Mathematical Modelling and Simulation of Chemical Engineering Process
Doctor Sourav Mondal
Department of Chemical Engineering
Indian Institute of Technology, Kharagpur
Lecture 52
Dispersed phase modelling – Aerosol dynamics

Hello everyone in this class we are going to talk about aerosol dynamics and aerosol is something that is you know, very common chemical engineering dispersant which is normally you could see in foaming solutions, you could see in the cloud formations, you could also see in foams, in sprays and there are many such instances where it was always used in our daily life.

Now, this aerosol actually is a dispersed phase system where you have small particulate matters that are present and there leads to the formation of new particles by aggregation of these aerosols or, these results can also break down due to some breakage phenomena. And essentially, this aerosol dynamic is a very important problem in chemical industries as well as in process industries, because he wants to have a stabilized aerosol system. And for that modeling this dynamics of the aerosol behavior or the characteristics is very, very vital.

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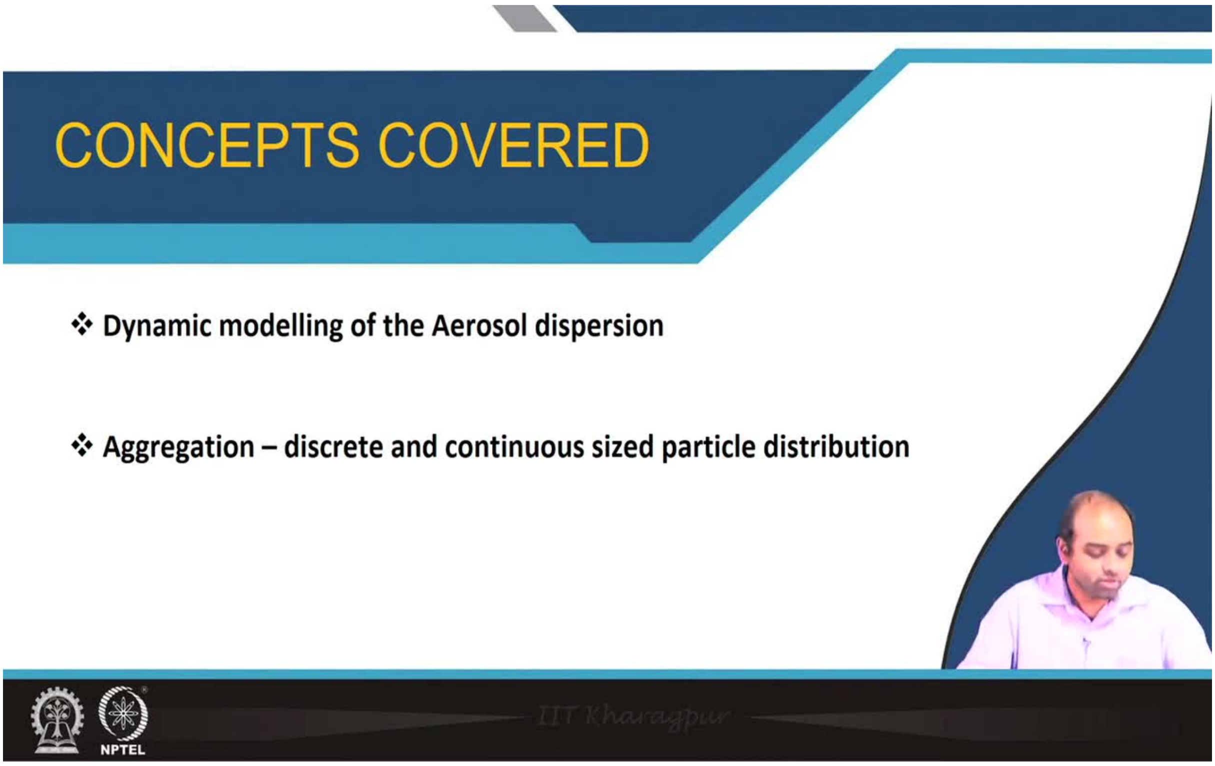

So, you can think of this aerosol as a sort of a dispersion of solid liquid particles in the gas continuous phase and generally aerosols which involves dispersion of solids in fluid medium has size ranges varying over several orders of magnitude, right I mean particle sizes in the aerosol can vary from micrometers to almost millimeter level scales.

