Mathematical Modelling and Simulation of Chemical Engineering Process
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Lecture 47
Population Balance Equation

Hello everyone, in this lecture we are going to talk about, will take forward from where we left off in the last class, and we will work with the Population Balance Equation and try to see, I mean try to use or try to understand the different boundary conditions with respect to this population balance equation.

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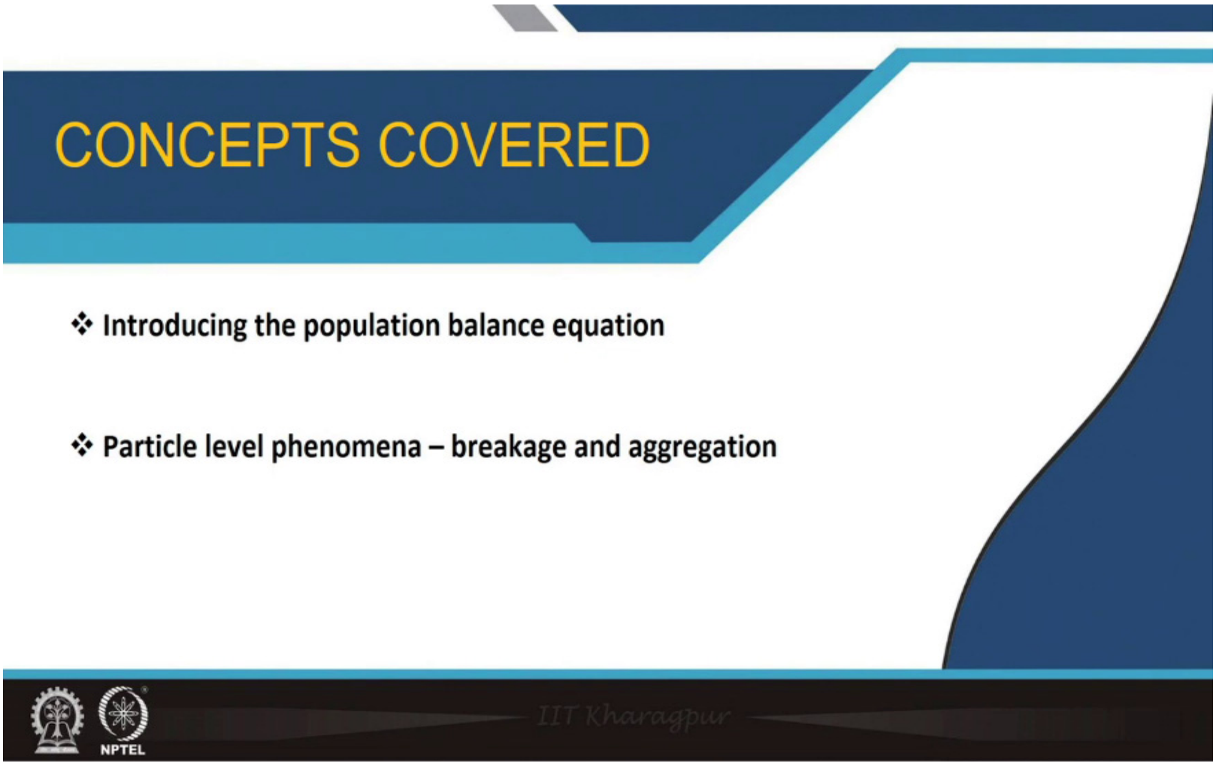

And then we will talk about the breakage and the aggregation behaviour, which is actually very interesting as well as exciting concepts in the dispersed phase models.

