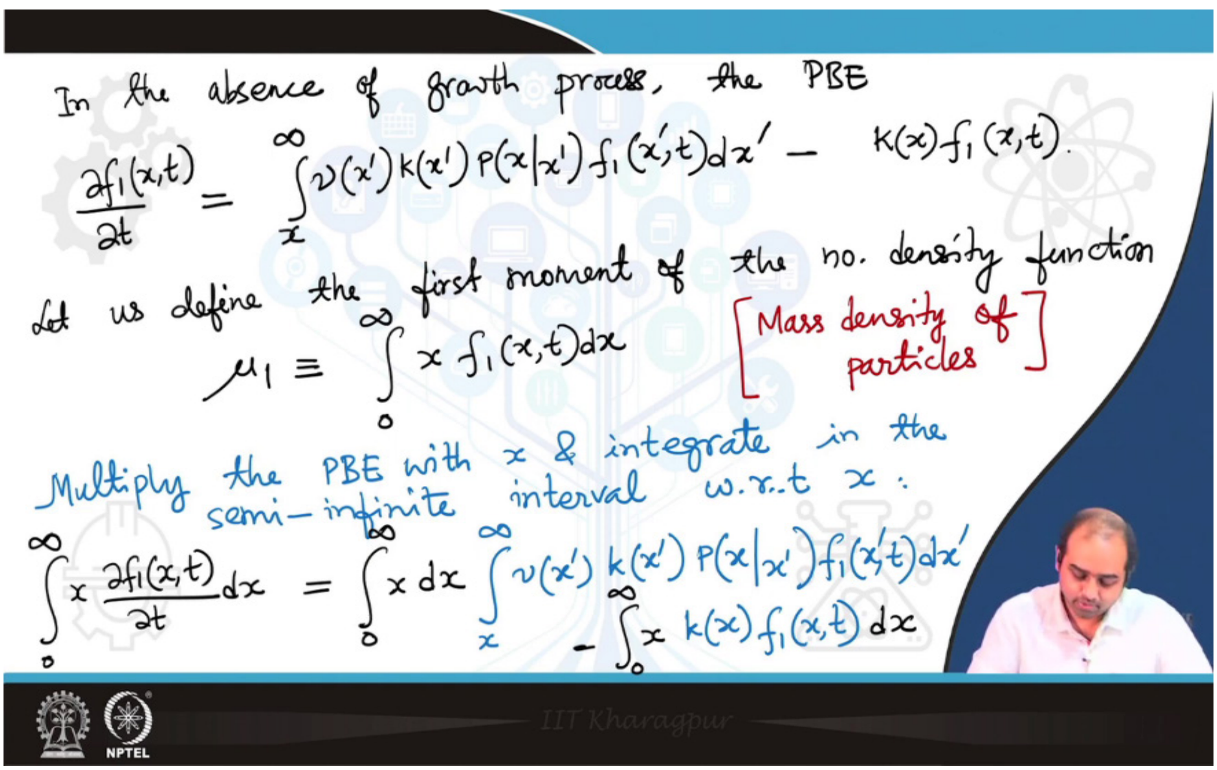

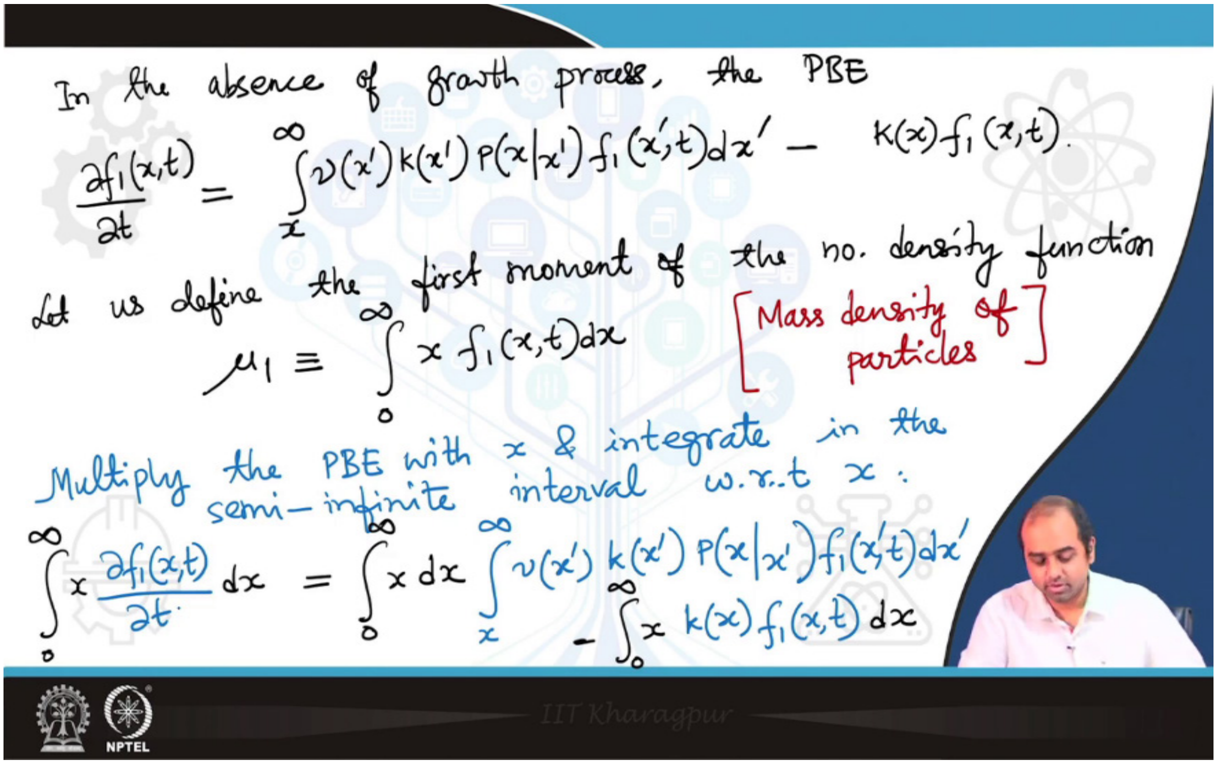

So, now, let us look into the PBE equation and let us try to understand the first moment of the number density function. So, in the absence of the P in the absence of the growth process, but we have breakage. The PBE can be written as this one. So, there is no growth so nothing on the lefthand side, then we have the right-hand side. This is h plus term, and this is the h minus term, breakage frequency into the number density function. So, this is the PBE equation in the absence of growth but with breakage. Now let us define the first moment of the number density function. So, I am defining the first moment as nu 1, which is like this.

From 0 to infinity, this is I am defining as the first moment of the number density function. So, in a way physically this represent the mass density of particles. So, we want to track that how does the mass density of the particle change with time during the breakage event. So, to do that, we what we can do is that we multiply the PBE, multiply the PBE with x and integrate in the semi final interval with respect to x. So, what do you get? On the left hand side we do the multiplication.

