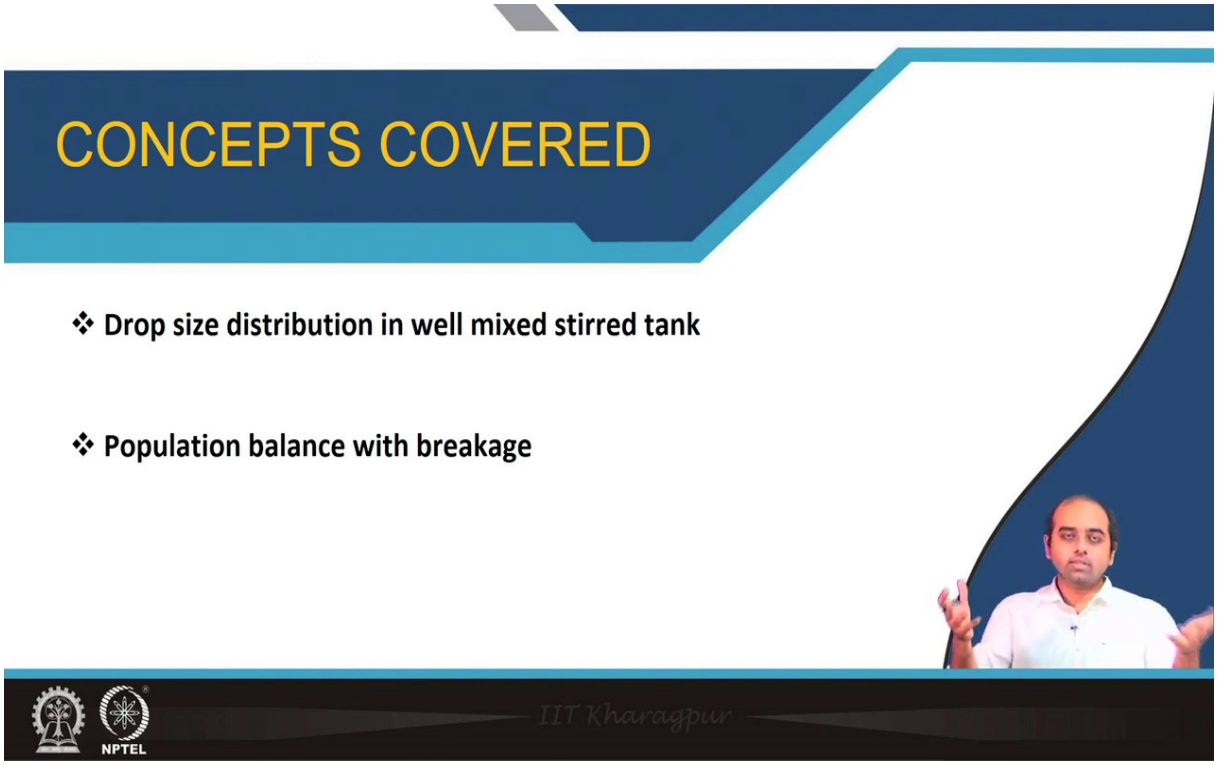
Mathematical Modelling and Simulation of Chemical Process
Professor Doctor Sourav Mondal
Department of Chemical Engineering
Indian Institute of Technology, Kharagpur
Lecture 49
Drop Size Distribution in Lean Mixtures