So, let us try to bring this aerosol into our, this population balance domain and they are we try to see that how does the aerosol physics can be actually modeled. Before we go into modeling the aerosol behavior I mean, mostly the aerosol behavior change by aggregation and there is as such, there is no such particle breakage event that you see, but there is a decrease in the size of the aerosol particles due to evaporation that is something quite also plays a big role in changing or reducing the particle size.

Because these are generally you know mixed or present in atmospheric system or gaseous systems where the chance of evaporation of these aerosol or the particles which generally liquid particles dispersed in gaseous mediums can evaporate and leading to their decrease or reduction in size.

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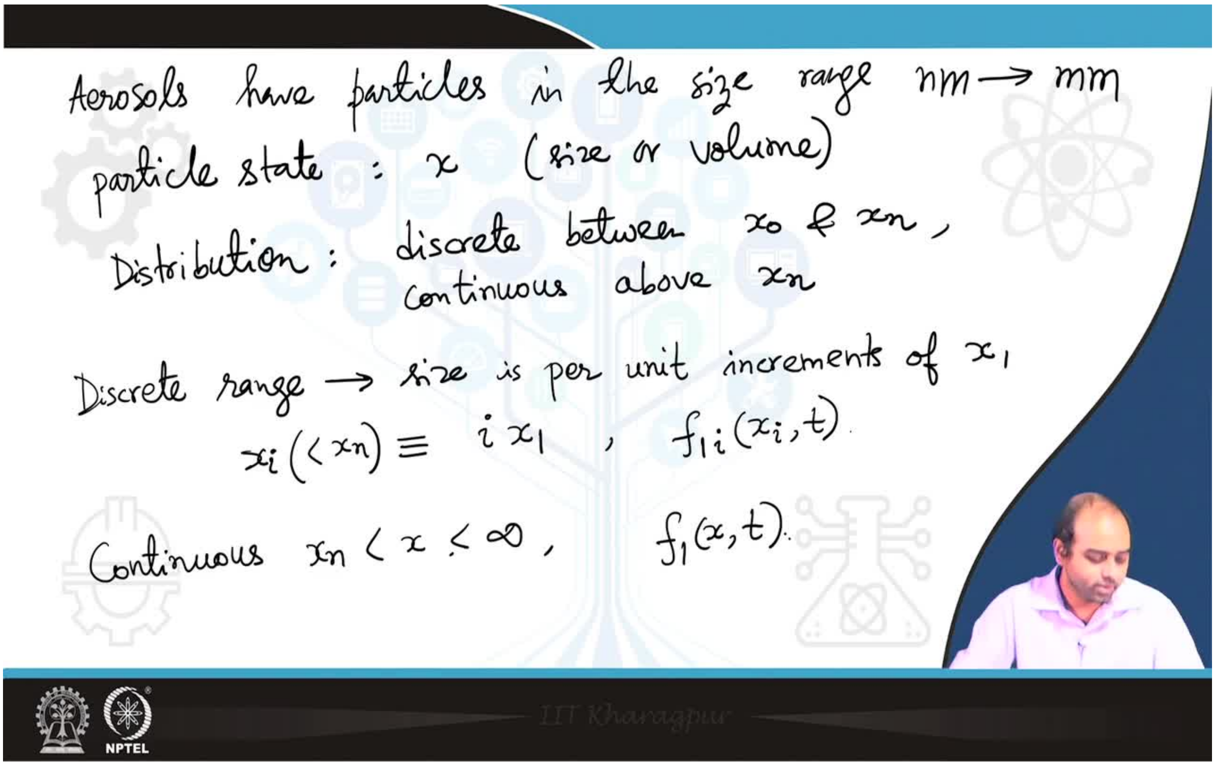

So, as I have said it results typically have a size range varying over a spanning over several orders of magnitude. So, let us say that any aerosols have particles in the size range spanning over let us say from nanometer scale to almost micrometer. So, there are a series of particles or there is a particle size, big particle size distribution in the actual world and normally, because of these, wide range of variation of the aerosol particles, it is often important that, there are certain, particularly in the lower size range, there are certain particles which exist and there is no such a continuous size range.