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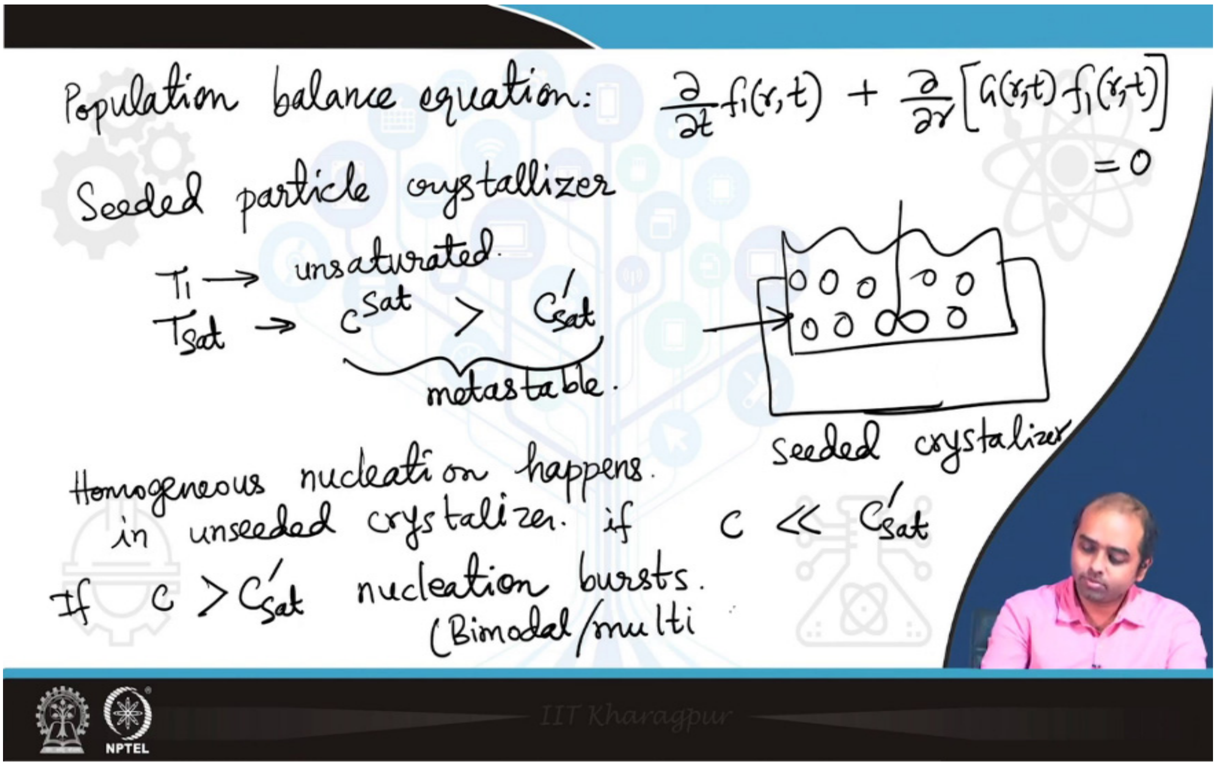

So, let us write down the particle population balance equation to begin with. So, the population balance equation, the differential form if you recall, where r is an internal coordinate that is the size and G is the growth rate. This is equal to 0, this is the population balance equation that we have, okay. So, I hope all of you understood the derivation of this equation and it is essentially a mass conservation equation for the particles of the number entities.

Here, this f1, the particle size distribution could be distributed a discrete could be continuous. So, if it is discrete then the partial derivative has to be replaced by the difference equations or there are difference form, the finite difference form. And but if they are continuous functions then we can write down the derivatives, okay. Now, let us look into the case of particle crystallizer, seeded particle crystallizer.

So, in the particle crystallizer, it is sort of the system, where you maintain uniform temperature, uniform concentration is maintained with the help of studying, so if it is a batch crystallizer and the particles are allowed to grow. So, T actually determines the saturation concentration, so at a particular temperature, things can be unsaturated it can be saturated or it can be supersaturated also.

So, let us say we maintain the temperature that things are in unsaturated state and that temperature is denoted as T1. Tsat is the saturation temperature, so the saturation temperature is concentration, I mean whatever this temperature we talk about the saturation temperature will lead to saturation concentration. And this saturation concentration is generally lower, I mean is greater than this C sat Prime and this is generally the metastable region we call it.

Now, these seeded, in the seeded crystallizer, we generally add seeds to the, so that the particles, the initial size of the particles or the crystals is more or less uniform, and the growth is more or less uniformly it grows, I mean most of the, so I mean the growth is more or less homogeneous both spatially as well as with respect to time.

Because the initial starting their size is provided into the system and it is sort of uniform, so you add seeds of uniform size or distribution into the system which acts as the starting condition and over those things grow and as it grows, the size more or less forms a uniform distribution, and the growth is also homogeneous or uniform in the spatial dimension. Also there is no heterogeneous nucleation.

So, this is sort of a homogeneous nucleation that you stimulate by adding the seeds into the system. So, generally this homogenization or this homogeneous nucleation happens in period if there are no seeded system crystallizer, if this saturation condition is much smaller than the super saturation con condition. But if this C, sorry, if C concentration is below the super saturation condition, if the concentration is above the super saturation limits, then nucleation burst happens. And, if this nucleation burst happens, you generally expect to see bimodal or multimodal particle distribution.