So, I can take d dt outside x f1, is not it? 0 to infinity. This is the lefthand side we have, that I can do, or better to write the d dt function inside. We go step by step, this is the lefthand side the first term I write x dx and then I have the remaining so, this is the remaining part that is from x to infinity. This is the first time that I have multiplied with x t and integrated out and the second term also I am having the, this integration x and then the remaining term is there k x f1 x comma t. So, let us, this also change let us change the colour of this one.

So, whatever is written in blue, represent the PBE equation whatever extra thing we are doing multiplying with x and then integrating in a semi-infinite interval is written in shown in black. So, let us look into what happens to the left-hand term.

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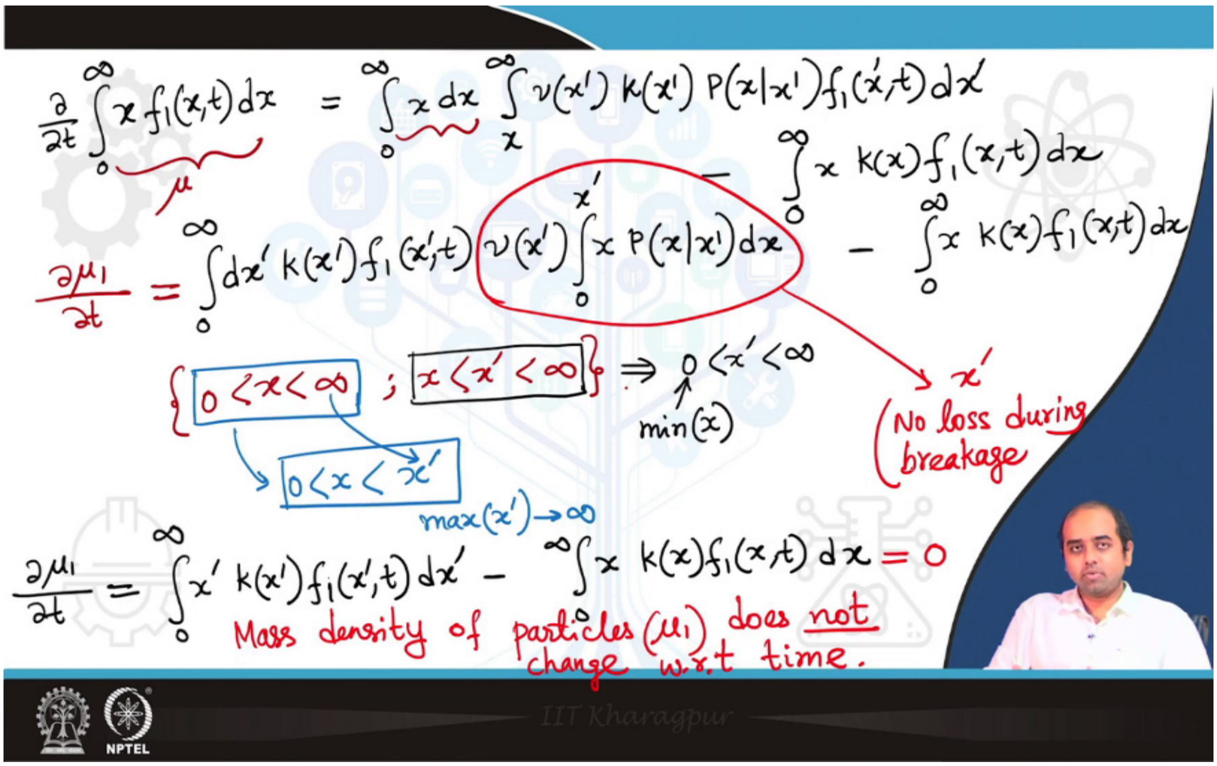