So, the distribution of the particles cannot be treated I mean particularly when it spans over several orders of magnitude cannot be treated as a continuous size range. So, whatever this particle state we are considering. So, the particle state x which could be size or volume, this does not have variation over this wide range continuously. So, it means that, in the smaller size regions, generally the particles, the particle size or volume is very discrete, and you only you have certain particle size which exist in the smaller size, but in the large size you do expect to get wide range of particles and almost concrete that distribution range to be continuous.

So, what do I mean that in the smaller state the particle size is like discrete. So, the distribution is let us say discrete between the range of this x 0 and x n and it is like uniform or it is continuous above x n. So, you can treat let us say this range of x n to be like from 1 to 100 nanometers. This is like the discrete range and beyond 100 nanometers we see that there is a continuous size distribution on means that the size difference of two particles is very very small.

And this also quite practically if you think or if you try to understand is also quite practically irrelevant in the sense that these small sized particles whatever is present, they actually agglomerate or aggregate and form the larger particles of course, the larger particles also exist by themselves, but since these smaller particles has a tendency to aggregate and form larger particles, these larger particles have a wide range of distributions.

So, as the particle size grows, the difference between two particle size is very small, which is not the case for small sized particles. So, if you have let us say a particle of 1 nanometer, 2 nanometers 3, 4, 5, 10 nanometers, and then you have particles let us say from 1 micron to you know 1000 microns to that if you are adding continuously 1 nanometer particles, so, the difference in of the particle size in the continuous range is very small. The relative difference of the volume or the size of the particles in the continuous range is very small compared to the size relative size differences in the discrete range.

So, naturally the discrete range size particle is in the smaller size domain whereas, in this larger particle size do exist in the continuous range. So, now, we consider that this discrete size whatever this discrete size that we have, this in the discrete domain, in the discrete range the size is per unit increments of x 1. So, you treat x 1 as the smallest size.

So, any particle let us say any particle in the x i where x i is less than x n in the discrete range I am talking about is equal to integer multiple of x 1. So, this is what we are defining as the discrete range whether the size ranges of the particle in the discrete range is in integer multiples of i 1. So, that is how we are defining the discrete particle size ranges and the particle size distribution is denoted by f, there is f 1, there is a number of size densities instead of writing.

So, just to denote that this is a discrete size number density function we write in terms of i, so, this means that you have all integer multiples of particles which exist at discrete range, I mean integer multiples exist for the smallest size particle. So, if the smallest size particle is of let us say 2 nanometers, then you have all like 2, 4, 6 or integer multiples of 2 nanometers, that kind of particle size we are expecting in the discrete range.

So, this is a consideration that we are making it may not be true always, but it is definitely true that, the integer, that this particle size do exist in certain integer range. So, it is like you cannot have a continuous distribution. So it is like quantum states it is very similar. It is certain integer states of the particle or integer size of the particle does only exist and these are multiples of the smallest size is that something which we are considering here.

So, generally the smallest size particles is, I mean it is very small like 1 nanometer or equivalent. Think of these particles like 2 nanometers or whatever and most of the other particles is in size ranges of these particles of the smallest particles, because match they are formed during aerosol preparation is by aggregation of these small particles itself.

So, that is why these existence of the smaller sized particles, happen by aggregation you do not have a breakage phenomenon in the aerosol formation or its aerosol dynamics. So, naturally the particle does not break up into smaller particles, it is only you try to create smaller sized particles and from there by aggregation the larger particles form.

So, in the smaller size regions, they are naturally expected to be integer multiples of the smallest particle size present in the system, that is how this is relevant or that is how this is described or it is actually practically relevant and in the larger (continuous), I mean the larger particle size even though they are formed by aggregation, but since the size becomes so large and the relative difference becomes so small, because of the small sized particles is very small compared to the larger particles.

So, any extra aggregation or addition will normally does normally lead to a small variation in the particle size and that is something what we denote as well a continuous range of the distribution. So, for the continuous range this x is in between x n to infinity and for the continuous range distribution we denote the number density function as f 1 x comma t. So, this is how we denote the continuous and the discrete size range. So, discrete size range does have a subscript i both in the size range as well as in the number density function, the continuous is just the variable x and the number density function does not have any specific subscript.