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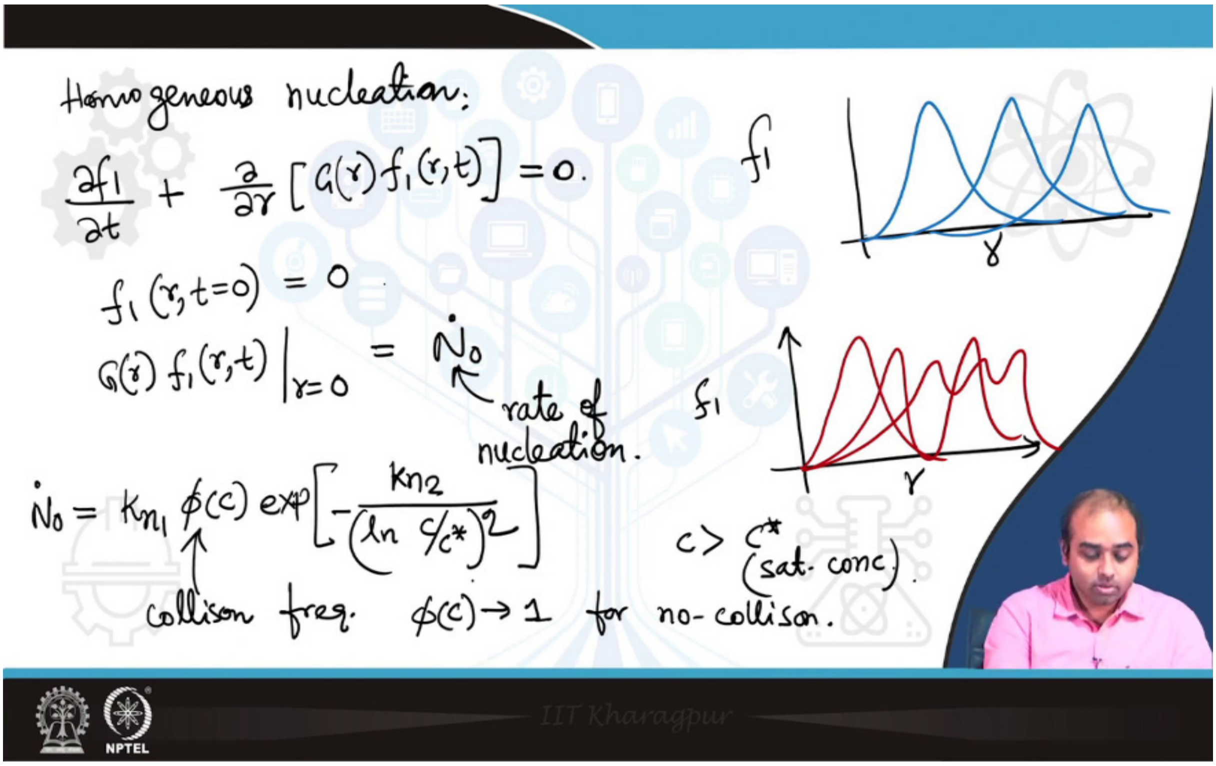

So, what is this bimodal or multimodal? So if you try to draw the number density function, normally for the case of seeded crystallizers, you would expect to grow things like this, this is the seeded crystallizer case. But if you have unseeded crystallizer, normally things go out of hand, so initially things may be like this, but slowly it will look something like this, like this with time, multimodal peaks, okay, bimodal or multimodal peaks, okay.

So, in this case we are discussing about homogeneous nucleation, so let us take it from there. So, homogeneous nucleation, so the particle, the population balance equation we have, let us write that as r, dr. So, this growth rate is only a function of r that is normally the case with respect to crystallization process, so the growth function is not function of time.

So, what about this boundary conditions? Initially at t is equal to 0, there is no crystal, so we call that 0. But this G of r, f1 r comma T at r is equal to 0 is some value and this is the initial nucleation rate, so that is the rate of nucleation provided by some initial seats. So, typically this depends on the concentration, so typically this n dot depends on these sorts of functions that looks something like this, this is crystallization physics, so of course C is greater than C star, so C star is the saturation concentration then only the crystallization starts actually.

And here, Phi C is essentially the collision frequency between entities, so Phi C tends to be 1 for no Collision. Other values of Phi C could be, it could be C, it could be a function of concentration, those are the possible values of this Phi C. So, this is just to get you an overview of how particle, sorry, how this population balance equation can be used in real world explaining problems or application of the, of in engineering problems and this is the case of the nucleation.

