Mathematical Modelling and Simulation of Chemical Process
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Lecture 50
Mass transfer in lean liquid-liquid dispersion

Hello everyone, in this class we are going to talk about mass transfer process or mass transfer in a lean liquid-liquid dispersion.

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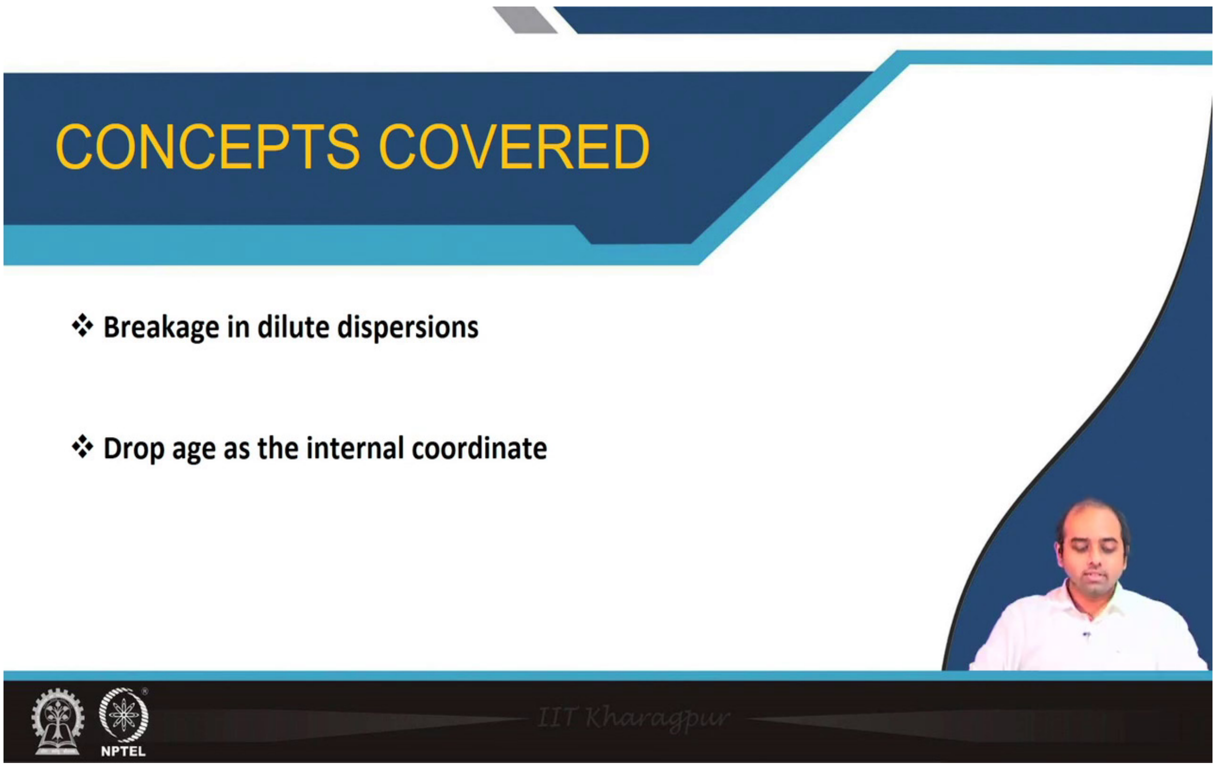

So, consider I mean the situation where you are having a dispersed phase and then we want to study that how much is the amount of solute that is removed from the dispersed phase as it flows through a vessel. So, this is very relevant to the to a, this practical situation where we try to see that there is a continuous flow device into which you feed I mean feed to this continuous device is in the form of a continuous phase as well as a dispersed phase.

So, it is a liquid-liquid dispersion and in the form the dispersed phase is in a present is in the form of uniform droplets and this mixture is getting well stirred during this process. So, as this liquid is withdrawn from the vessel, how much of the dispersed phase is actually getting removed?

So, it is you can think of a dispersed phase CSTR. And in this case you can think of this to be as a sort of extractor or removal of the dispersed phase, things like that. And here the objective of this exercise is to find out that how much of the or the amount of the solute that is removed from the dispersed phase?