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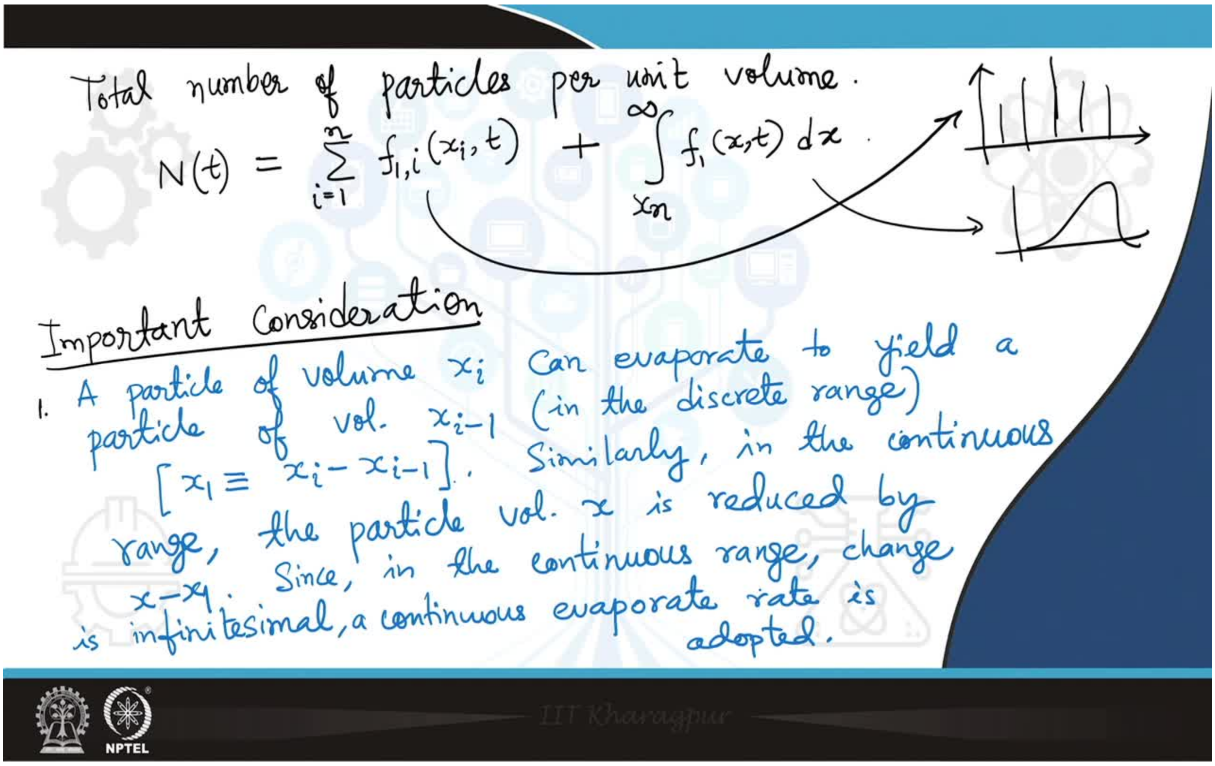

So, now, the total number of particles if you try to estimate total number of particles per unit volume, this does increase the contributions from both the discrete range as well as from the continuous range. So, for the discrete range it is f 1 i where i is from 1 to n and so this is the discrete contribution whatever I have written as a summation form and continuous summation is the integration.

So, this is how we denote the continuous size distributions. So, if you recall in the first class where we talked about dispersed phase systems, we talked about the histograms discrete size distribution, that is how something looks like and the continuous looks something like this. So, this part represents the continuous the discrete size range represents the sort of this histogram behavior.

Now, important considerations in the aerosol behavior or assumptions you can think of, let us list them down first before we start writing down the this their breakage sorry their h plus and h minus function. So, the first one is that I mean I will list it down as well as try to explain to you that a particle of volume x i can evaporate (is related to the evaporation) to yield particle of volume x i minus 1, in the discrete range of course.

So, any evaporation will reduce the particle size by x 1 amount, x 1 is the smallest size of the particle that is what I am writing the subscripts are different. So x 1 so, how do you write so x 1 is the difference of x i minus x i minus 1 is not it? So, any evaporation will lead to reduction of the particle volume equivalent to the size of the smallest particles.

