Mathematical Modelling and Simulation of Chemical Engineering Process
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Lecture 55
Numerical solution of the population balance equation

Hello everyone. In this class we are going to talk about the numerical solution and the framework of the, this numerical solution technique for handling the partial, this population balance equation. Of course, this numerical technique cannot be solved out explicitly, I mean right I mean this class for which you need to set up some of your course. But, in this class, we will try to look into the, some of the features of the highlights of this method of discretization or trying to discretize the population balance equation or essentially the number density function into some discrete intervals and see how this can be handled in a numerical framework.

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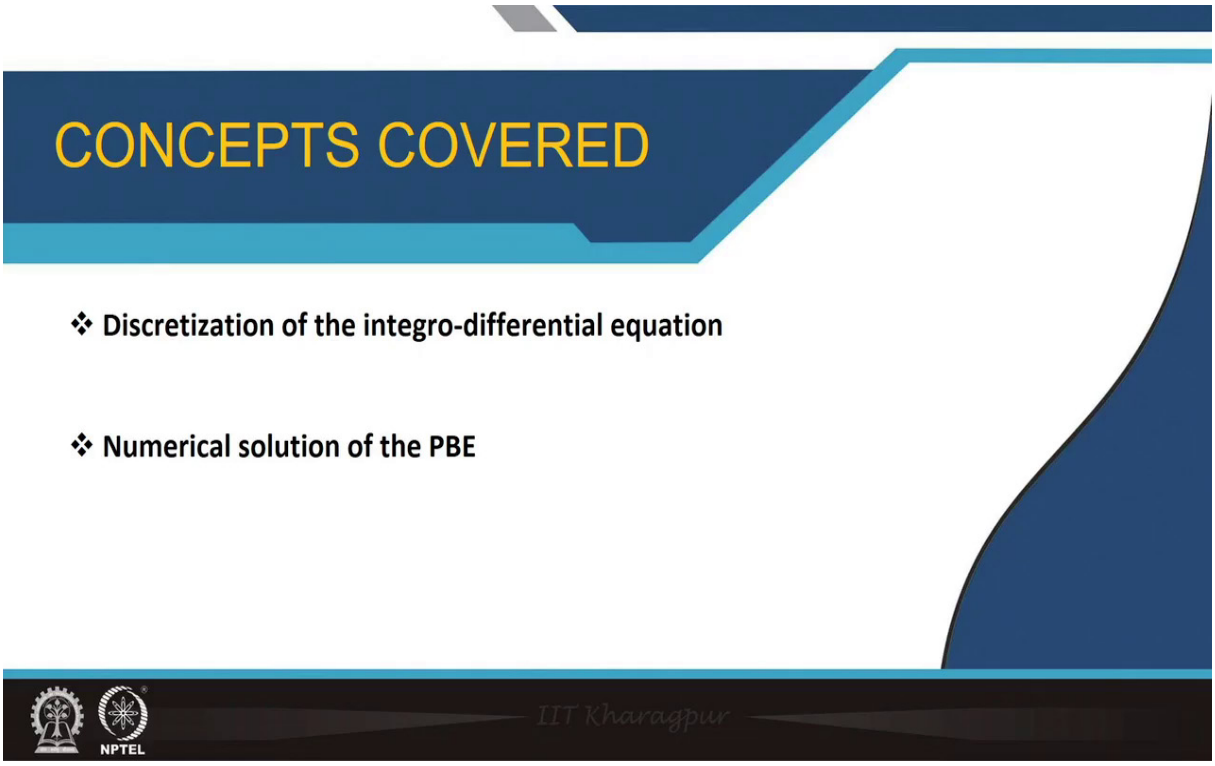

So, let us begin for today's class and we will be talking about discretizing this integral differential equation, ultimately with the addition of the source and sink terms the population balance equation is an integral equation, essentially integral differential equations that we will talk about the discretization of these integral limits. And then we will try to see the framework of the numerical capabilities here.