So, there is also mass transfer that is taking place in this process that is removed from the dispersed phase as it flows through the vessel under steady state condition. So, you can realize that in these problems since it is a flowing through the vessel drop age or the residence time of the dispersed phase is very important. So, this drop age distribution is very similar to the residence time distribution that we normally study in chemical reaction engineering essentially.

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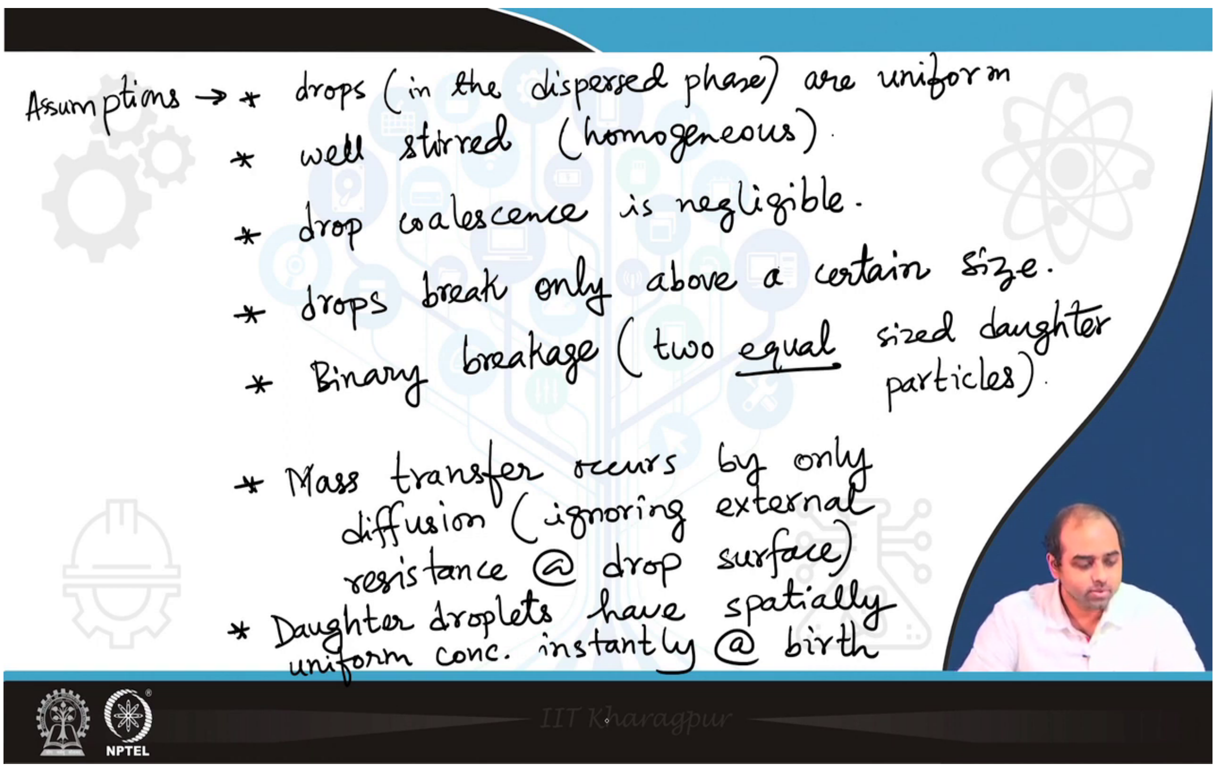

So now, let us try to understand or write down the different assumptions in this process before we try to describe the mathematics behind this process. So, the major assumptions are drops present in the dispersed phase are uniform, it is well stirred, can say to be like a homogeneous distribution, drop coalescence is ignored or negligible. Drops break only above a certain size, binary breakage. So, it forms two equal particles of same size. It is something which will be required later that the mass transfer occurs by pure by only diffusion.