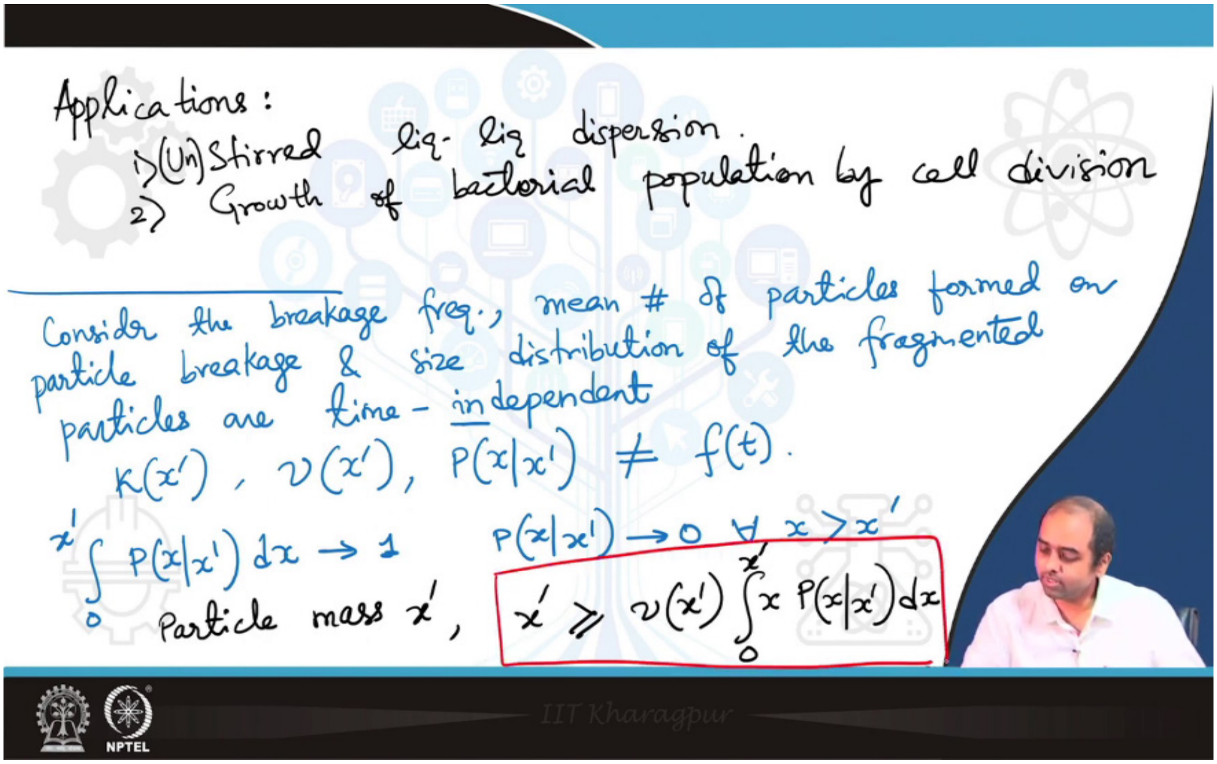

So, the left-hand side can be written down as I can take the d dt outside and multiply with x f1 x comma t dx 0 to infinity. Now, in the right-hand side this thing exists 0 to infinity then I have x dx integration of this thing is there, h plus and this is the corresponding. Please note here all the functions are independent of time.