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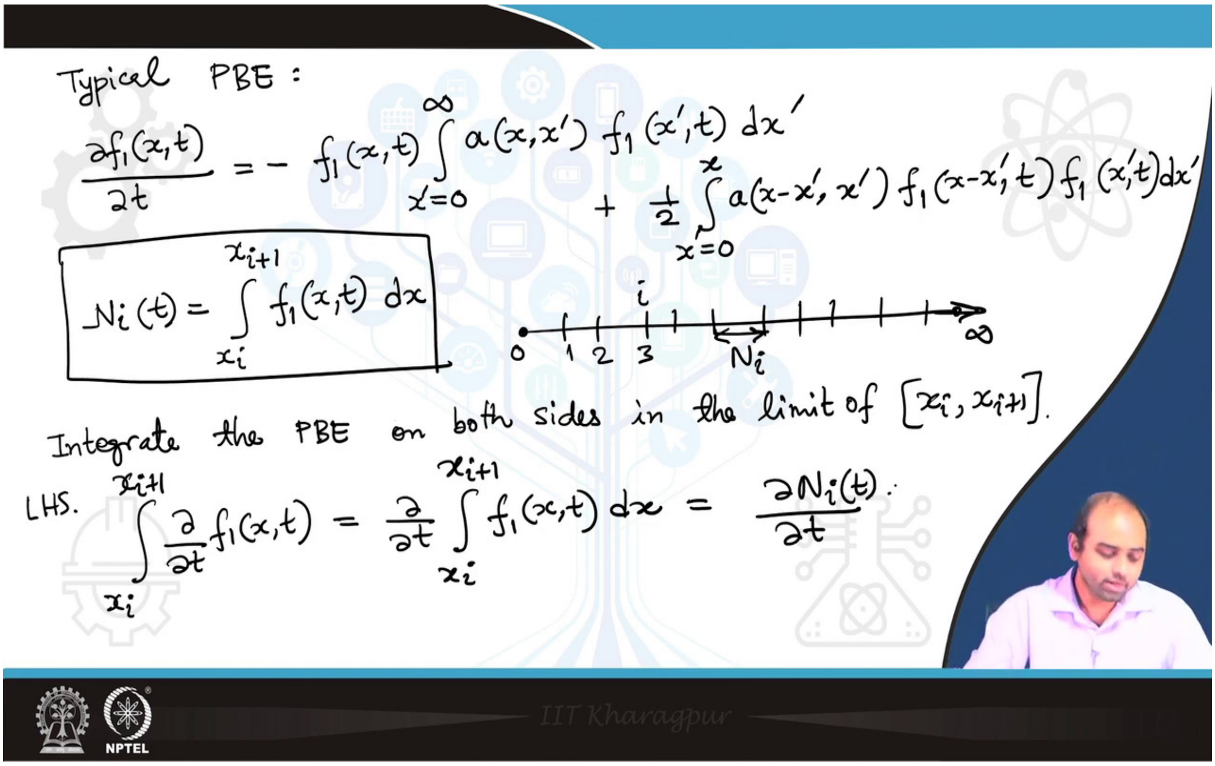

So, let us see that, it is the same kind of a population balance equation just what we discussed in the analytical treatment, in the previous class. So, the typical population balance equation with essentially with aggregation, we are now so fond of aggregation now, after so, much of intense discussion on aggregation, this is how it looks like. So, no growth etc. We are discarding any growth, so, no convective term, only aggregation.

Aggregation frequency instead of considering to be constant there is no such hard limit in the numerical capabilities, we can choose it to be a function. And this is the sink term and then we have the source term, these are the pairs x minus x prime, and x prime are the pairs. So, this is the population balance equation, you are all used to this.

So, the first part is the sync term on the hand side, and the second part is the source term and here I considering aggregation by pairs and this is something we mentioned in the beginning also that for when we started the class on aggregation that we will consider all pairs aggregation only not triplet and multiple particle aggregating. So, the pairs are x minus x prime and x prime. So, this is what gives you the contribution of x. So, that is why the limits that you see in the source terms is from 0 to x. All the particle size within this range has to agglomerate or aggregate and form x only.