So, we are actually ignoring external resistance at drop surface, some more important assumptions also exist and these are also to some extent important, even though they might sign sound quite obvious or trivial, that the daughter droplets which is formed have spatially uniform concentration, almost instantly at birth. So, as soon as the daughter particles are formed, they have spatial uniform concentration,

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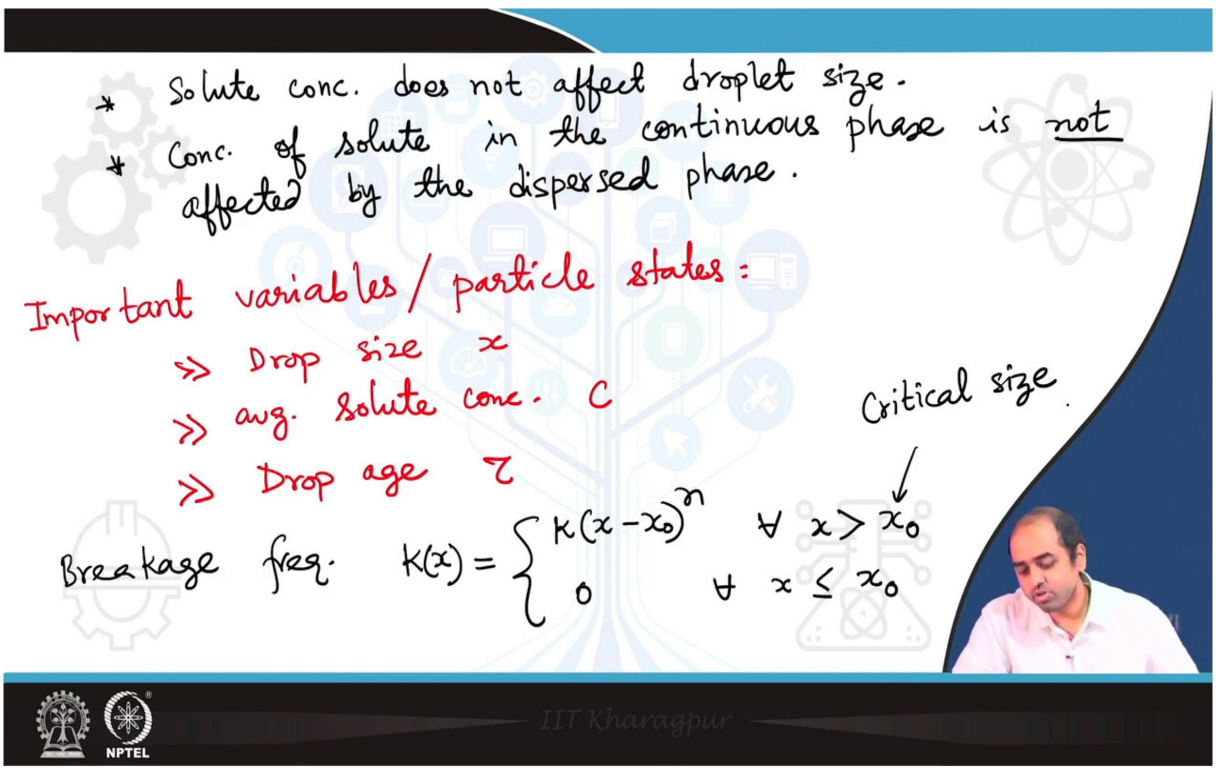

Then solute concentration does not affect droplet size and concentration of solute in the continuous phase is not affected by the dispersed phase. So, whatever is there in the concentrated in the continuous phase will stay there it is the there is no mass transfer or I would say this transfer of the solutes is actually influenced by the presence of the solutes in other phase.

So, concentration of the solute whatever present in the continuous phase is not influenced by the solute that is present or the by the presence of the dispersed phase. So, there are no interaction between the dispersed and continuous phase. Now, what are the important variables that is relevant for the problem, So, one is the drop size that is very critical, let us denote that by x. Second is the average solute concentration because we are talking about this mass transfer in this system and third is the drop age or the residence time. Let us mark it as tau.

In this case, since we have said that the particle only breaks above a certain size. If you recall one of the assumptions or consideration that is made is actually practically irrelevant. So, in a practical problem not all the particles that actually breaks or tries to disintegrate into smaller particles. Only when it attains a certain size or it is beyond a certain size it actually breaks down, leading to the formation of daughter particles.

So, there is a critical size above which these drops essentially breaks, I am saying for fluid droplets or liquid droplets. So, in this context you can consider that the breakage frequency in this case is defined as something like this. So, only if it is beyond this size of x0, then we write then the breakage frequency is non-zero.