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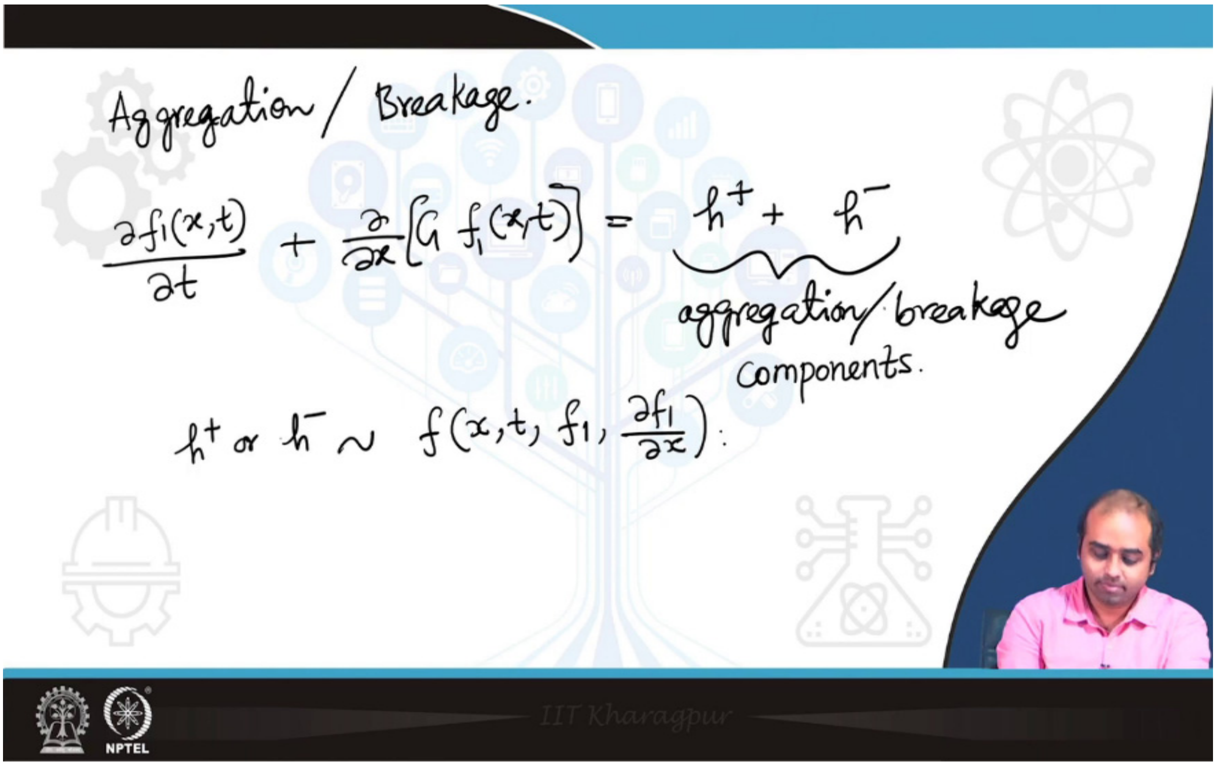

So now, we will talk about the aggregation or the breakage phenomena. As the name suggests, aggregation means joining of two entities or two particles and forming a new one, two or more particles in forming a new one. Breakage means this integration of a particle or an entity into two or more entities. Of course, whenever this aggregation or breakage happens let us say, a large particle breaks into two smaller particles, so the number density of the large particle will change.

Because the large particle is no longer exist, it had led to the formation of two smaller particles. So, two smaller particles I mean the and maybe the there are other particles of the similar size of these second-generation particles or the first-generation particles after the breakage, so they will be added up to that distribution. So, the distribution of the mother particle or the parent particle will be reduced, and or the numbers will be reduced, and the number of the daughter particles, or the first-generation particles will increase, just the reverse happens in aggregation.

So, whatever this entity that forms agglomerate, agglomerates and joins and from a larger entity, so the initial state whatever you are having that numbers will decrease because they are now lost from the system leading to the formation of new particle. So, the numbers of the new particular the larger particular aggregated particle will increase, okay.

So, generally the population balance equation in the presence of or when you have breakage and aggregation functions, generally, you have these two functions, h plus and h minus. These are like the source and the sink contribution to this population balance equation aggregation or breakage, whatever happens. In both cases, you will be having some particles which are added to the system and there are some particles which are lost from the system.

So, this is like source and sink terms to these to this population balance equation that happens. So, this h plus or h minus they are generally functions of coordinates, time, it could be functions of the distribution function itself, d f1, dx, anything all the possible combinations. Next, we will focus mostly for the breakage now and then a couple of classes, later we will talk about the aggregation behaviour, okay.

