Mathematical Modelling and Simulation of Chemical Engineering Process
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Lecture 53
Dispersed phase modelling – Aerosol dynamics (Contd.)

Hello everyone. So, in this class, we are going to have a more detailed view of the different terms that is appearing in the source and the sink functions for the aggregation behavior in aerosol dynamics. So we will start of from where we left in the last class.

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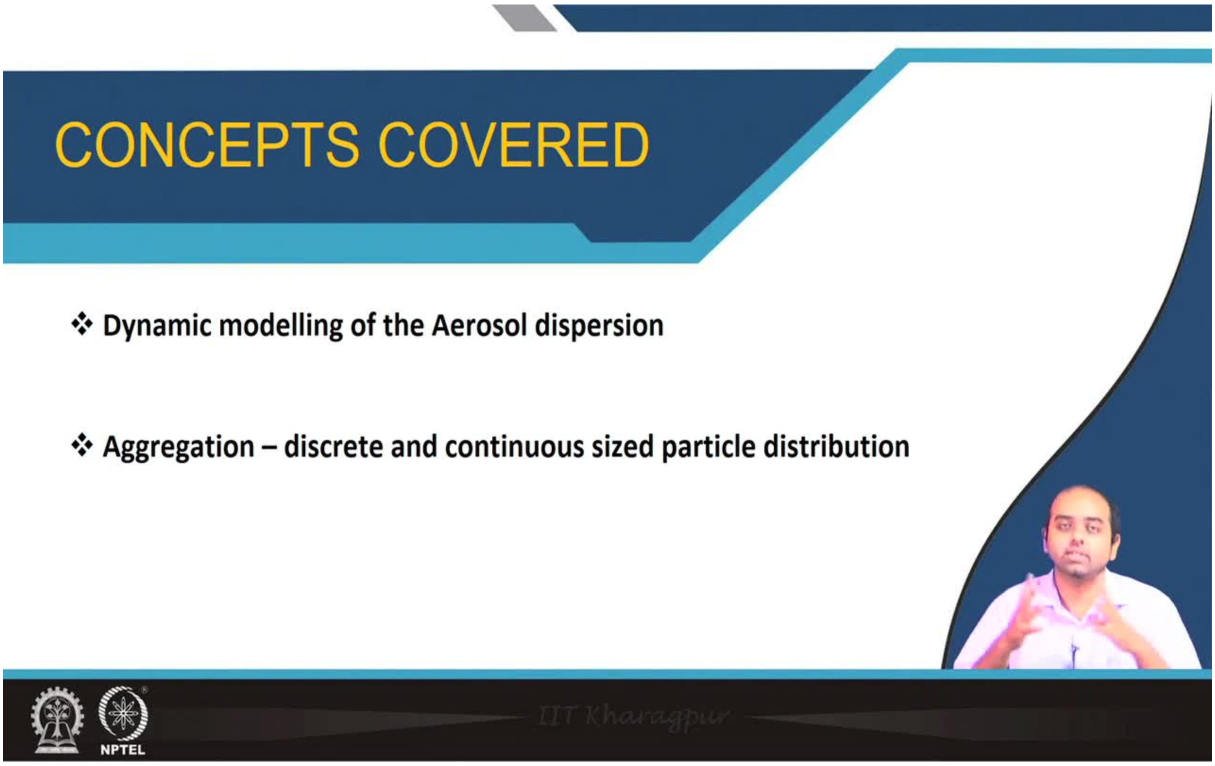

So, if you recall, we talked about the discrete range particle size, we talked about essentially the how we do we handle the smallest particle because there is no this source term or the source contribution to the smallest size particle by aggregation. So that that process does not exist it exists for starting from x 2 onwards, since the smallest x 1, 2 x 1 can aggregate and form x 2, but it does not there is no particle smaller than x 1 that is why there is no aggregation or the source contribution by aggregation does not exist.