And in the case of the first term or the first thing term the limit says from 0 to infinity. So, any particle, I mean can essentially aggregate, I mean particle and x, particle x can aggregate with any particle x prime, noted as x prime in the entire range and that particle can get, I mean, it can get we can lose that particle x as it get aggregates with another particle of x prime. So, that is why this entire limit of 0 to infinity does exist for the lost term.

Now, let us define this Ni t as total number of particles in the size range of xi to xi plus 1. So, this is very similar to the kind of concepts now, we are invoking to the scenario, where we describe the discrete size range of the particles in the aggregation model, where we have all discrete size. So, essentially this partially, this population balance equation, we are trying to discretize or these whatever the internal coordinate that we have of the size range from 0 to infinity, we are trying to discretize into certain segments of intervals, this could be uniform, this could be non-uniform also. So, that is a separate issue altogether.

But at least we are trying to discretize them or segregate them into certain size intervals, and these size intervals can be small, can be large whatever depending on how many number of search intervals we are talking about. And then this total number of particles in each size interval. Let us call that size interval as i, so, we are something trying to say that this is, the size interval from 0 to infinity and that is something we are dividing as all are same size range as i in this case is 0, 1, 2 and whatever the number, total number of particle in each size range that is something we are denoting as Ni. So, that is the integration of f1 over the size range i to i plus 1.

So, please note that here we are not considering the particles to have only discrete size range, please do not get confused with the scenario of the discrete size any other particle that we have described in the last-to-last class or couple of classes back, it is not the same. Here, the size of the particle sees uniform and continuous, but we are imposing or we are segregating them into different size domains.

So, considering, we do not consider that particle size, only need to exist at this fixed interval sizes. And that is why I do not write, the subscript i to the number density function or we do not write in terms of xi or f1 i, I am writing this in Ni as the size range from xi to xi plus 1, but it does not mean that particles do not have I mean, there is no particle that does exist between the size range, it is not the case or the particles are only there in the case of these discrete size range, it is not like that, this discrete size range could be anything, we can choose the entire domain to be discretized into 10 parts, we can choose it to be discretized into 100 parts.

So, this has nothing to do with the size of the particles it is only we are segregating them into certain groups. And this group size can be uniform, can be non-uniform whatever, and the number of particles that belonging to that size range i to i plus 1 is denoted by this Ni, that the total number of particles.

So, with this idea, we try to integrate the PBE, both sides in the size range or in the limits of i to i plus 1. So, integrate the PBE on both sides in the limit of xi to xi plus 1, in this limit we directly integrate. So, essentially the left-hand side, whatever we have will look like this. So, integrating from xi to xi plus 1, so, this can be, I can take out that time derivative and I can write this as this and this is nothing but equal to the Ni dt. This is what the left-hand side turns out to.