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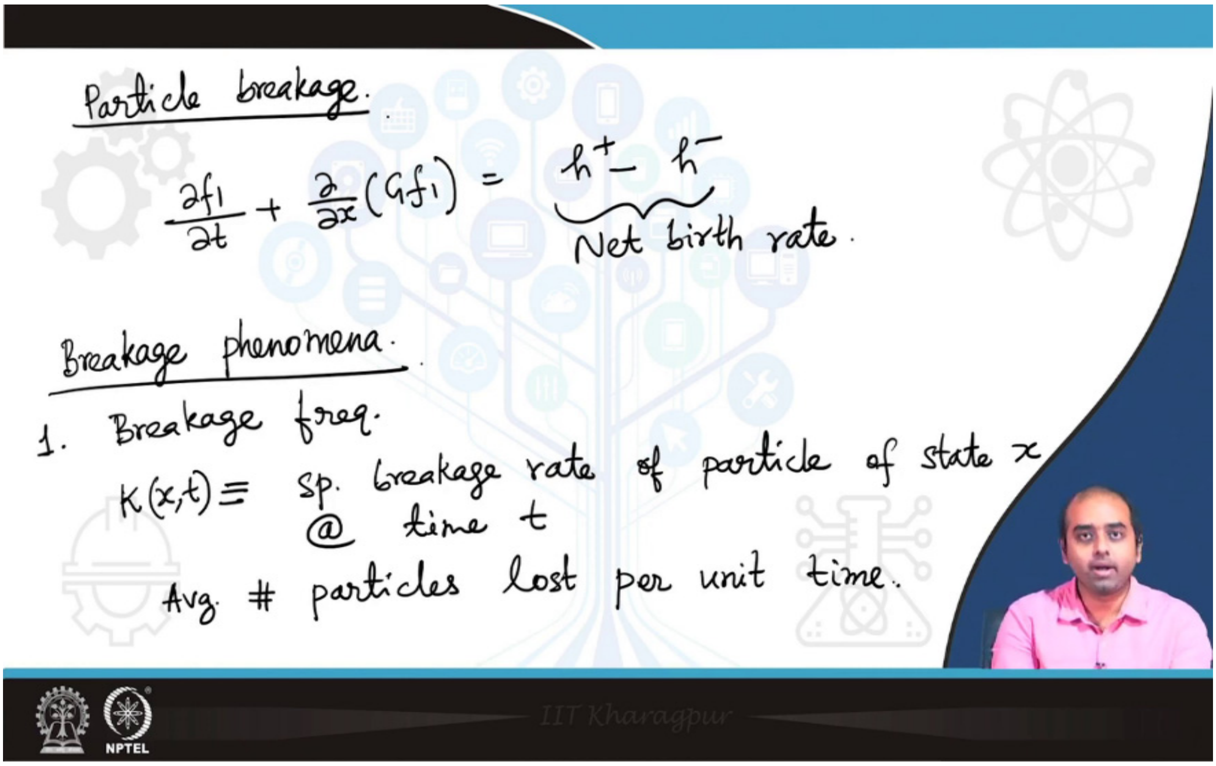

So, let us talk about the particle breakage phenomena. So, in the particle, so breakage could be, breakage of disintegration of droplets, forming new daughter droplets, degradation of polymers by UV or some reaction ultrasounds breakage of particulate matters like glass beads, talcum powder any Milling operations that you do pulverization, then you have ball Mills or any rotary meals, all are examples of particle breakage phenomena.

So, the population balance equation in this case is, sorry, G into f1, so you can consider this as the net birth rate, h plus is the terms which are added to the system by this particle breakage, of course of smaller particles and h minus is the function which add, I mean which is taken away from the system or which is like the data of the particles which is essentially the larger particles because it is a breakage phenomenon.

Now, this breakage I mean there are some breakage functions, let us talk about the breakage functions. So, this breakage phenomenon depends on three factors or you can say three functions, the first function or the first factor is the breakage frequency. So, this is again a physical parameter, so what does this breakage frequency tells you, that we represent that by K (capital K), so this is the specific breakage rate of particles of state x at time t.

So, it is the breakage rate essentially of is written, as x comma t which means that whatever the particles as there at the particular size, I mean x represents the internal coordinate for this problem. We are talking about that the breakage rate is a function of the particle size as well as the time, so it is essentially the breakage frequency. Next is the, so breakage frequency is the average number of particles that you can think of, average number of particles (is another way of putting it) lost per unit time.