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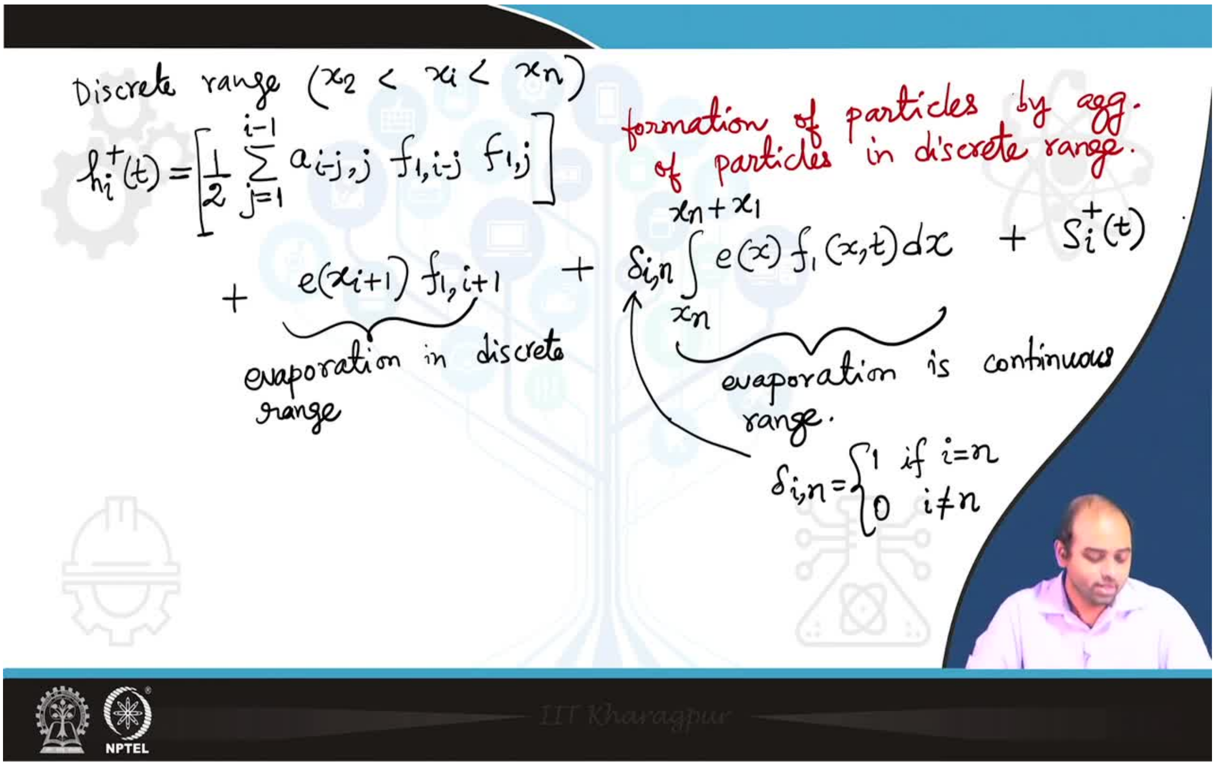

So, now, let us try to look into the discrete size range from 2 onwards and then we move to the continuous range. So the discrete range from x 2 to x 1 x n in this size range, this will give us a generalized picture. So, this h plus h i plus the source term, we are focusing on the source term first. So, each will have contributions by aggregation and this aggregation we write as a i minus j comma j, 2 particles within the discrete range f of 1 i minus j into f 1 j. So, these are the pair of particles. So, this is ranging from j is equal to 1 to i minus 1 and since it is a pair we do it 1 by 2 to check for the redundancy I mean half this added for the pair of the particles.

So, this is the formation, this part describes the formation of particles by aggregation of particles from discrete range and it is not possible that 2 particles from continuous range will aggregate and form the discrete particles because the particles in the continuous range are larger than the discrete range there is not a possibility it can aggregate and form a continuous particle, but aggregating 2 continuous particle to form a discrete possible is not possible.

So, this is the formation from 2, I mean aggregation of 2 particles will lead to the formation of the particle i. So, this particle i can essentially, please note that this aggregate, this particle i can you know any particles from 1 to i minus 1 can essentially aggregate and form i any 2 particles can aggregate.

So, it could be like essentially particle i minus 3 and then particle 3 could you know combined together to form a particle i. So, similarly any combinations from 1 to i minus 1 will essentially form the particle i that is why the summation is done from i to 1, 1 to i minus 1. So, all the possibilities are included here and half contributes to avoid the redundancy factor.

Then we have the contributions when the second contribution generally contribution. So, this is actually this first part is actually missing for x 1 because it cannot be formed by aggregation. Next is the evaporation of particles large then x i can evaporate essentially i plus 1 can evaporate and form i, is not it? And particles in the continuous range can also evaporate and form this i. So, for that we write e of x f 1 x comma t.

But please note that this last term whatever I have written down here this last term that is evaporation of the particles from the continuous range is only valid for the case of x n. So, this evaporation range starts from, this evaporation range actually starts from x n. So, and the particles which is just larger than x n so, in the range of x n to x n plus 1 in this range any particle can evaporate and can form you know x n only.