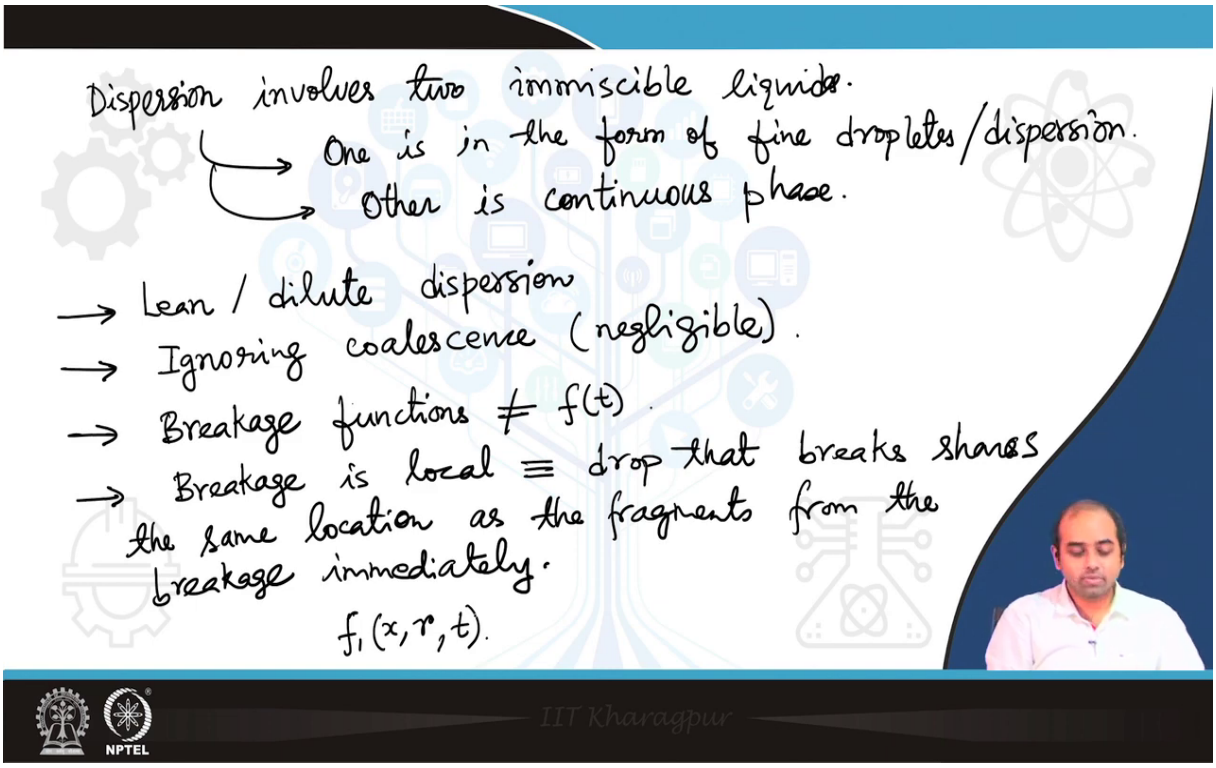
Hello everyone, in this class we are going to talk about the drop size evolution or the drop size distribute evolution of the drop size distribution in a stirred lean mixture or the dilute mixture.

(Refer Slime Time: 00:43)



So, here we are going to talk about that how does this drop size distribution actually evolves with respect to time and how do we frame the population balance equation considering the breakage phenomena due to this stirring of the dispersed phase.

(Refer Slime Time: 01:22)



So, before we start the model or try to frame the modelling aspect, it is very important to understand some of the assumptions involved in this process. So, this dispersion whatever we are talking about or this dispersed system that exists here. The dispersion involves two immiscible liquids, as I said it could be oil in water or water in oil.

So, essentially one is in the form of fine droplets or dispersion and another is essentially a continuous phase. This is the generally how do we describe our dispersion is that one always exists in the form of a dispersed phase or the quantity which is less in volume will form the dispersion and another will be in a continuous phase and the dispersion is often present in the form of fine droplets or fine particles like that could be a suspension could be a emulsion. So, this is how a dispersion actually looks like.

Now, in this case when we are having I mean when we are talking about a lean mixture, each means that the mass or let us say the volume fraction of the dispersed phase is very small. Essentially it is very dilute. So, it is a lean mixture, or other words it is like dilute dispersion. Then since we are having stirring essentially to break these droplets and create fine dispersions or fine droplets or reduce the average droplet size, in this process we are ignoring any