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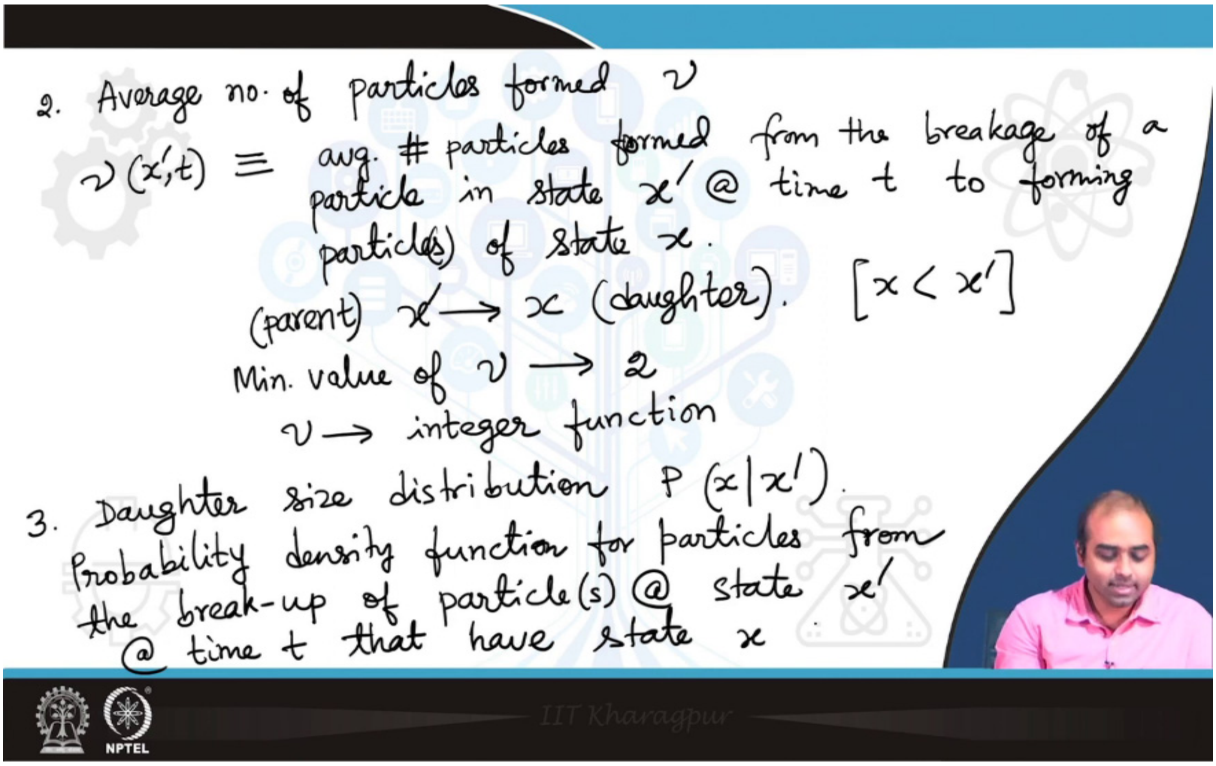

Next is something, the average number of particles that is formed after a breakage operation, so this is the second factor of the function. Average number of particles formed, form called the new, so these new, so is a function of x Prime. I will just say what is x Prime, so it is the average number of particles formed from the breakage of a particle in state x prime at time t to forming particles of state x.

So, you can think of x prime is like the parent state and x is the daughter state, so it is the transfer, it is the breakage of the parent particle to the subsequent formation of the daughter particles or the broken up particles, and of course this x is always less than x prime, total particles cannot be larger than the parent particles.

So, this is the quantity this nu tells you that what is the average number of particles which for which forms as a particle of State x prime or a parent of State x Prime is broken down to x State, what is the number of particles from? Of course, the minimum value, so the minimum value of minimum value of this nu is 2, at least it has to form two particles, one particle can break into only two particles, I mean minimum two particles less than two, it is not possible.

So, minimum value of nu is two and nu, this function is always an integer function, so it will always have integer values. A particle cannot break into having some fractional values, it will only distinct integer, into distinct number of particles, so it is it has to be integer, so if the integer value function and it is the minimum value is 2. And the third one is the daughter size distribution, which is represented as p as the probability density function of x, with respect to x Prime, with respect to its parent.

So, these daughter size distribution is the probability density function for particles that has formed from the breakup of particle at state x prime which is the parent, at time t that have state x. So, this is the probability density function of the daughter particles that have formed from their parent particles. So, we see these are the three important functions which helps you to describe the breakage phenomena.