Below that it is not possible to form and after x n it can further evaporate and form the other type of particles and other discrete range particles it can form but that part is already accounted for this in this term e x i plus 1 this this term is already accounted for there. So, this is evaporation in discrete range and this is evaporation in a continuous range. This part is very small, because here the contribution of the evaporation or contribution of the continuous range particle as to the source term of the discrete range particle by evaporation is only for the largest discrete particle size.

So, to do that, we essentially multiply this delta i comma n so, this delta i comma n actually represents so, this is the redundancy factor for this case of the x n so, this is delta i comma n is essentially equal to 1 if i is equal to n. So, this factor only exists for the larger, largest particle size and it is equal to 0 for i not equal to n. So, only for the largest particle size this evaporation term does exist. So, I hope all of you got this and then of course, you have that additional in this S i sorry plus t term.

So, this is the additional term that we have to this generation that the all of you are aware of. So, this is all the source contribution in the discrete range. So, therefore I will repeat once again the first term represents the contribution by the source and the contribution by aggregation by particles in the discrete range.

Next one is the evaporation of larger particles in the discrete range. And the last is the smallest contribution where evaporation of the continuous range particles producing the largest discrete size particles and that is why this delta i n factor, the delta function is there.

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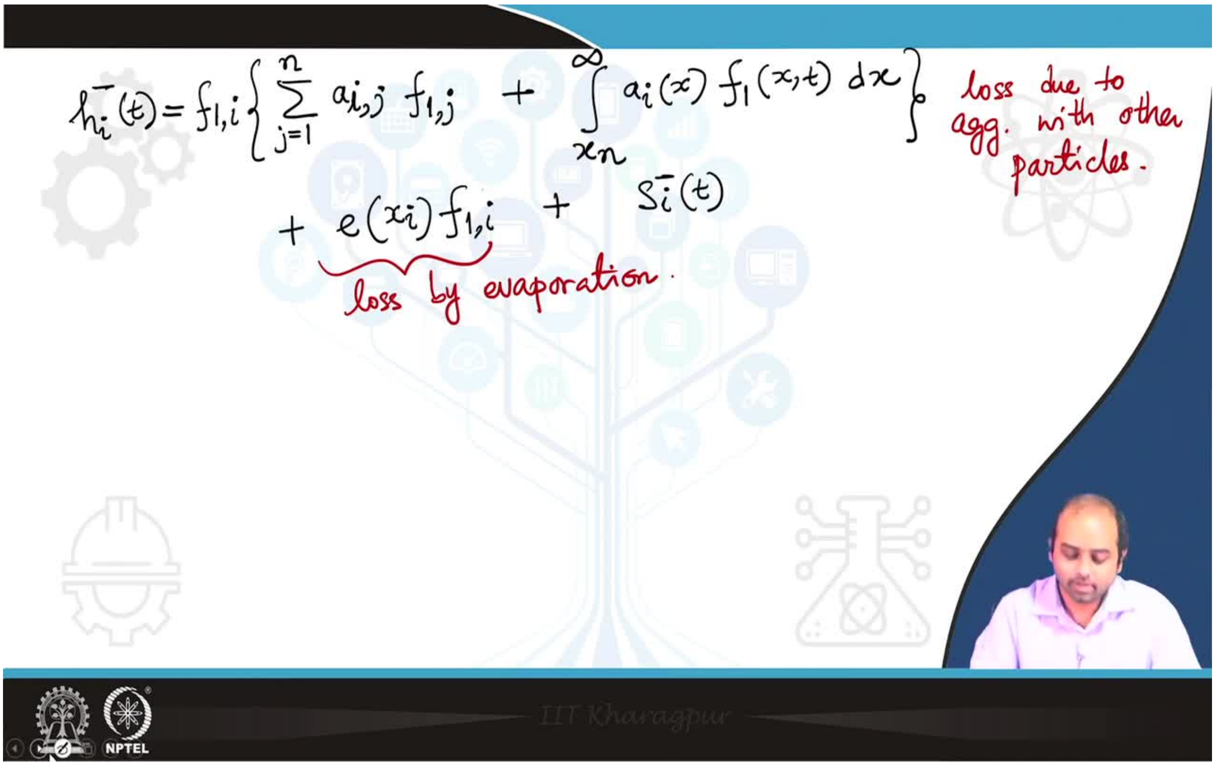

Now, coming to the h minus term so, this one is summation so, there again you know essentially two contributions one is lost by aggregation with all other particles. So, i x j it could be any particle from 1 to n plus a i x aggregating with a particle in the continuous domain that is a possibility by which a particle can be lost. So, aggregating with a particle in the discrete domain or aggregating with a particle in the continuous domain can lead to loss of the particle of size i to that will multiply on i.