So, similarly in the continuous range the particle volume x is reduced by x minus 1. So, in the continuous range even though I mean generally in the continuous range since this particle size reduction is vary infinitesimal the continuous evaporation rate needs to be adopted. So, since in the continuous range we see that change is infinitesimal, the continuous evaporation rate is adopted.

This evaporation rate we will talk about later when we talk about this writing down the h plus and h minus function. So, this is all about evaporation.

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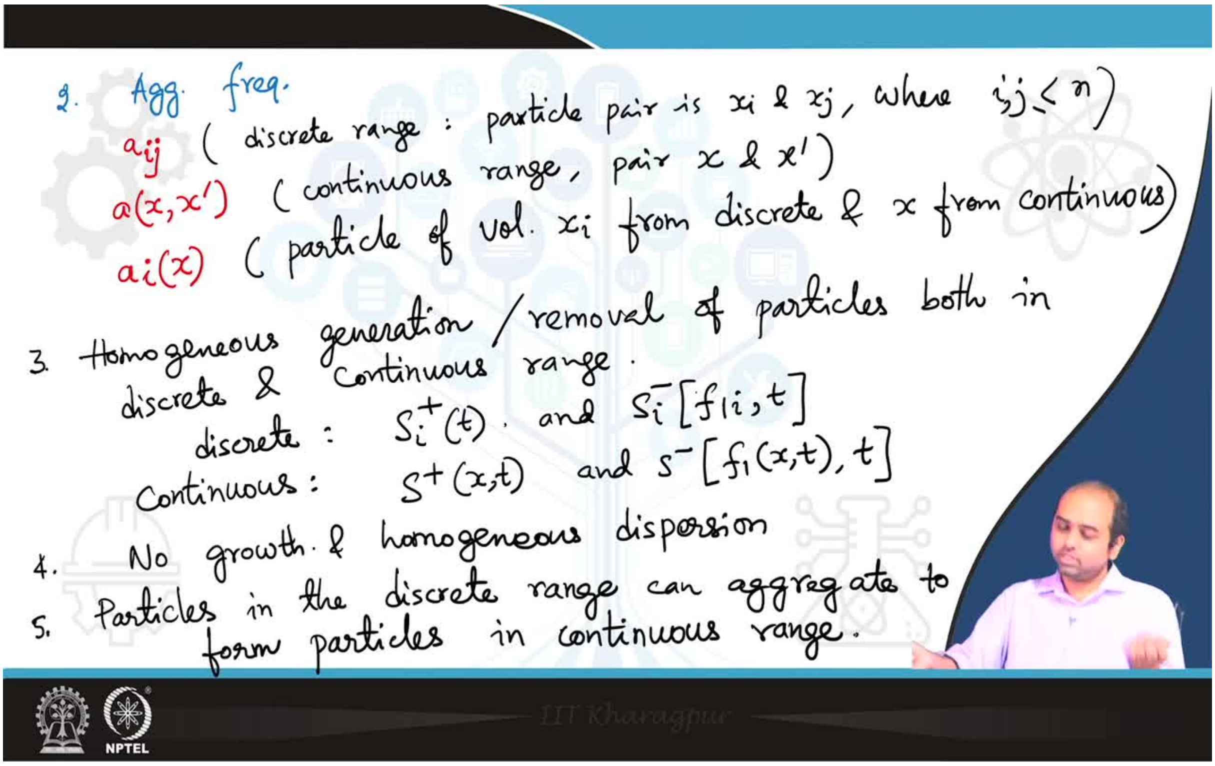

Next is the aggregation frequency so, we write in the discrete range the aggregation frequency is denoted by a ij. So, this is in the discrete range and the particle pair is x i and and x j where both i and j less than n. If we are talking about continuous range, then it is a x comma x prime. So, this is the continuous range, aggregation frequency of two pair of particles in the continuous range.

Here is x and x prime and there is also a (possible) possibility that one you know this particle from the discrete range is aggregating with one particle in the continuous range such a scenario can also happen. So, particle of volume x i from the discrete range and x from continuous range is actually aggregating and that frequency is denoted by both a subscript i as well as this continuous size variable x.

So, next is the homogeneous generation of the particles, this homogeneous generation or removal of particles both in discrete and continuous region. So, these functions are generally denoted as in for the discrete range is like S i plus this is like generation function of time and like S i minus these are generation or removal you know functions of the particles there could be due to some external factors.