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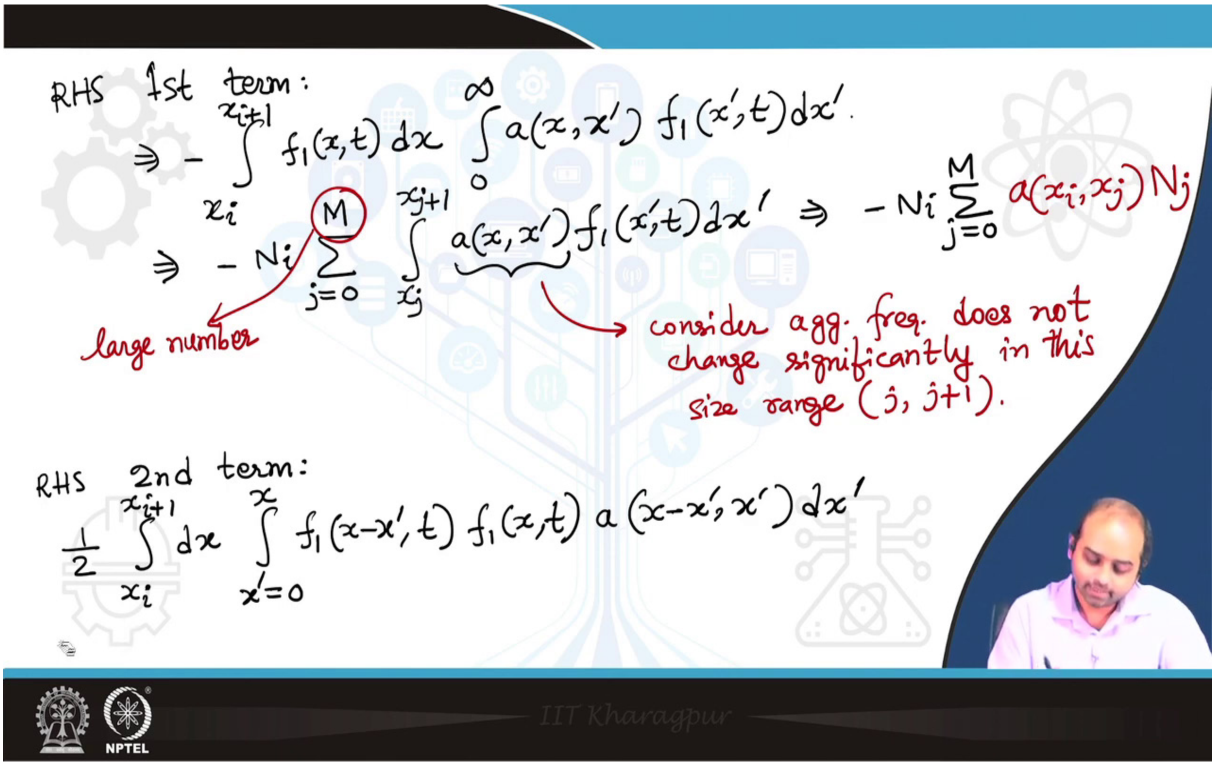