Else for all other cases x less than x0, there is no breakage frequency and there is no essentially there is no breakage. So, only beyond this critical limit so, this is like the critical size above which breakage happens, x0, the breakage takes place. So, that is how we define this breakage frequency and we have already considered that this breakage frequency the number of particles formed all these are particle size distribution all these are independent of time.

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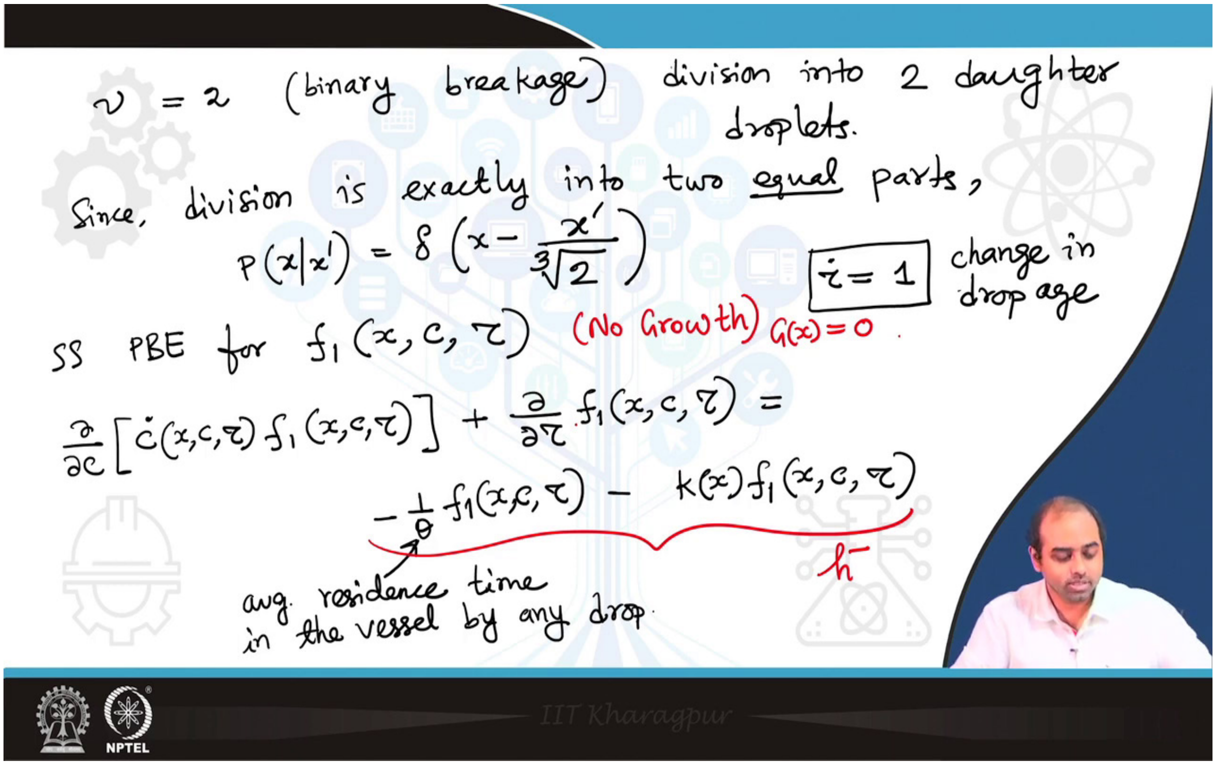

So, from here I mean further we can say that this nu is equal to 2 because we are having binary breakage. So, division into two daughter droplets and since the division is exactly into two equal parts, I would say. The drop size distribution is generally represented by the direct delta function. x represents the size or the volume of the particle and this is related to the daughter size particles essentially.

So, this I mean you can really understand that this direct delta function can take into I mean this can only lead to 0 and 1. So, there is no distribution as such, of the daughter size particles that is the reason why we wrote down a delta function that distribution is equal to 1 only in the case of when this matches on when these two are into equal half's.

So, in the case of two equal volumes, that is what you can we are thinking that x prime disintegrates into two equal volume and this is the equivalent size that we are talking about. So, if you have this this volume that we are talking about our x prime is the volume then you can find out that what would be the volume of the two equal daughter particles, that is what we wrote down that x minus x prime cube root of 2 and this delta function would be equal to 1 when this criterion is satisfied and else it is 0. So, essentially there is no distribution as such it is a single valued function. So, this takes 1 or 0.