So, this is loss of the particles with any particle in a discrete range or in the continuous range continuous range we are writing with the integration and the discrete range you are writing summation term. So, this is the loss, loss due to aggregation with other particles and then we have the loss due to evaporation.

Evaporation is actually very tricky, it has contributions to the source in the form of larger particles which produces ith particle that is why it is appearing in h plus term. In h minus term also the particular particle can be lost by evaporation and then you have the S minus terms that loss by removal. So, this is the lost by evaporation.

So, this is most of the descriptions that we have for the discrete range size distributions or the source and the sink term for the discrete range particles.

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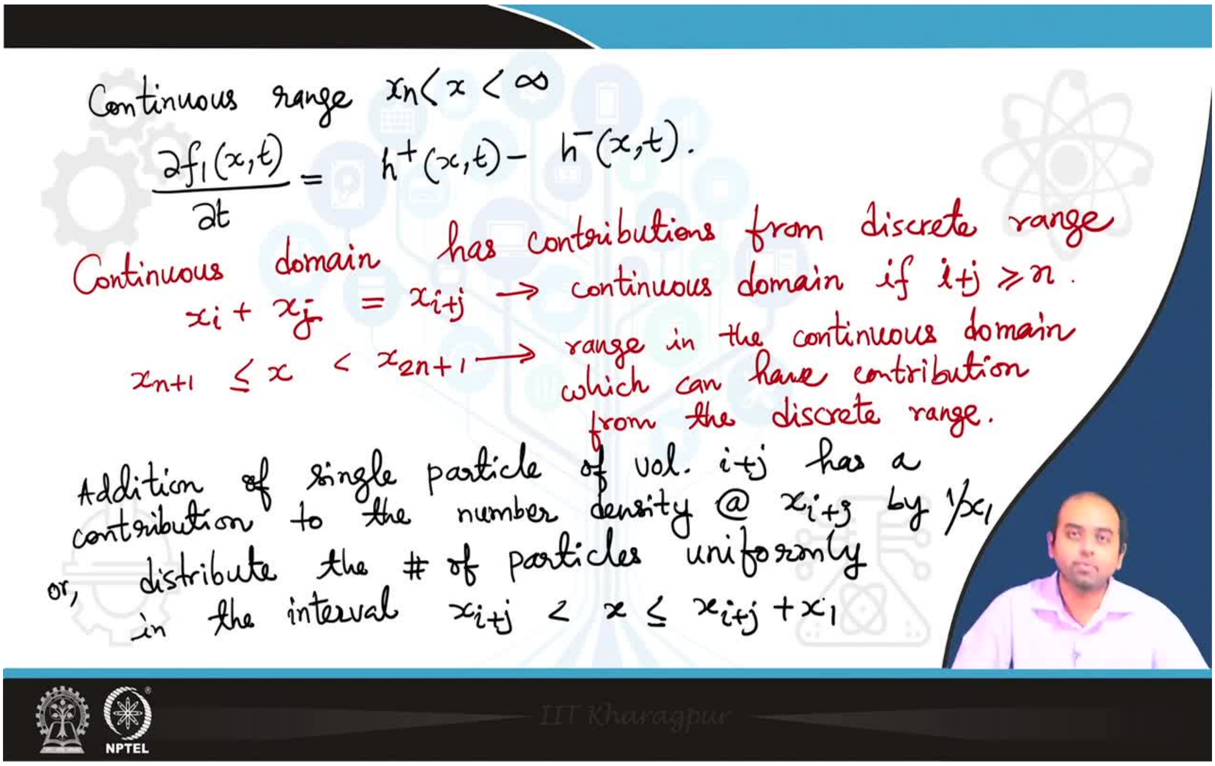

Now, let us talk about the continuous range. So, in the continuous range the particle size is larger than x n up to infinity. So, in this case, you drop all the subscript i the number density function is remember just f 1 these are the h plus and h minus. Now, please note that the continuous domain, continuous size domain has contributions from discrete range which was not the reverse way round. So, there was no contribution of the, in the discrete range by continuous domain but there are contributions of possible contributions of particles from the discrete domain to the continuous range.