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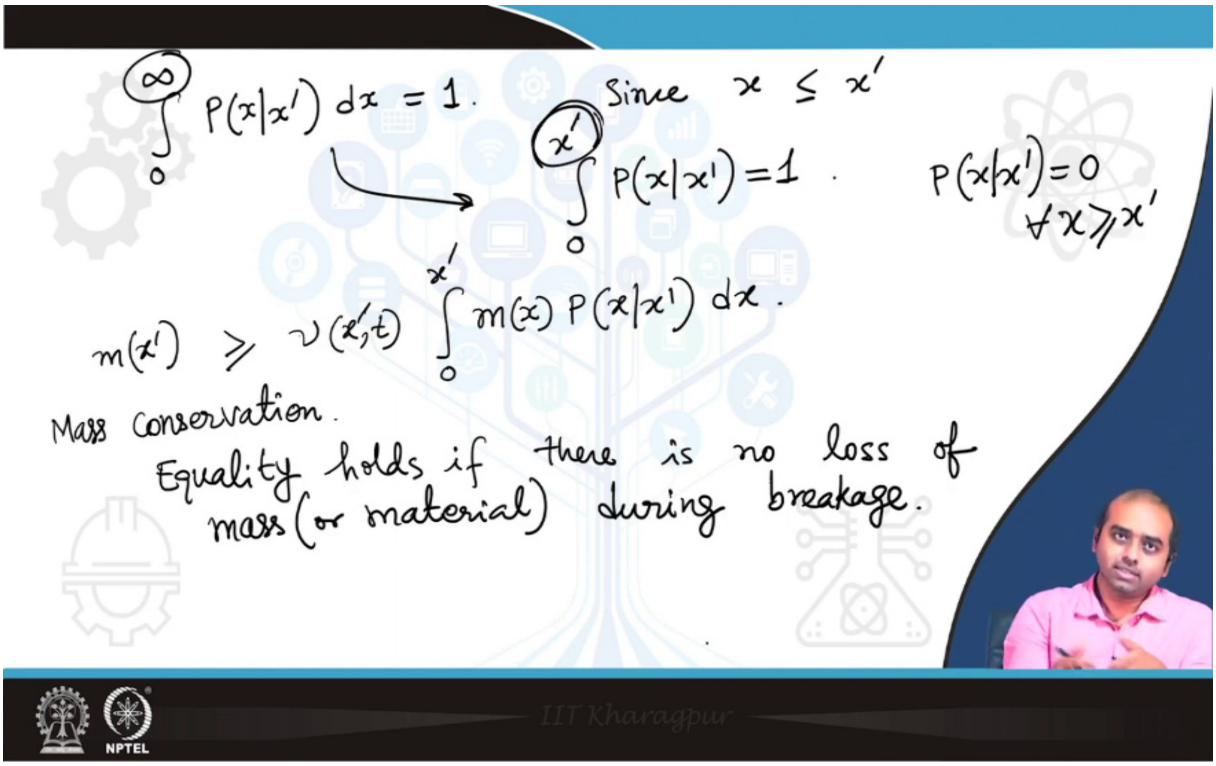

So, some of the important things we should also note here is that this breakage function which represents the daughter size distribution has to satisfy the mass conservation, so what do we mean this mass conservation? so over this I mean it is a probability density function, so all the daughter particles, summation of all the daughter particles is equal to 1, over the limits of 0 to Infinity, this is true for any probability density function.

So, what is interesting is that since x is always less than x prime or less than equal to I must say, this integral can be written down as 0 to x Prime only, because beyond x Prime there are no daughter particles. So, P of x Prime is equal to 0, for x greater than x Prime, this is not possible, one sorry, this is one, so the infinity whatever we are saying is replaced by x Prime, because beyond x Prime there are no particles. The probability density function of the daughter size particles, beyond x Prime is not possible, because x Prime is the parent size particle, so all the daughter size particles are below that size.

A particle cannot have size larger than its parent, and I mean do not take this sense in the literal meaning, but whatever particle that is forming from its original state after this integration, after breakup, cannot be larger than the original particle isn't it? So, that is the reason why these particles or this probability density function is 0 for all such cases.

Now, it will also satisfy the mass conservation, so what do I mean by this mass conservation is that, the total number of particles that is formed, the mass of the particles that is formed, so let us write it like this m of x Prime, the mass of the parent particle should be greater than equal to the total number of daughter particles form. So, what is the number, how do I get the number? First, we multiply the number of particles that is formed, in this breakage, multiplied with the mass of each particle, and the integration of the probability density function.

So, this is the mass conservation that has to hold always for this breakage. So, these are some very important correlations or let us say equations or relations that we are talking about here, and as we use in the subsequent classes. Why I have written down this greater than equal to? That it may be there may be some losses during this breakage, where they do not account for any discrete particles or any particles, those losses can get lost.

If you are doing a ball meal operation and you are trying to break a larger size particle into smaller size of particles, some there may be loss of material in the form of dust, etcetera, that is the reason why that equality sign is there. So, equality holds if there is no loss of material during breakage, then the equality will hold or if there is no loss then always you will, I mean if there is loss then that this inequality will be there and it will be always mass of the parent particularly always be greater than the total number of daughter particles that is formed.

It could be in different size ranges, so the particle size distribution is important and m x is the mass a size function, that needs to be multiplied with the particle size distribution across the overall size ring, that is from 0 to not Infinity, it is up to the size of the or the dimension of the parent particle, and everything should be multiplied with the number of particles that is formed, so that is this function nu.