So, now, in this case, the steady state since we are dealing with the steady state problem, the PBE equation the population balance equation for the number density function, number density function has x as the size, c and you have this tau which is the drop age. So, there are like I mean, with respect to time, it does not make sense but in this case drop age is other important variable in this case.

So, drop age is one coordinate for the problem concentration is another and x is the size. So, the left-hand side as will be written down in terms of the respective gradients. So, x dot x c tau then we have f1 x c tau. So, there is no d dt term plus you have this with respect to the d delta and this one would be equal to only x c tau because this, f of this d tau I mean this is something writing in terms of I mean this tau dot. The change of the drop age with respect to time does not happen.

So, any function with respect to tau or change in the drop age is equal to essentially what I am trying to say is that this tau dot in this problem is equal to 1. So, and how this is possible? So, which means that a drop which appear in the vessel either by entering with the feet or by breakage of the larger droplets, whatever it is the new drops that are appearing in the system whether it is entering into the system or it is getting disintegrated, it is form are necessarily of age 0, they are of age 0 and they are only I mean they are only accounted for in the boundary condition corresponding to age 0, that is something very important to note here and this is f of theta.

So, theta is the average residence time in the vessel by any drop, minus you have this k x f1 x c tau. So, please note here that in this case there is no new drop that is forming in this problem. Because the new drops which is forming is of age 0 and that will come as a boundary condition because age, tau is essentially one of the independent variables or coordinates of this problem. So, the drop generation term. So, whatever we are seeing here everything that we are writing here in this case contributes to the h minus term.

So, there is no h plus term in this scenario, because whatever the new drops that is forming in this system is considered by the boundary condition because what as I said whatever is entering or whatever is forming in this system are is at age 0, and that becomes a part of the boundary condition, not as a part of the source or addition term to this. So, there is no actually h plus term here. I hope all of you get this idea, since there is no growth in this process. So, it is also the case of no growth. So we do not write the growth related terms.

So, g of x is equal to 0, and the change in the drop age, d tau by dt I mean essentially that is equal to 1, because you are drop age, I mean what is this drop age? Drop age is nothing but time. So, integrating time with respect to time will only give you 1. So, that is what this tau dot function which was present here, I am supposed to present here is equal to 1.

So, that is the reason why I have written only this d of f1 with respect to time. So, drop age and timer are same essential in this problem. So, this is how the formulation looks like and as this boundary condition now or particles at drops at age 0 is very important. So, maybe we should try to write down that essential boundary condition to this problem, because of that, only there is no generation term in this problem or there is no h plus term.