So, essentially x i plus x j can form something like x i plus j and these can be in continuous domain if i plus j is larger than n that is a high possibility. So, these contributions do exist I mean this whatever the contributions that we are talking about will lead to particles in the continuous size domain it is possible that there are contributions coming from the discrete range will land up particles up to from x n plus 1 till x n to n plus 1. So, up to this much. So, this is the limit or the range in the continuous domain, range in the continuous domain which can have contributions from the discrete domain is not it? Because, it is only 2, I mean x 2 n is the largest particle size that can be formed by discrete particles beyond x 2 and it is not possible is not it?

So, that is the maximum possible size range that can have, that can form in the continuous range by contributions from the discrete range because 2 x n particles can agglomerate together and form x 2 n that is a maximum contribution can have contributions from discrete range and beyond that, it is all you know the continuous-continuous interactions or particle and 2 particles only in there. So, beyond x 2 n it is only particles that are present in the continuous domain will interact each other. So, further contributions from the description is not possible.

Now, the case is that the discrete particle size have very multiples or discrete size ranges whereas in the continuous size range it is not like that. So, how do you account for the change in the number density function by the addition of these discrete sized particles in the continuous domain this is an important part.

So, we say that any addition, so addition of single particle volume i plus j has the contribution to the number density at x i plus j by 1 by x 1 amount, because x 1 is the smallest particle size and all are integer multiples of x 1 only the discrete size. So, whatever particle that we are getting, I mean this new particle that is added to the continuous system is i plus j so, that amount or that particle the number density I mean the contribution of that amount is only 1 by x 1.

So, any addition of any discrete particle is having a contribution of 1 by x 1. So, in other words, we can see that this particle I mean essentially what we say that we distribute the particle density, distribute the number of particles uniformly in the interval of this, so, whatever i plus j this particle is present in the continuous domain, we are trying to distribute it evenly and that size is broken and that particle distribution is already uniformly into this size range of i plus j plus x 1 whatever the size because in the continuous domain there is no discrete sizes which are present.

And that is why these uniform distribution has to be maintained. Whatever addition we make has to be uniformly distributed because this x we are talking about is in the continuous range now. So, mathematically this distribution is represented with the help of this Heaviside function. So, we will just tell you.

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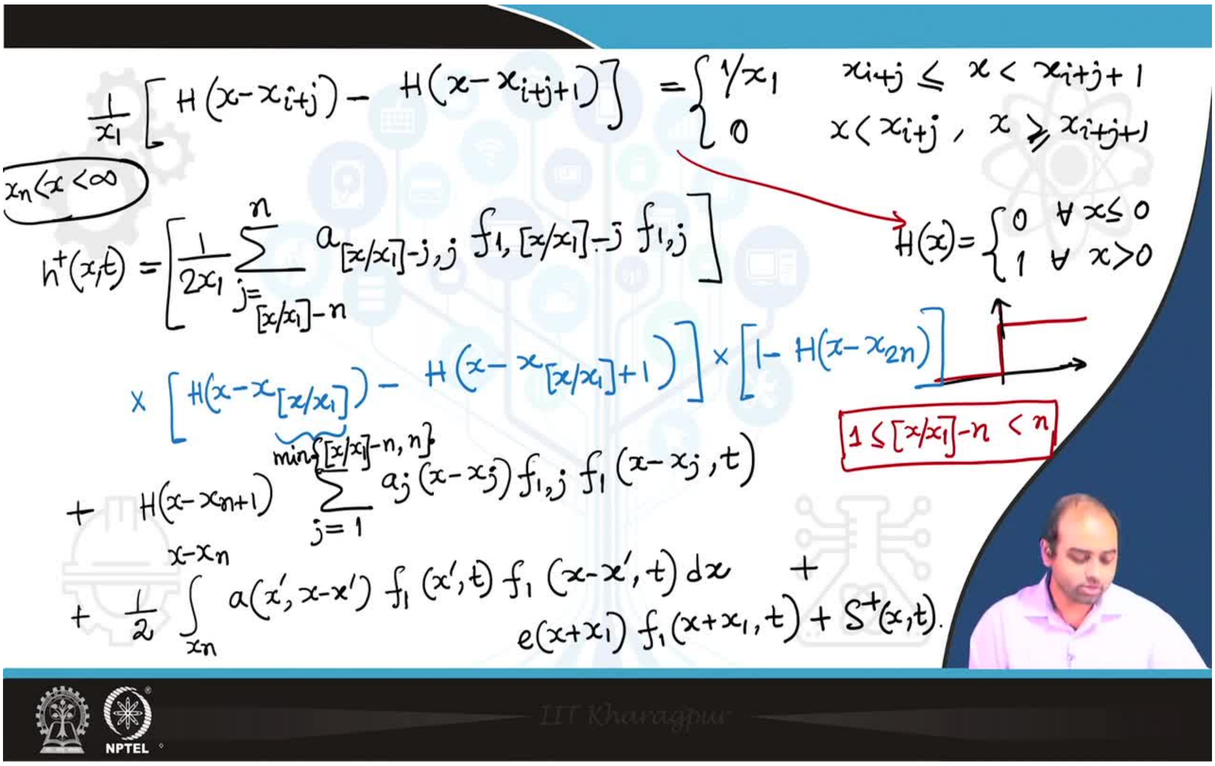