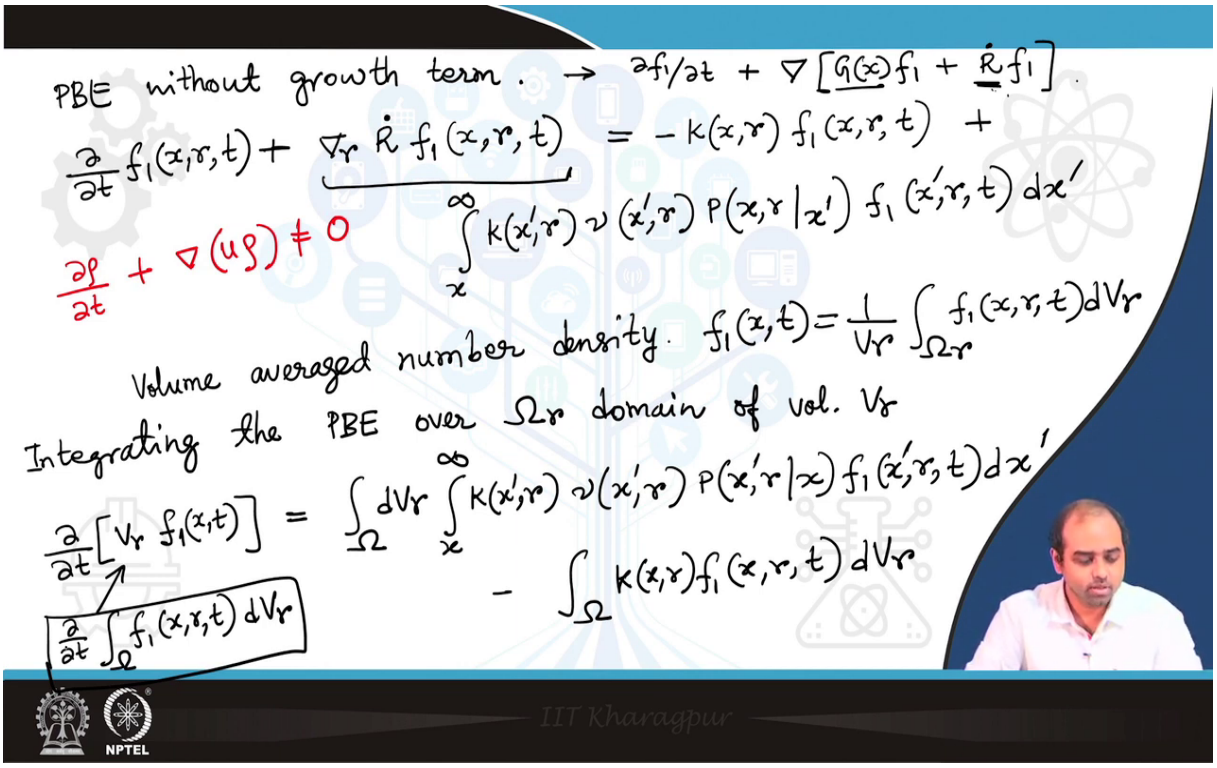
coalescence. So, we are ignoring any coalescence that may be taking place or even if it takes place we consider them to be negligible.

Next important thing is that we assume that the breakage function, this number of particles that is breaking the average size distribution of the daughter particles, then the breakage frequency et cetera all the breakage functions are not a function of time. So, they are independent of time. Breakage is local. So, this means that that drop that breaks a shares the same location as the fragments from the breakage immediately. So, this is the these are generally the major I would say assumptions in this breakage phenomena

So, the population balance equation that we try to write for the number based of a number density equation, it will have its internal coordinate as x, but it will also have an external coordinate that is r and r represents the location of the particles or the spatial location of the particles in the system. So, I mean dropping the growth term, assuming that drop size I mean does not grow.

So, we are removing any growth effects in this phenomena, as a growth is generally relevant only in the cases of crystallisation or the particles grow in their size. But other than this discrete phenomenon like breakage or aggregation this cannot be termed as any sort of negative growth or positive growth. It is only the particle without any breakage or aggregation they grow themselves and that is the case mostly in crystallization that you see. So, these number density function is a function of the particle size which is represented of x, r, r is the spatial external coordinate and time.