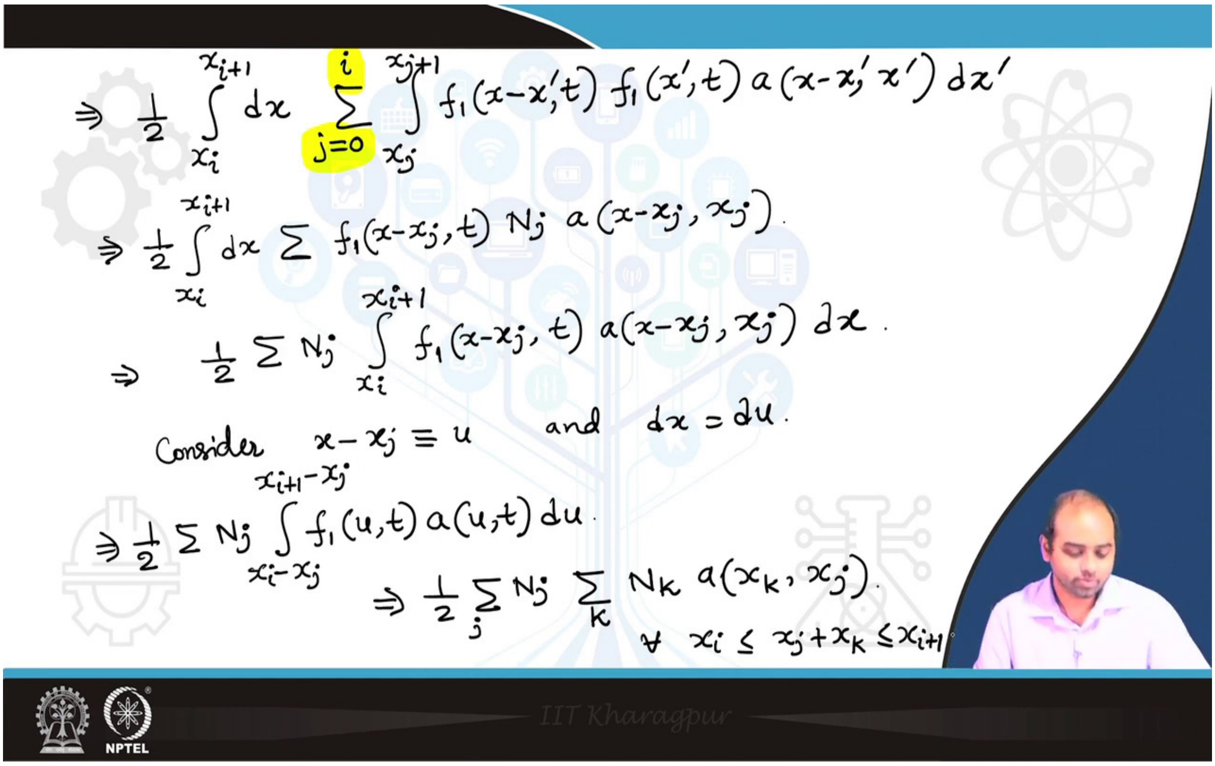

Now, coming to the hand side or essentially the hand side fast down I would say. Let us take it term by term, the first term, if I try to integrate, I am having f1 x comma dx in the limit of xi to xi plus 1, this a x x prime, 0 to infinity, is the first term. Now, this is converted to something like minus Ni, the first term is converted to Ni that is easy. And next this entire integration over the range of 0 to infinity is marked as 0 and j is equal to 0 to not infinity, but a large number, where you can choose this M to be a large number, let me write it out explicitly here, this is a large number or the largest number, it is not infinity, because there is nothing infinity that is possible in numerical solution, any sort of numerical solution.

And then we say that now, this integration 0 to infinity is converted to as xj to xj plus 1. So, this entire domain of infinity from 0 to infinity is again segregated, I mean with a different index now, because already i I have used, so in the limits as in this is this integrated or, this segregated into different fractions of j and we say that again this small interval j to j plus 1 and then entire thing is summed up separately from 0 to M, where M is a very large number.

So, xj can take any values from 0 to very large, and then we segregate these into small, small segments. So, instead of having a continuous integration, which is numerical not possible as we can see in this case, we take the help of this summation essentially, of small segments. Now, what is the thing that we are going to do in this small segment is very interesting. So, in this small segment, we assume that this aggregating frequency this a, a in this zone does not change significantly, in the small segment of j to j plus 1, a does not change significantly in this interval, let me write it down, we consider, which is also quite practical provided this zone of the segment of the particles is very small.

Consider this aggregating frequency does not change significantly in this size range of j to j plus 1 and with this idea in mind, we write this part as a x i comma x j and then the other part is Nj. So, this entire integration, so, previously Ni was defined only for integration of f1 dx over the intervals of i to i plus 1, but in this case we consider that a is not changing significantly. So, if a is not changing in this integration, we can assume a to be constant and then in the interval j to j plus 1, f1 dx prime can be integrated and written down as Nj and that is what we are writing here this.

So, this is what the first term looks like, I hope it is clear to everyone. So, these things this a is constant, I can take out of this integration and but of course, it will be inside the summation. And these integrating part xj to xj plus 1, f1 x prime, dx prime is written down as Nj for this a different subscript j and this entire thing is within the summation region of 0 to M, where of course, M leads to a very large number and represents the theoretical limit of the infinity.

Now, coming to the second term, the second term of the right-hand side. So, you also do the integration over the limits of i to i plus 1 xi to i plus 1, on the second term also. So, you write half integration xi to xi plus 1 dx, this is the second term. So, what we are going to do immediately, this second term, integration we are going to write down in the form of the summation. So, this is half.

Let me write in the second slide, next slide. So, this is converted to half xi to xi plus 1, this is there what is. Now this part I am doing a summation of xj like the previous case to xj plus 1 and then I write the same things, I mean whatever the functions are there f then I have f1 x prime t a x minus x prime, x prime dx prime. And this summation is varying from j is equal to 0 to, if you remember this was the integration limit was from x prime is equal to 0 to x and these x is essentially, this is from 0 to x.