And similarly in the continuous you drop that subscript you write it as S x t and S minus of x comma t sorry in the case of S it is, sorry S minus depends on the number density function at that current value, so, it is f 1 i and here also this is f 1 x comma t like this generally the removal rates are dependent on the number density function depending on what we are trying to remove or how much we are trying to remove.

Another important thing is that we consider no growth. So, this means that there is no convective term no growth and homogeneous dispersion. So, that means, there is no role of any external coordinates we assume that these particles generally you get dispersed very fast and more or less uniformly so, there is no source of you know heterogeneity in their spatial locations or their spatial distribution and there is no growth process. So, essentially this leads to no convective term in the population balance equation.

And last consideration is that particles in that is also something we have said in two but just let me write down explicitly particles in the discrete range can of course, aggregate with some particle in the continuous range is something you already said. Also particles, 2 particles in the discrete range they are pair of particles in the discrete range can produce a particle in the continuous range.

So, particles in the discrete range can aggregate to form particles in continuous range. So, this is a possibility that does exist in this case, because since we are doing a different treatment to the continuous range particles and this discrete range particles, so, it is very vital to separately identify that what are the possibilities in each of these ranges. So, now, first we will have a treatment or first we will try to discuss the source and the sink term h plus and h minus term for the discrete range and then we move to the continuous range.

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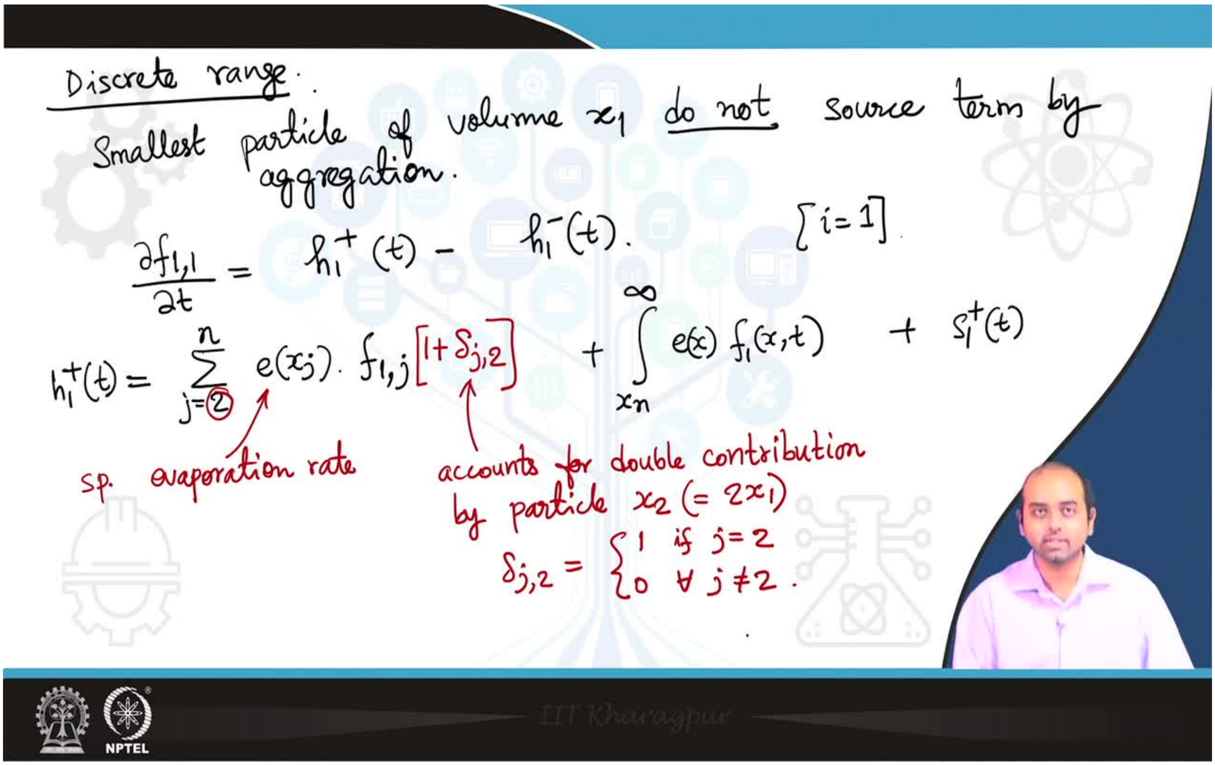

Now, in the discrete range case, please realize that whenever we try to write the h plus or the h minus functions in a discrete range, you will write them as h subscript 1 or h subscript i. So, typically for the first particle and the smallest particle let us have a closer look into the situation of the smallest particle in the system, the smallest particle x 1 do not have source term by aggregation.