(Refer Slime Time: 07:26)



So, we try to write down the population balance equation just write it down first and then we see from take it from there. So, the population balance equation without the growth term whatever we have is, sorry, this I missed the r here. So, you must be a little bit intrigued at why I wrote the second term. So, if you recall that the second term of the, this population balance equation generally the term contents the growth function, and growth is sort of the rate of change of the particle size or the internal coordinate in this case this is x.

Similarly, if there are external coordinates present then the then their rate of change of the external coordinates would also needs to be taken into account. So, if you recall the generalized PBE equation we discussed like it is d f1 by dt plus grad of there is some function which is related to the particular coordinate, whether it is an internal if it is internal coordinate and then we have G of f1.

If it is external coordinates present, then ideally it is like G for the internal coordinate and then something would be there for the external coordinate also, which is denoted as R dot in this case. So, if depending on the number of kind of coordinates we are having. So, there could be this presence of these additional functions that present the rate of change of that coordinate.

So, in this case R dot is a rate of change of the spatial coordinates you can think of that to be like the velocity, you can think of that R dot as a function of the velocity. So, the left-hand side if you think is very close, I mean this looks very close to the continuity equation, I mean you can find a close analogue to the continuity equation, where you have the continuity equation in fluid flow as something like this.

So, in this case, u is represented by R dot and rho is the number density function. So, in the case of there is some mass generation and mass accumulation then this, hand side term is not 0 and that is what exactly we are seeing here in this case. So, there has to be this depending on the spatial variable or which this this equation, I mean this PBE we are writing since there is no growth process. So, the function or rate of change of the internal coordinate that function G is not there, but since we are having an external coordinate in this system, this additional R dot does exist and R dot to some extent here relates the velocity of the individual particles. And on the hand side we have the breakage function.

So, let us write down the breakage functions on the hand side as minus k x comma r. So, r represents the spatial coordinates where it is the essential essentially this is the external coordinate for the system. So, f and all other functions are not only functions of x and t, but there is also additional this r is there to denote that what is the distribution number density function at different locations in the tank or in the system.

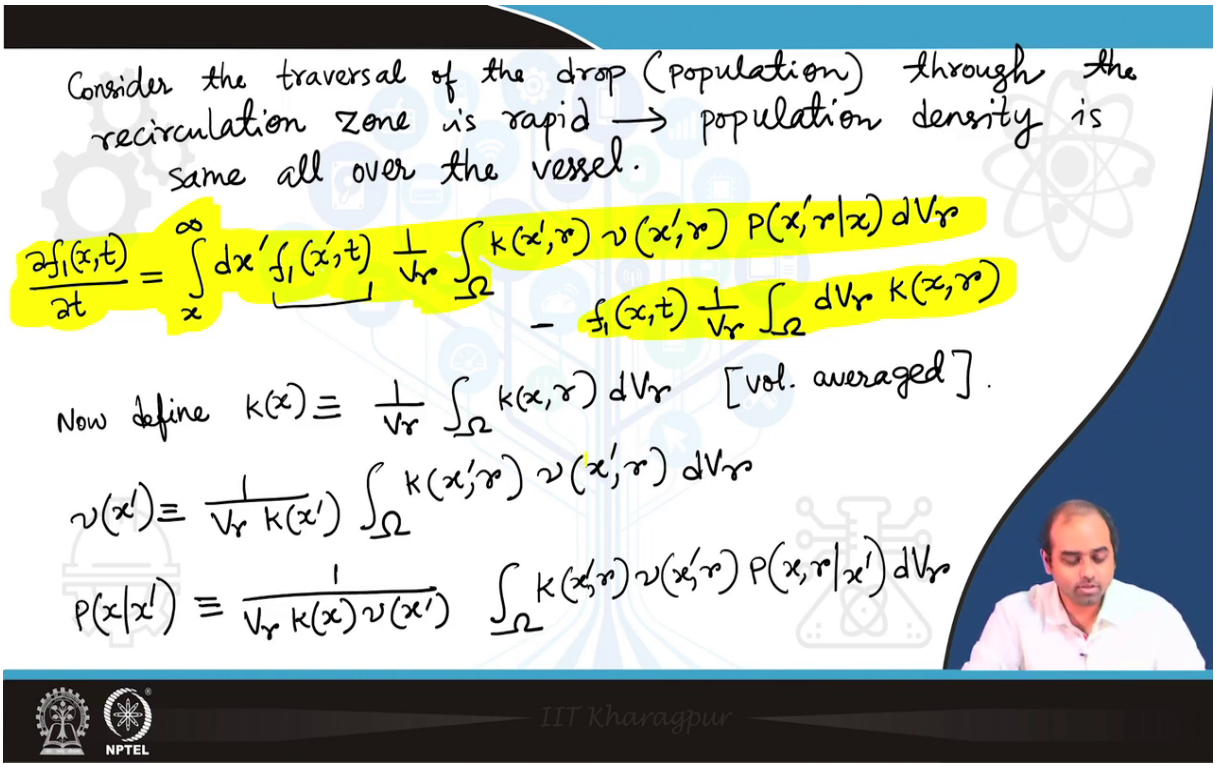
And then we have this integration term x to infinity k x prime r mu x prime r. This is the h plus term on the hand side and the term with the minus sign is h minus term. Now, let us try to define the volume average number density. So, let us define this new volume average number density as same as f1 or if you wish I can also write in to f but let us let us continue with f1. But please note that when I write this volume average quantity, I am dropping the r term, why? Is because I am integrating over the whole spatial domain. So, this is this integration over the whole r domain or whatever this is spatial external coordinate domain.