And x is something we are already representing in terms of i. So, that is the reason this limit from j is equal to 0 to, it will be not infinite in this case on a large number, it will be i. So, I hope all of you realize this because this is, this limit of integration was from 0 to x and that is why we are writing this j is equal to 0 to i, because i is something is there in the outer integral and this is everything is written down in terms of i now, because we have already defined Ni as the integration of this quantity.

So, with this idea, we proceed next and we do some more algebraic steps. So, this one is half of integration xi to xi plus 1, dx still exist. Now, we have the summation, summation of 0 to i j is equal to 0 to I, I have f1 x minus xj comma t Nj and then I have a x minus xj. So, all the x prime is converted to xj, this is possible to write, Nj is the integration of x prime, integration and a once again is assumed to be constant within this small range of j to j plus 1.

So, then we are, what we are trying to do I mean is once again I am trying to take out these Nj from this here. So, I am getting half summation of Nj integration xi to xi plus 1, f1 x minus xj comma t a x minus xj, xj dx. Now, if we consider that x minus xj is equal to u and dx is equal to du, then what we get is half summation of Nj f1 u comma t a u comma du, and this integration limits is something very interesting.

So, this one would be xi minus xj and this limit would be xi plus 1 minus xj that is how the limits should be in terms of u, so, it is like u to u plus 1 something like that and this ultimately leads to the formation of half summation in Nj and we are doing a summation once again here, this quantity as Nk a xk comma xj. So, please note that inside integral is of k and outside summation is in terms of j.

So, where we assumed that xj plus xk is in between xi to i plus 1, this is the understanding or this is the condition for which this is valid. So, now, we have two summations representing these two integrals. So, ultimately these two integrals is reduced into the form of two summations in this case.

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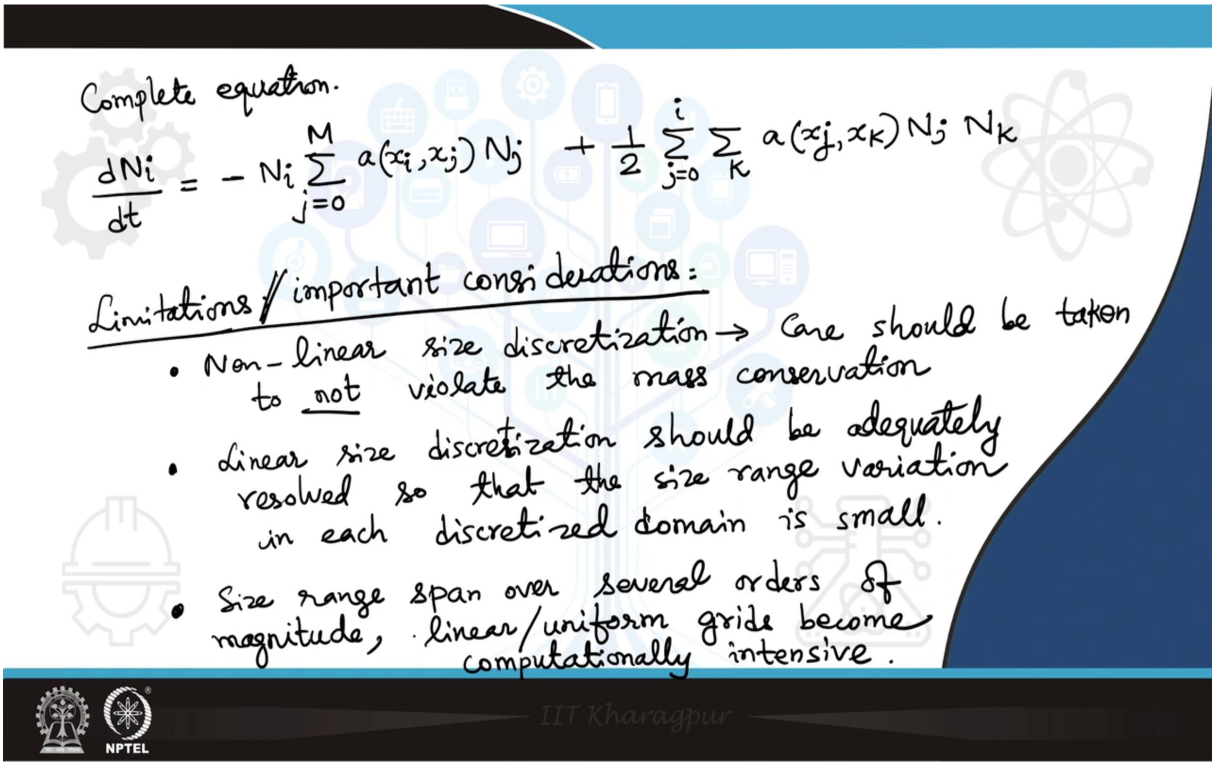