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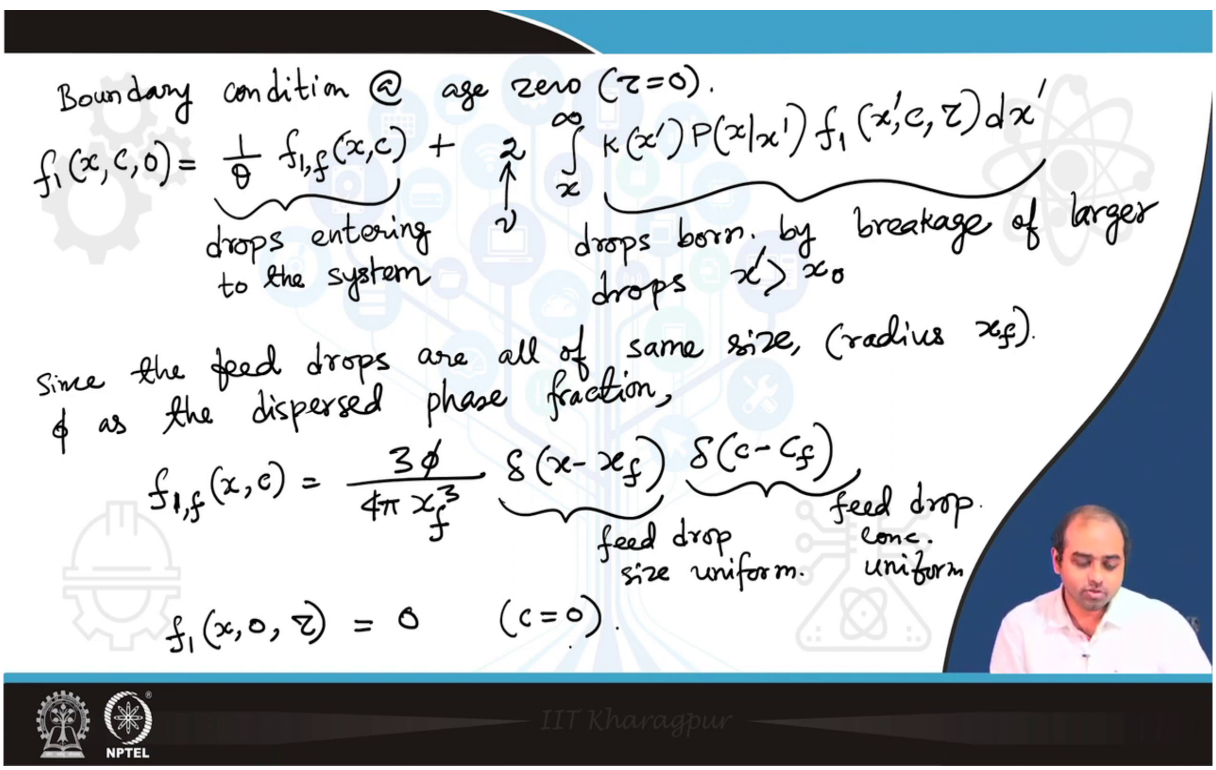

So, boundary condition corresponding to age 0, tau is equal to 0. So, essentially, we are talking about a scenario f of x, c, 0. So, this is equal to I mean this f of x, c represents sort of the flux of the particles at age 0. So, this is let me first write down the equation then I tried to explain it. So, this is an equivalent to saying that the particle velocity along the age coordinate is identically unity.

That is what we are trying to write down as like the particle flux on the left hand side, is what we're trying to write as a balance of this first term is representing the drops of age 0, that is what we do not write any I mean, this what the average this residence time and exceeds the amount that is entering into the system.

So, this is the contribution to the drops are the drops that are entering to the system. So, whatever is entering is at age 0 and the second term is whatever is forming by this division. So, that is k x prime P x x prime which is a unit valued function f1 x, c, tau. So, this is whatever is forming from in between x to infinity, this is whatever is forming. So, this is the contribution by the drops that are born, drops born. So, this is nothing but our new born by breakage of larger drops, of course larger than x naught.

So, this is the to contribution of the, this boundary condition or the particle density distribution at age 0. So, one is the part that is entered into the system or the contribution of the terms due to the entering the system and another part is due to the breakage of the larger drops both of which are essentially I mean they constitute particles of drop age 0, but please note here these particles which are breaking they may have a different age.

So, that is why this tau exist here in the second term, but this is essentially the new particles that are formed are of age 0. Since, the feed drops are all of same size say radius let us say x, f then considering phi as the dispersed phase fraction. We can write f1 this first feed entering function x comma c as like 3 phi by 4 pi xf cube delta x minus x f x sorry then again delta c minus Cf, Cf is the feed concentration. So, this is sort of the volume density function that we can write of that unless x is off radius except there is no distribution or the there is no particle in the system and unless c is of Cf which is a feed.

So, these are these delta functions which says that unless x is equal to xf this will be equal to 0 for all other cases. So, this is how we represent this feed function. Now, coming to the final part that what happens. So, this is like the I can also write it here that the feed drop size since it is uniform this is like either 0 or 1 and here this case is feed drop concentration which is also uniform.

So, the other condition that x 0 that concentration 0 whatever is there is 0 because this represents c is called to 0 and for x is equal to 0 which is the sort of the initial bubble state that you need to describe. So, this is how the three boundary conditions are described for this problem.