This is a very important statement I want you to understand and note that see that a particle whatever this volume is there, what are the possible phenomena that can happen. So, the particle can form by aggregation with another particle. So, particle state x can form by like to other particles smaller than x, it can form by evaporation of a larger particle, these two are the only possibilities and by of course, some generation mechanism if you have in the system or by some external presence if you want to add them.

So, these are the only three possibilities by which a particle can be added to the system. So, the source term will have contributions of (I mean) by particle addition due to aggregation particle forming by evaporation it is by from a larger particle evaporates and forms these present particles any particle whichever we are talking about x it can only form by evaporation of a particle larger than x and by this external this removal or generalization terms.

But for the case of the smallest particle, it is impossible to form the smallest particle by aggregation because particles smaller than x 1 does not exist in the system. So, two particles cannot form x 1 the smallest particles have that possibility is ruled out. So, in the case of the smallest particle, it can form only by evaporation of larger particles larger than 1. So, from x 2 to x n or from particles from the continuous region can also evaporate and form x 1, is not it?

So, that is the only possibility that the smallest particle can form. So, if the population balance equation in the absence of the growth term looks something like this. Now, we are talking about the h plus term here. So, the h plus term which 1 plus essentially the smallest particle and we are doing a separate treatment for the 1 particle because there is no growth. So, there is no formation due to the aggregation of the smallest particle.

So, what is the possibility of the formation it is e, e is the evaporation rate. So, let me write this as the evaporation rate, evaporation rate multiplied with f 1 j and this is across all the particle size from 2 to n in the discrete range. So, e is the specific evaporation rate to the number density function appropriate number density function we are multiplying. So, that gives us the so, that gives us essentially these particles which are formed by evaporation.

So, this is possible from the particle size larger than 1 because they only can evaporate and form this particle 1, particle 1 cannot itself evaporate and form particle 1. There is the reason why this 2 is starting number of this summation. Also please note that there is I mean a double contribution of evaporation particularly for x 2. So, for that we have to have this additional term to account for the double contribution. So, these term accounts for double contribution, is not it? Only specifically by particle x 2 because x 2, x 2 will evaporate and form 2 x 1.

So, whatever this so, this delta is a delta function. So, it means, so, delta j comma 2 is equal to 1 if j is equal to 2 and is equal to 0 for all j not equal to 2. This is for the delta function relates to. So, in the case of this, particularly for x 2, one additional extra contribution needs to be added down based on whatever the number density function we have for 2, one additional term, one additional number will come it will be doubled, is not it? So, that is the reason why this contribution is added specifically to the case of the evaporation of x 2 because generally x 2 relates to the case where it will produce 2 x 1 particles this is something which we already discussed that this is to account for the double contribution.

So, it is essentially not like this 1 plus this one right because it will be doubled essentially, let me write it properly so, only for the case of 2 the number density function should be doubled, because, that is something which we see that is possible when you have 2. So, this is accounting for the double contribution x 2. So, next is the contribution from the continuous side. So, the continuous evaporation rate is given by e x multiplied with f 1 x comma t and this will be integrated in the entire range from x to infinity this is the contribution by the continuous range particle to produce x 1 they also can evaporate substantially and produce the smallest size particles.

And finally, if there are any generation of the x 1 particles that is given by this additional function S 1. So, let me also try to write down the, you know this h sink function h 1 minus function.