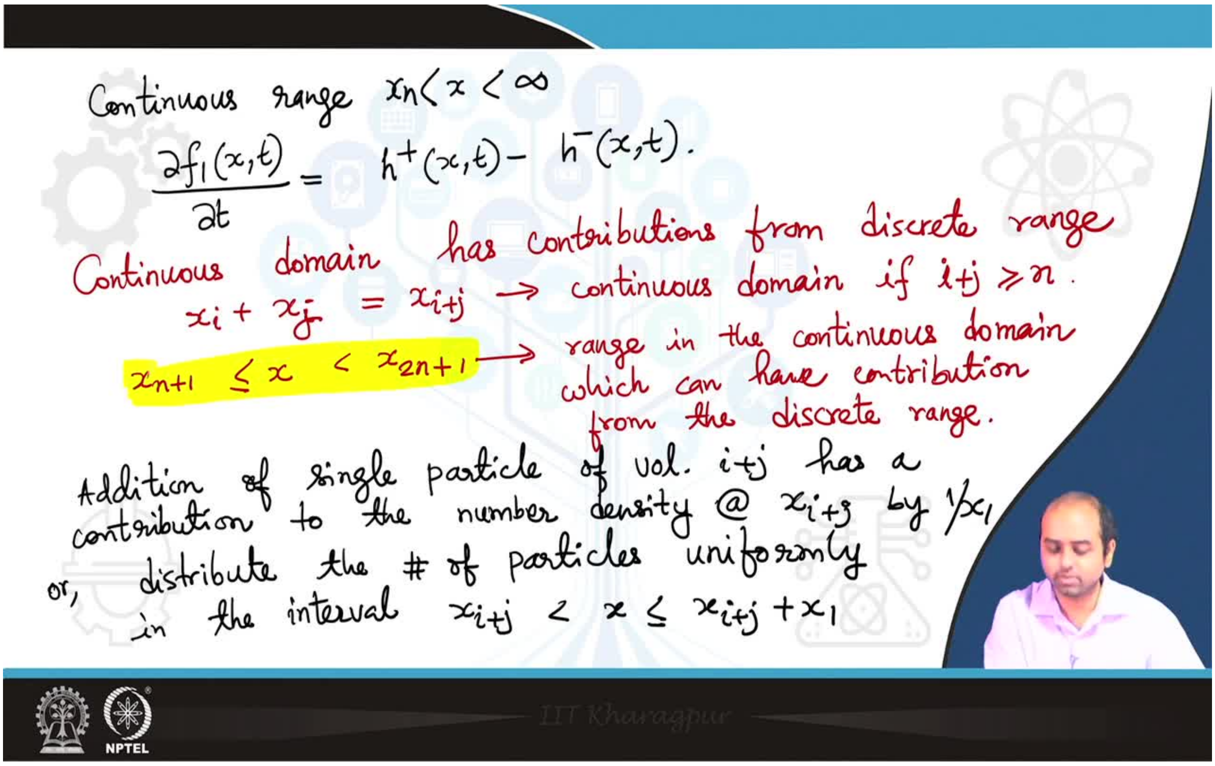

So, make this distribution as is equal to 1 by x 1 if x is in between i plus j plus 1 or 0 if x is either less than x i plus j or x is greater than x i plus j plus 1 in all other cases it is equal to 0. So, this is what the Heaviside function means, I mean essentially this in any Heaviside function is almost equivalent to the delta function you can think of.

So, H x is equal to 0 for all x less than 0 and it is 1 for all positive value of x so, it is like a step. So, this is like a step function so for all positive values it is essentially 1 and for all negative values of x it is 0. So, this is how we make this description of addition of I mean try to handle the addition of a particle from the discrete range, particle agglomerated or aggregated particle from the discrete range in the continuous range.