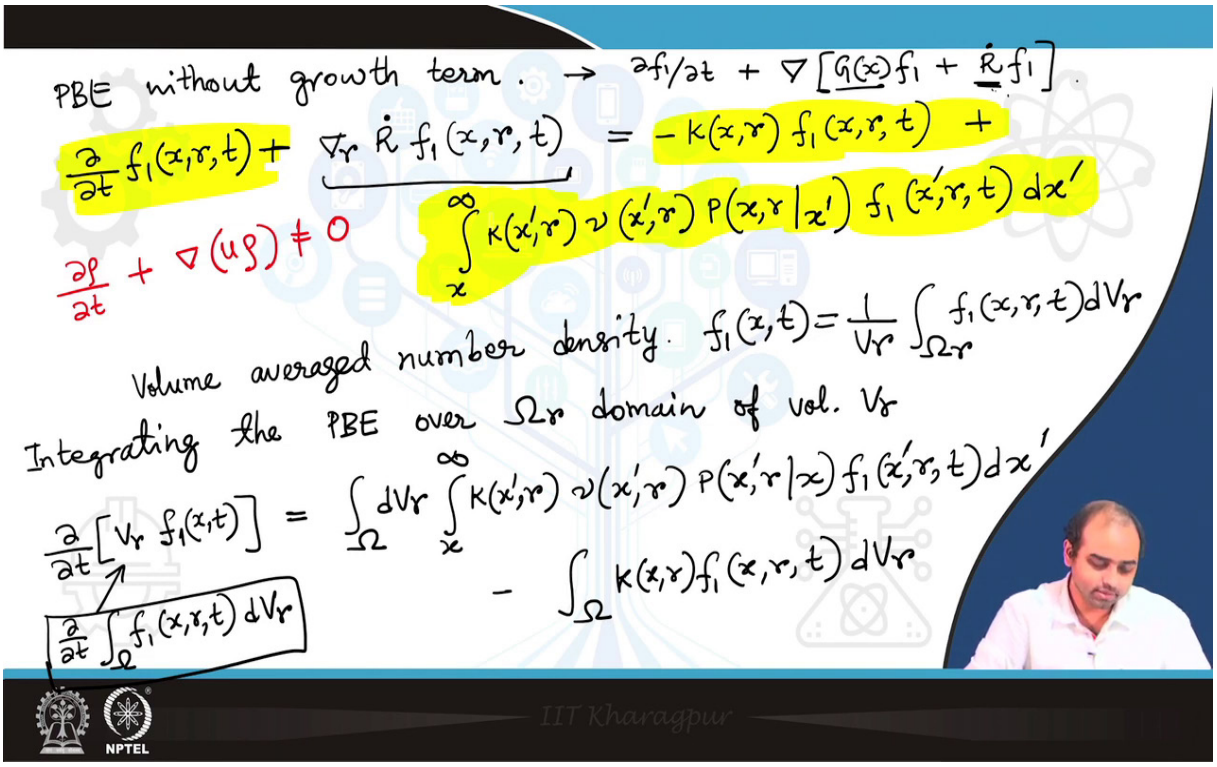
So, if I integrate this quantity and I am trying to get something like a volume average quantity, so, I do not wish to worry about what is happening in the different spatial locations in my system. I am interested to find out the volume average quantities or essentially what is the total average number density in the entire volume.