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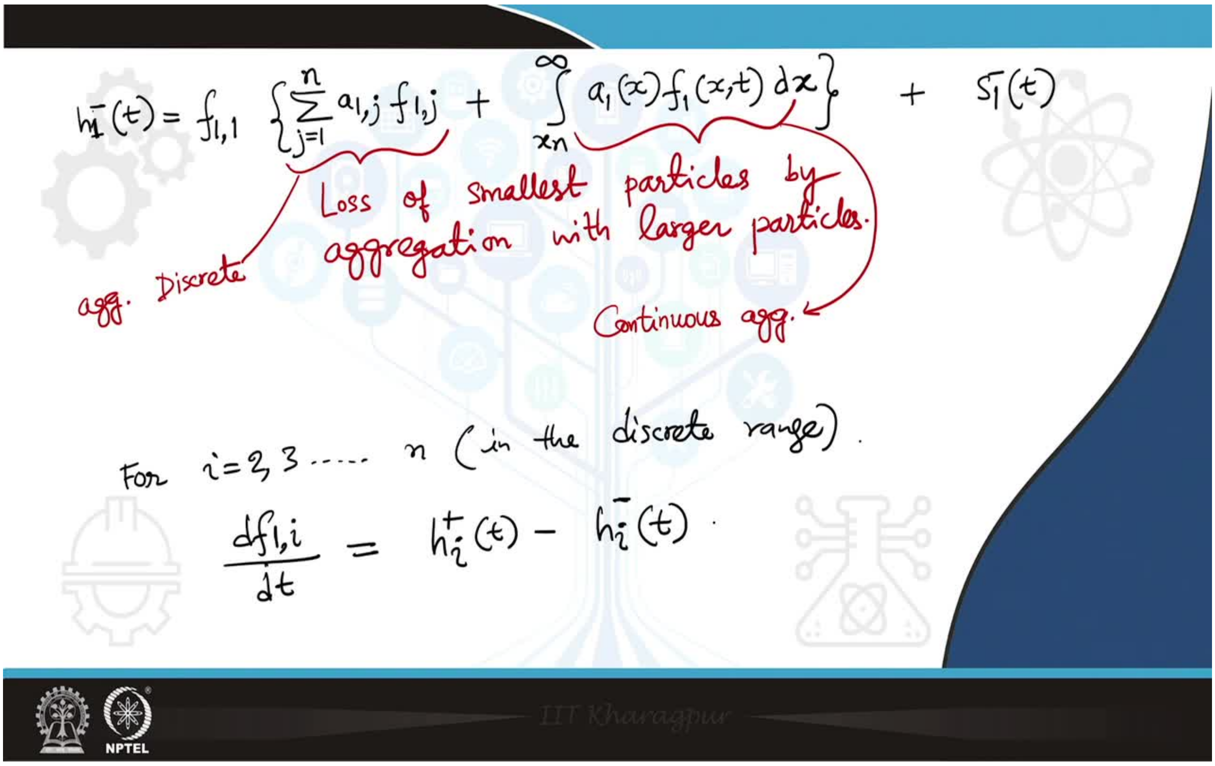

So, this h 1 minus function whatever this loss, so, this loss of the particles are x 1 particles can be due to aggregation with another particle in the discrete range as well as aggregation in the continuous range. So, this is the discrete part.

So, this is 1 comma j, f 1 comma j and this is from 1 to n. So, this is like any particle which is agglomerating with f 1 so, to that we will write f 1 comma 1. So, this is the lost due to the discrete part and this is the part of the continuous range. So, this is the loss of particles, this is the loss of particle. Loss of smallest particle by aggregation with larger (with larger) particles I mean it can also aggregate with himself, I mean itself I would say in that way and this is the actually aggregation with the discrete part and this is the aggregation with the continuous part.

So, both of these are possible and you have essentially along with that any loss due to removal of the particle this is 1 minus. So, this is essentially the sink term for the smallest particle. So, in the next class, we are going to talk about the generalized expression or this description for any particle other than the smallest particle, so, for i is equal to 1, sorry from 2, 2 onwards to 2, 3 up to n in the discrete range. How do you write the source and sink function? So, in that case the population balance equation looks like this h i. So, other than the smallest particle, the h i functions plus both source and the sink term functions should be described in a generic way and then we see that how the particles of the continuous range can be handled in the population balance equation.

So, I hope all of you get a fair idea of the aerosol dynamics particularly in the case of the aggregation behavior and how we have a differential treatment to the particles belonging to the small sizes or in the integer size in the small size range and particles in the continuous size range.

So, in the next class, we will talk about the detailed description of the both the discrete and the continuous size range particles due to this aggregation phenomenon. And, I hope this will be quite interesting for all of you, so, stay tuned. Thank you.