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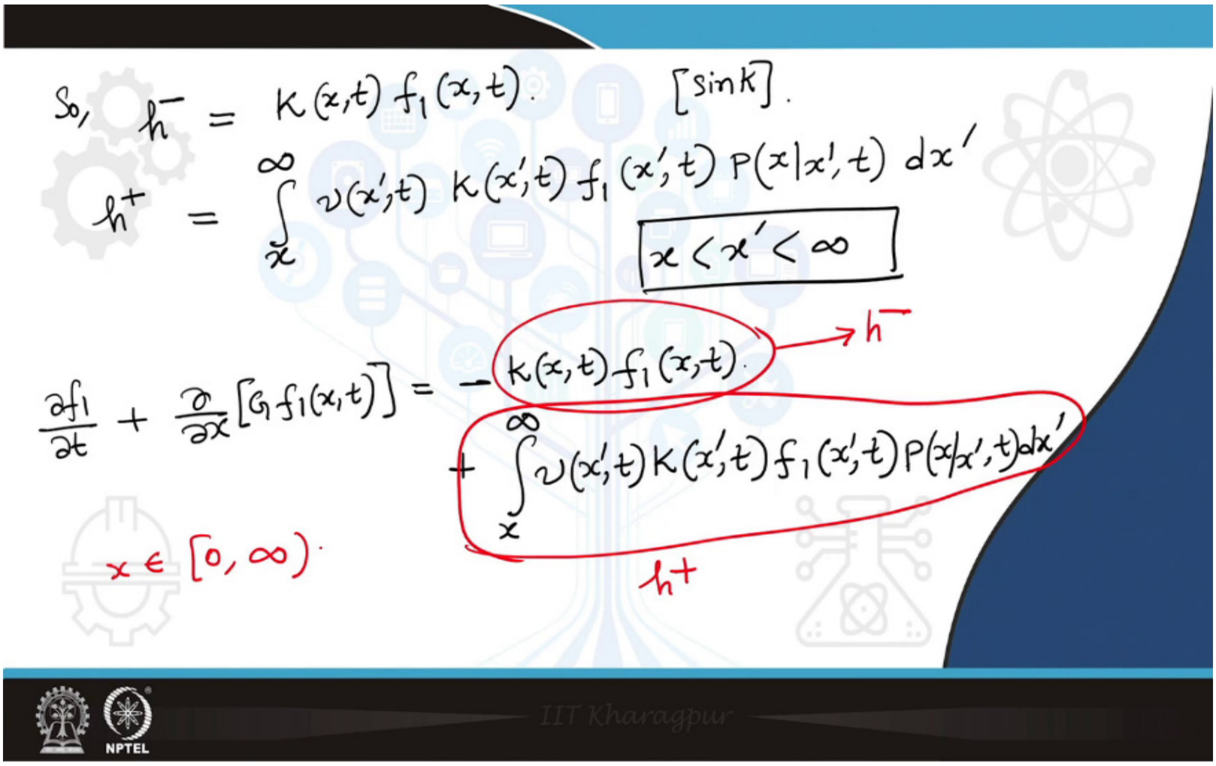

So essentially, these particles that are lost, this h minus function can be written down as K, which is the number of particles that is formed, multiplied with the number density function. So, this is the number of particles that is lost, so at any particle, so please do not get confused with x Prime and x, x Prime in the generic frame is also and x do not treat x Prime to be very different, and x is the general coordinate that we always talk about.

So, x Prime and x, I mean even though we are trying to designate x Prime as like the parent State and x as the daughter State, just to distinguish these two. But when we try to write down the generic population balance equation, this parent State could also be x, isn't it? So think it in that way. And this is the sink part, so these particles would be lost by the breakup, so K is the specific breakage rate, and this is a, this is like the number of particles which is lost part time.

So, K has, this K has a unit of power per time, like number of particles that is lost per time, so this will be equivalent to df dt, when we write in the population balance equation. h plus is the particle that is added to the system by this breakage process, so what are the particles that are added? So we are talking about nu, then we have K, the specific breakage rate, f1, number density function, P the nu probability density of the nu particle size this, I mean particle size distribution.

So, this is like integrating the whole range of the, this is like integrating the parent I mean whatever this x Prime we wrote down here just to represent that it is the parent particles that is getting disintegrated, in that respect we wrote all these functions, this nu, and K, and the probability density function and everything. But these should be essentially integrated, these should be integrated from the limits of x to Infinity.

So, above the daughter size, that is the size range because the limits of x Prime, this x Prime exist only from x to Infinity. The daughter size exists only from the above the size of the daughter I mean, the parent size exists from the daughter size to Infinity, it cannot be below the daughter size, so there is no point from 0 to Infinity. So, that is the value of the amount or that is added to this system.

So, the total net population balance equation in this case that comes out as like this, G into f1. So, this part represents the particle that is lost, that is h minus, and this part represents the h plus, and x can have values from 0 to infinity. So, this is the overall population balance equation accounting for the breakage process.

So, in the next class we are going to talk about some application of this breakage phenomena, in the context of the population balance equation. And we will see some examples from there how specifically this equation can be formulated for the case of some real-life applications. For example, let us say a liquid dispersion or a bubble coalescence or a bacterial growth, cell division and things like that. I hope all of you liked this lecture, and thank you for your attention.