So, the final complete or the composite equation looks like dNi, dt is equal to minus of Ni summation of j is equal to 0 to M, where M is a very large number xi minus xj N j this is the first term and this is the second term. So, this is over j is equal to 0 to i, this is over k a xj comma xk Nj Nk. So, one of the limitation, I mean this entire, the sort of discretized population balance equation I would say is valid when we try to discretize or segregate the particle size interval into some designated portions and the limitations of this equation of course, you can understand that non grid size particles whatever if they are something present with violate the mass balance.

So, you need to consider, that is why we need to consider the summation here. And again, linear grid points are very difficult if you have a very large variation or size variations of the particle, it needs to be appropriately segregated or this captured properly. So, when you have several orders of magnitude of the variation, then the discretization is tricky, you cannot have same resolution of this discretization of the particle size. So, these are some of the limitations I would see of this technique or the numerical technique.

But nevertheless, it works best when you have, you do not have a large size variation and you do not need to have so many discretization of this space or this j is going to 0 to M. So, this discretization is very, very vital and you know that based on this discretization only we made the assumption that the aggregating frequencies not varying too much in this discretization. So, the discretized zones of the particle sizes needs to be very small and that is why if the particle size varies too large, then we often land up with some difficulties related to the fact that, it is not resolved adequately or some of the approximations which is considered during this, numerical framework or the discretized numerical equation or the summation equation or you would say in this case is not valid.

So, under no circumstances you can violate this mass balance. So, whatever the total mass that is present in the system, and we know that the mass density, in fact does not change in time. So, that is something needs to be taken into account that whatever sort of discretization we are trying to do, what are our type of solution that we are trying to do, it should be adequately resolved.

So, resolve means, the size variation of the particle distributions should be sufficiently small as well as they should cover the entire span of the size range, such that the mass density of the particles do not change with time. Since, there is no growth process, so, you know that from the first movement or first order movement analysis that has mass density does not change with respect to time.

So, the total number of particles even though that can change, but the effective mass density should not change with respect to time. So, that is the reason the limitations are is that if you have non-linear, nonlinear size discretization let us say, in the case of non-linear size, care should be taken to not violate the mass conservation, because the mass cannot change.

Secondly is that, the linear size discretization should be adequately resolved, so, that the size distribution or the size range variation in each discretized domain is small. And of course, this is another limitation that you say when that size range span over several orders of magnitude, linear or uniform grids become computationally intensive because there will be lot of grids or size ranges, even that the large size range also needs to be discretized into small segments such that the second criteria is taken care of. So, limitations are important considerations I would say.

So, I think we will close this class with this note here. And on the dispersed phase modelling of course, in the next week we are going to talk, one class we are going to talk about the kinetic Monte Carlo. And this has particular relevance with respect to particle level simulations. But in general, the population balance equation and its treatment is something that I wanted to emphasize to all of you in this entire week, as well as in this course. And I hope all of you found this quite interesting and useful and quite relevant for engineering processes. Thank you once again for your attention. I hope all of you enjoyed this class.