So, the left one side this is nothing but mu 1 so the lefthand side I can write d mu 1 by dt. Now for the right-hand side there is something I want to discuss here, let us see that in this part of the integration x dx, I mean we are having over the limit of 0 to infinity. So, the limits of x that we are having here is from 0 to infinity, this is the limit of x. And for x bar we are having the limit x to infinity. These are the limits we are having in the above integration at least the first term in the above integration, the limits of x prime is from x to infinity and the limit of x is from 0 to infinity.

Now, carefully think on this part, that if x prime is from x to infinity and the lower value of the x is 0, then it is equivalent to saying for the x prime at least x prime it is starting from 0 because the minimum value because that is the minimum value of our x. Since x can reach 0, x prime can also reach 0. So, the lower limit of this x prime from x to infinity is same as saying the lower limit is from 0 to infinity because x prime also reaches sorry x also reaches 0.

So, these limits can be modified in this case after x prime from 0 to infinity and for this case, this case we all know that x is the daughter size particle. So, infinity I mean x is only restricted up to x prime beyond x prime the existence of this x or the daughter size particle does not there I mean does not arise. So, the higher limit of x is only up to x prime. Of course, I know x prime can also reach to infinity. So, this is also seen as or equivalent to saying that x is restricted up to x prime and where x I mean x can reach infinity provided x prime which is infinity then only it is possible.

So, this is the change I can make here. So, the x prime max value of this is possible because the max value of x prime is infinity. So, instead of writing infinity, I can write that as x prime. So, for the case of x, I can change the limit instead of 0 to infinity I can write 0 to x prime where x prime of course, which is infinity and in the case of the x prime instead of writing x to infinity I can write from 0 to infinity.

This change or this recasting of the limits of the independent variable can be done in this case this top equation that you see here or the h plus term corresponding to the H plus term. So, if I can do this, then what happens is that, from 0 to infinity I can write k x prime, and also write, let me write the dx first so not to confuse you. So, I can write something like this. All the x prime things. This is all x primes, and I can put that limit from 0 to infinity that is like becomes like the now the outer limit of the problem because that is like covers the entire domain and in the internal limit, we have 0 to x prime x P x x prime dx.

Because please note that the existence of P is only up to x prime. So, it does not make sense to put it in the outside because that value would be 0. So, P x with respect to x prime only exist up to the limit of x prime not beyond that. So, even if I say that extends up to infinity that part will be 0.

So, P x beyond x prime is essentially 0. So, this and then the remaining part all exist as it is. So the remaining part is x, kx, f1 x comma t dx. So, this is 0 to infinity. Now, please note that this part this part of the integral, this is x prime from the mass balance. If you recall, this is nothing but our mass balance, is not it? For no loss during the breakage, I think this is something we already talked here.

So, if you recall this relation, this is what we get as x prime. So, this quantity is nothing but our x prime. So, the left, so, the equation now looks as d mu by dt is 0 to infinity x prime then I have k x prime x prime t d x prime and minus off this, is not it? And if you follow closely these two functions, these two integrations are equal only in one case it will expand another case is x, but in the limit of 0 to infinity, I mean, I can always change the independent variable and these two are equal.

So essentially, this means that the change of the mass density of the particles does not happen with time during breakage. So this is the important conclusion that we draw here that the mass density of particles does not change mass density of particles that is mu 1 does not change with time during breakage. So, this is an important conclusion that we get from the first moment analysis of the population balance equation of the breakage phenomena. So, the mass density of the particles does not change with time.

So please remember this one that even though if you have breakage, the mass density of the particles does not change with respect to time. So, it remains constant or time invariant. So, even though if you have breakage, the average mass density does not change with respect to time. So, I hope all of you understand this that this is an important part here that no loss during breakage then only this equality holds. And x prime we have said already is the mass of the particles.

So, I hope all of you got this idea on the first order moment analysis of the breakage process and we have proved that the loss or the there is no change in the mass density of the particles during these breakage phenomena. And this is based on the fact that there is no loss of particles during the breakage event and all the mass that is present in the parent particle and that the summation of the all the rotor particles or the mass of all the rotor particles is equal to the sum is equal to the parent particles. Unless there is loss of mass, the mass density does not change. So, thank you for your attention. In the next class we will talk about realistic problem on how to explain the drop size distribution in a lean mixture so dilute mixtures. Thank you everyone and see you in the next class.