And please note that all these contributions are only in the range as I have already said only in the range of x n plus 1 2 x 2 n plus 1. Whatever discrete contributions we are having is only in this range, beyond that there is no existence of these sorts of interactions.

Now, let us write down the H plus and H minus expressions. So, the H plus for this case first it will have the contributions by the particles in the, from the discrete range and that is valid only up to x to n. So, I write half 2 x 1 summation x a so, this is the integer function or round of integer function just to have the corresponding integer version of the particle that is aggregating with respect to x 1 f 1 x by x 1. So, this x by x 1 is essentially the integer function.

So, since x is a continuous variable it does not have integer multiples of x 1 just to convert it into the integer multiples of x 1 we have written down this integer function. So, x by x 1 is sort of you can think of it as the smallest possible integer or this smallest possible I mean this sort of rounding of function. So, if x is like 2.5 and x 1 is 1, so, then x by x 1 I mean this integer function will give you 2.

So, that is what we mean by the this represents the largest integer smaller than x by x 1 actually. So, it is essentially that smaller side of the I mean truncating the decimal point actually. So, when we do this and this minus j and then we have f 1 comma j this summation is also from x j is equal to x by x 1 minus n to n. All the possible values we are including here.

So, to this function to this function we are multiplying to this function we are multiplying the Heaviside function. So, what are the Heaviside functions it is a multiplication written here to this term Heaviside function is H minus sorry H of x just since we do not have this concept of i here so, i can only be found out by the this since it is a part of the continuous system, so, this is the variable x.

So, here we can only get i by writing so, this essentially gives us a sort of the i in this case equivalent to the discrete range particle that could form the continuous range so, there is no i in this continuous range. So, x by x 1 gives the sort of the i in the continuous range, but that is not something you should not treat that as the i or the discrete thing, but this gives you some approximate idea on the size of the particle if we are to consider in the discrete range because the contributions from the discrete range can only be mapped with respect to this integer multiples x by x 1 plus 1.

So, this is the Heaviside function we just describe to distribute these contributions uniformly in the as 1 by x 1. So, maybe I should write 1 by x 1 in this way anyway you understand I have already written on 1 by 2 x 1 in the beginning and to that there is another Heaviside function just to take into the fact that all of these processes is only up to x 2 n. Beyond that, these sorts of things does not exist.

So, this entire term now represents whatever you see on the screen represents the contribution by the particle pair in that discrete range to the continuous range. Next is the contribution of the particles from I mean from one discrete and one continuous that is also high possibility. That is why we write subscripts as well as this continuous variable. So, f 1 j is a continuous variable and 1 is from the discrete range, sorry f i 1 j is the discrete number density and f x comma x j is the number density of the continuous particle. So, one continuous and one discrete particle can form and produce another continuous particle and this subscript I mean this super summation range from j is equal to 1 to this is the limit of this summation at the minimum of x by x 1 minus n comma n is the range of the summation.

And please note that, this I should write somewhere here that this x by x 1 minus n this quantity varies from 1 to n, is not it? So, essentially what we are writing here is that any value 1 to n can actually participate and provided that particle is not beyond in. That is why only the discrete particles so, let us say there are 2 particles we do not know which one is from discrete and which 1 was from continuous.

So, this minimum function which helps us to identify that if that particle is I mean this minimum I mean this x by x 1 minus n this quantity if it falls within n that value, then we know that, that is the discrete particle so, that will be chosen and if not, then we know that

that particle is the continuous particle. So, whatever the size that we are choosing for the, there is one continuous and one discrete.

So, to take which one is the discrete can be identified by this minimum function. So, up to that those many number of possibilities can exist. So, this is like the contributions due to the aggregation of one particle from the discrete one particle from the continuous and finally, we have the term from the continuous-continuous aggregation. So, this is the range of the continuous-continuous aggregation.

Here it is both the particles are from continuous range they are identified as x prime and another one is x minus x prime is a pair of particles half is already written on account for the redundancy. So, this pair is from the continuous range there is one more term due to the evaporation of the particles is not it? So, e of x plus x 1 larger particles than x and f 1 x plus x 1 comma t and of course, you have this term, generation terms.

So, this is the contribution or the source contribution for particles in the continuous domain is the h plus contribution.