So, I volume it out I mean I essentially integrate it out across the whole volume. So, the r dependencies now lost, I get the number density function which is now volume average quantity. So, if I try to integrate over the volume this entire PBE equation, so, integrating the PBE over the volume domain of the volume Vr that contains this dispersion, then what you get?

So, we do we multiply both sides on, this is what I get when I try to multiply I mean try to integrate over the domain of this one, I mean if I just do an integration and the left hand side becomes Vr f1 x comma t this is the first term which is equivalent. So, this term is equivalent to integration of and then on the hand side we have this is the first term and this is the second term, is not it? This is what I get by doing an integration of that PBE and this is that is how I replaced the left-hand side of this equation.

(Refer Slime Time: 17:04)





So, now, we consider now assume or you can make an assumption or consider that the traversal of the drop or essentially the drop population through the recirculation zone is rapid, such that it

is so rapid that the population density is same all over the vessel. So, by this what I mean that the region that contains I mean this Vr that we have, Vr is nothing but the volume of the vessel and there is the number density function or the transfer of these drops in all locations of the vessel which is essentially a recirculation zone is so fast that it is uniform.

So, whatever number density function I have in one corner of the vessel is same as that it is present on the corner of the vessel. So, the immediate mathematical implication of this assumption is that in the left-hand side this Vr is not a function of time. So, Vr is essentially the size volume of the domain, essentially the vessel size, but this has to be ensured that this domain is essentially the location over which we are making the averaging of the number density.

So, if I can ensure that only when that the drop distribution in the or the drop movement or their transfers in the entire domain whatever this domain that is denoted or marked by Vr is same. Then essentially here is not changing with time do not consider it is like equivalent to the vessel size vessel size is constant.

But essentially it is Vr is the volume over which we are trying to compute all these this PBE and everything, or the distribution we are trying to track. So this zone of tracking is not changing with respect to time or in other words, we try to say that the drop movement everywhere in the vessel everywhere in this vessel is so fast that this domain whatever we considering everywhere it is same. So, essentially now, the domain that we are looking into is essentially the vessel size and vessel size of course, is not changing with time.