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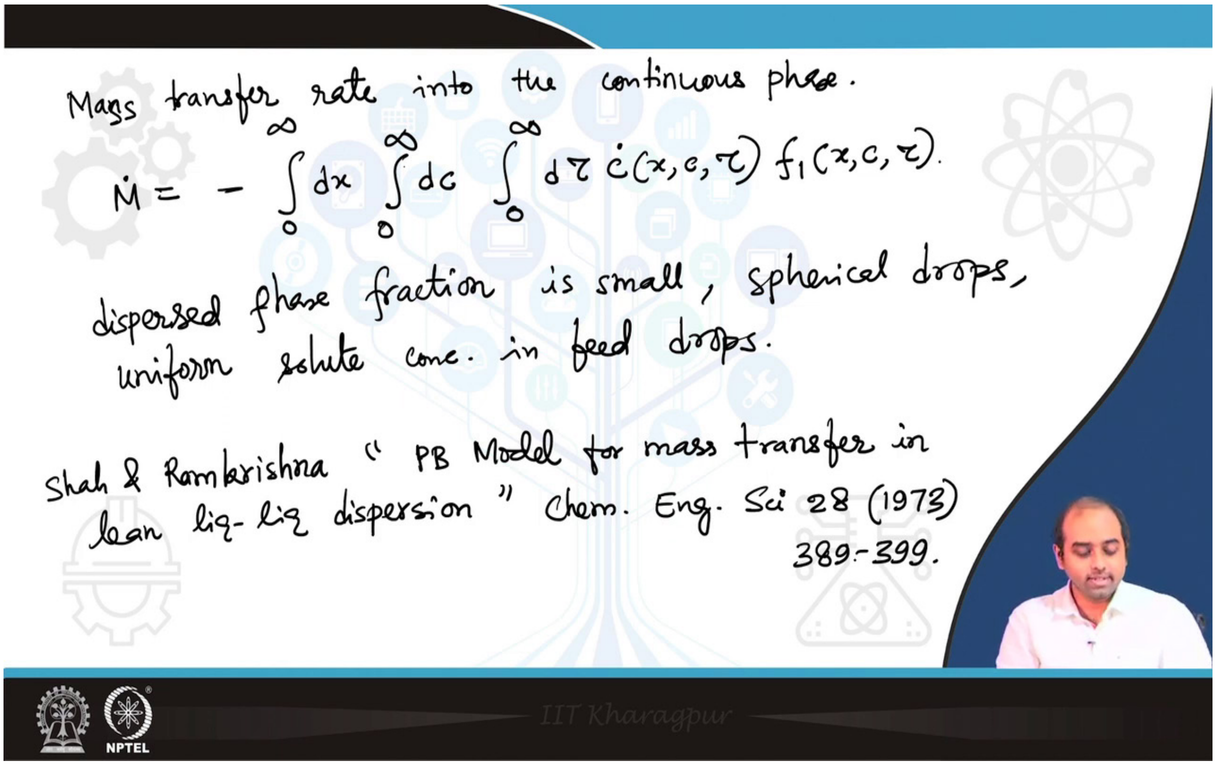

So, with this assumption of the spherical droplets and uniform concentration of the drops, unform concentration of the solutes in the feed drop, the mass transfer rate in this case. So, mass transfer rate in to the continuous phase this is the mass transfer rate in the, is actually given by this derivation and this is a true for spherical drops and uniform solute concentration in the feed drops. So, this is based on the assumption that the dispersed phase I mean whatever this dispersed phase function, dispersed phase fraction is small or lean this assumption is very crucial.

And spherical drops and uniform solute most of them what is something we defined in the beginning, uniform solute concentration in feed drops, and the concentration of the solute in the continuous phase is unaffected by the dispersed phase. So, based on this assumption for this particular case this is how the mass transfer rate can be determined in this case.

So, if you want to know that how this relation is actually developed analytically. I mean this is something beyond the scope of this lecture. So, you can you can look into this reference by Shah and Ramakrishna on this population balance model for mass transfer in the lean liquid-liquid dispersion this is a fantastic research article were these two guys. That describes the purpose of mass transport of solute during this dispersed phase system and that is taking place at steady state.

So, I hope all of you got a quick as well as the detailed overview on the breakage phenomena and different circumstances. So in the next class we will be talking about the process of aggregation. We had a lot of discussion on breakage so far. So in the next class we will talk about aggregation and we will that how the aggregation function can essentially be modelled or described and that how it fits in to the population balance equation. Thank you, see you everyone in the next class.