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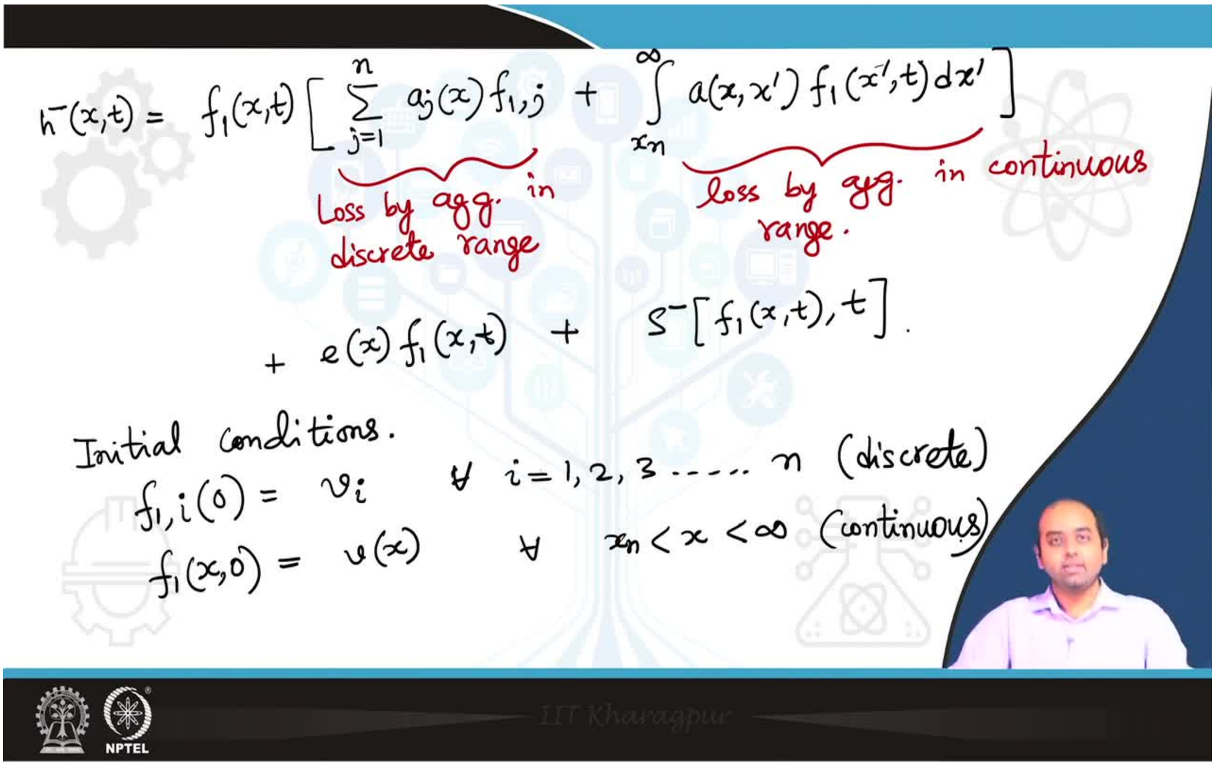

Next we are going to talk about the loss of the continuous domain, the h minus function so, which is given by the loss by aggregation with particles in the discrete range that is a possibility see particles can form by aggregating with another particle in the discrete range. Similarly, it can be also lost by aggregating with another particles in the discrete domain. So, please note the aggregation frequency 1 subscript and then again x. So, this is for all particles in the aggregating in the, this discrete range and we have also contributions from the discrete range x and x prime.

So, everything would be multiplied with f 1 x comma 2. So, this is another pair of the loss of the particles by aggregation in the discrete range, is not it? Loss by aggregation in discrete range loss by aggregation in continuous range. Next, we are having the lost due to evaporation. So, that is e x f 1 x comma t and the lost due to this removal terms.

So, this is how the loss function looks like in this case, to solve this problem you will always need some initial conditions or initial size distribution. So, let us say for the discrete part you will have discrete size distributions where i is equal to 1, 2, 3 like that up to n so, this is the discrete part.

Similarly, the continuous part but continuous size distribution so, this is all about aerosol dynamics, we talked about how the system can be described by the help of the loss and the source functions h plus and h minus both in the discrete range and in the continuous range. The continuous range things were little bit more intensive, because there are a lot of contributions or interactions of the particle both in the continuous range as well as in the discrete range.

I hope all of you get a fair understanding of the process, the aerosol dynamic process, considering this discrete, I mean the different size range of the particles spanning over several orders of magnitude, leading to their classifications as discrete and continuous range particles.

So I hope all of you liked this lecture. In the next class, we are going to talk about the solution methodologies of the population balance equation in some very simplified scenarios. Thank you, and see you all in the next class.