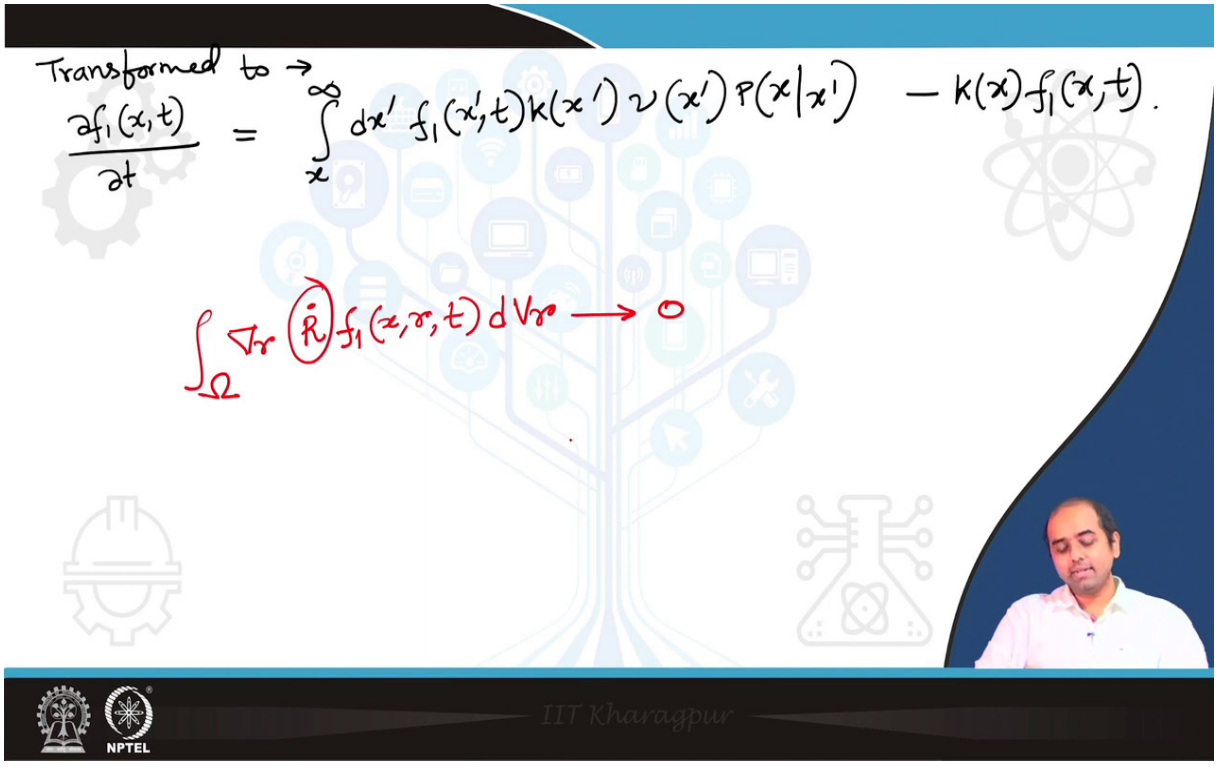
So, with this condition only we can say that Vr is not a function of time and this is only ensured when there is rapid traversal or the movement of these drops all throughout the vessel or at high stirring conditions you can say. So, in this case, we take Vr out from the left hand side and the left hand side now becomes d f1 x comma t dt we drop that fr thing goes over integration in the hand side now becomes sorry x to infinity

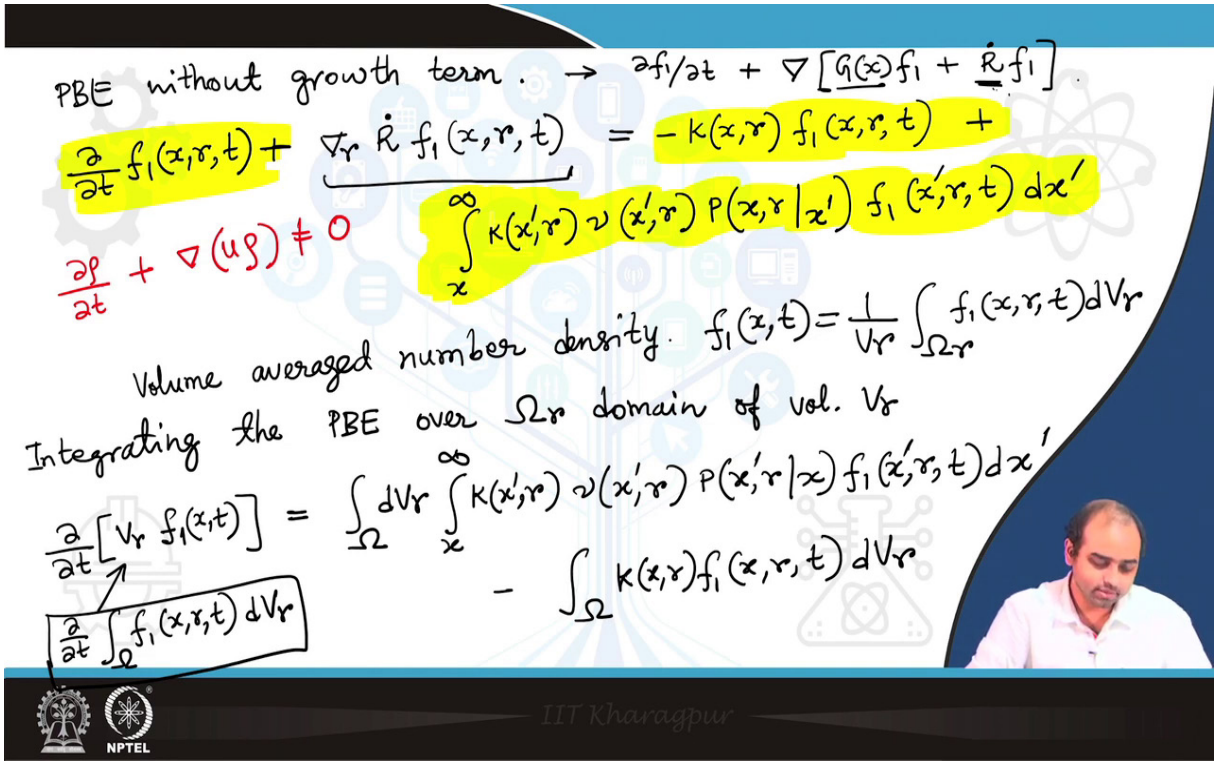
We have the dx prime and f1 x comma t. We have 1 by Vr integration k, then we have mu x prime r P minus f1 x comma t. So, in all the places I am replacing that since we are already having that integration I am replacing one of the integrations and replacing that from f1 from x prime comma r comma t to just f1 that is something I can always do.

I am doing the integration on one part and trying to take out that instead of writing this f prime I can always I mean f x prime r comma t, I can always write in terms of f1. Because I am just integrating it out. So, this part you can now define your new kx if I volume average out this k x I can write something like this. It is like the volume averaged k x, is not it? I can do this volume averaging.

Similarly, I can also do it for mu and this is slightly different, and the probability density function can also be treated as like a volume averaged quantity. So, if I define them in this way. So, then what do I get? So, this entire equation here. So, entire PBE equation whatever we are trying to write in terms of the volume average quantities and everything, possibly this is not the equation. But at least you can get it from here also this entire equation or maybe this equation that we have written down here, this equation. This entire equation, here. It is getting here.

(Refer Slime Time: 25:01)





And then with the definitions of these is converted into something like this. So, in terms of the volume average quantities I get this equation like this. So transformed. So, this equation is identical to the standard case of the particle breakage. But this is what we are getting as the transform equation in the absence of any this r coordinate or the external coordinate.

So, please realize that even though there is an external coordinate in the system and we are trying to track or trying to understand the different locations, where the particle distribution can be different or this k, f, P and mu et cetera these functions k are all functions of the size as well as the external coordinate or spatial location.

But in terms of defining as the volume average quantity. In terms of defining a some sort of volume average quantities for each of these terms into some representative definitions these equations the volume average transformation if we try to do we can have the same equation which exist for the standard PBE case without any external coordinate dependents.

Here one more thing I must emphasize that when we are trying to integrate over when we are trying to integrate over the PBE, there is this term, if you recall. But this term on integration. So, when we to integrate this term over the entire volume essentially the term actually vanishes. So,

in this case, we can say that even though there is this additional term present because of the this sort of the velocity that you can talk about in this case.

But when we try to integrate over the entire domain of these recirculation and circulation for the case of uniformly mixed and homogeneous dispersion, this time essentially will go to 0. The volume integration of this term will essentially go to 0 for this case. And that is why that term does not appear in the final transform the equation. So, I hope all of you understood and realized this important process of breakage in a stirred, lean mixtures and there we also tried to describe what to try to frame the population balance equation in this case 2.

And for this problem, we have seen that if you try to transform in terms of the volume average quantities. The dependence of these functions or the breakage functions on a spatial coordinate vanishes and an equivalent representative volume averaged quantities can be estimated or can be used in this case and it reverts back to the classical population balance equation, where you have the only the internal coordinate and without any growth process. Thank you for your attention. In the next class we will talk about mass transfer in a liquid-liquid dispersion.