Mathematical Modelling and Simulation of Chemical Engineering Process
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Lecture 46
Dispersed phase modelling - introduction

Hello everyone, in this week we are going to talk about dispersed phase modelling. So far, we have been talking about systems which is related to Continuum Dynamics, where we do not identify or we do not look into the particle level events or molecular level events, whatever you can think of. But in this week, we will try to look into the situations where the phenomena happening at the particle level or with the particles is important and significant.

So, for example you know Emulsion systems, so what is the interaction of the particles or the colloidal particles is distribution is very important. Then, this solid powder, talcum powder, this again interaction of the particles their aggregation this is very important. Bubbles is another important phenomenon, you cannot describe bubbles in the system as like a gross, a sort of one unit or one system, because each bubbles will be of its different shape or size, bubble-bubble interactions are there, the whatever this flow, etcetera, around one bubble is different from the another double, two bubbles can coalesce, they can break up, and things should be changing and bubble is the important product here.

Another important example of a dispersed phase system is crystallization. So, crystallization involves the growth of the particles and each of these particles is not necessarily, not necessarily same as the other one, so their distribution, their size, their mass, their density, are all can be different. Again, polymer is also another system which is at the molecular level which say, but again polymers, polymeric weights, they are chain length, they are size, etcetera, distinctly different from another polymer. So, here the size distribution of these particles is important, their interactions is important, one particle can generate another particle, and then the size distribution can change essentially, so all these things are very important and that is where the dispersed phase systems or phenomena is very relevant.

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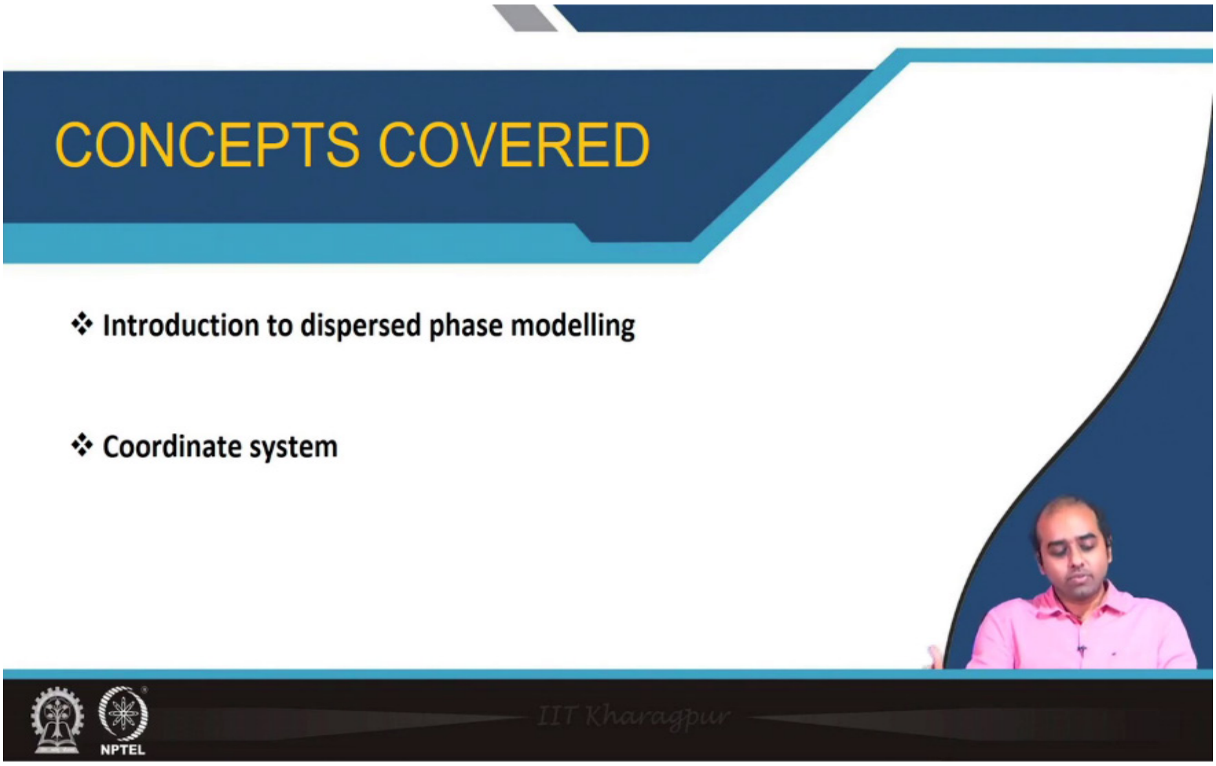

CONCEPTS COVERED

- Introduction to dispersed phase modelling
- Coordinate system

So, we in this class, we will talk about and essentially in this week as well as the following week, we will talk about how the dispersed phase systems are essentially different or what are the different types of physics of phenomena which takes place in the dispersed system. We will talk about in this class also about the coordinate system, so coordinate systems could be of two types, external and internal, and we will talk about what are these essentially. And then slowly we will move into the purple and swim, balance equation as a sort of equation that describes the size distribution in a, with a differential equation, I would say or put it this way.

Then we will look into the aggregation behaviour, then we look into the breakage functions, and slowly we will also look how the population balance sequence equation can be solved analytically or numerically, okay. So, the first thing that we want that these are the idea of the display is talking about a population.

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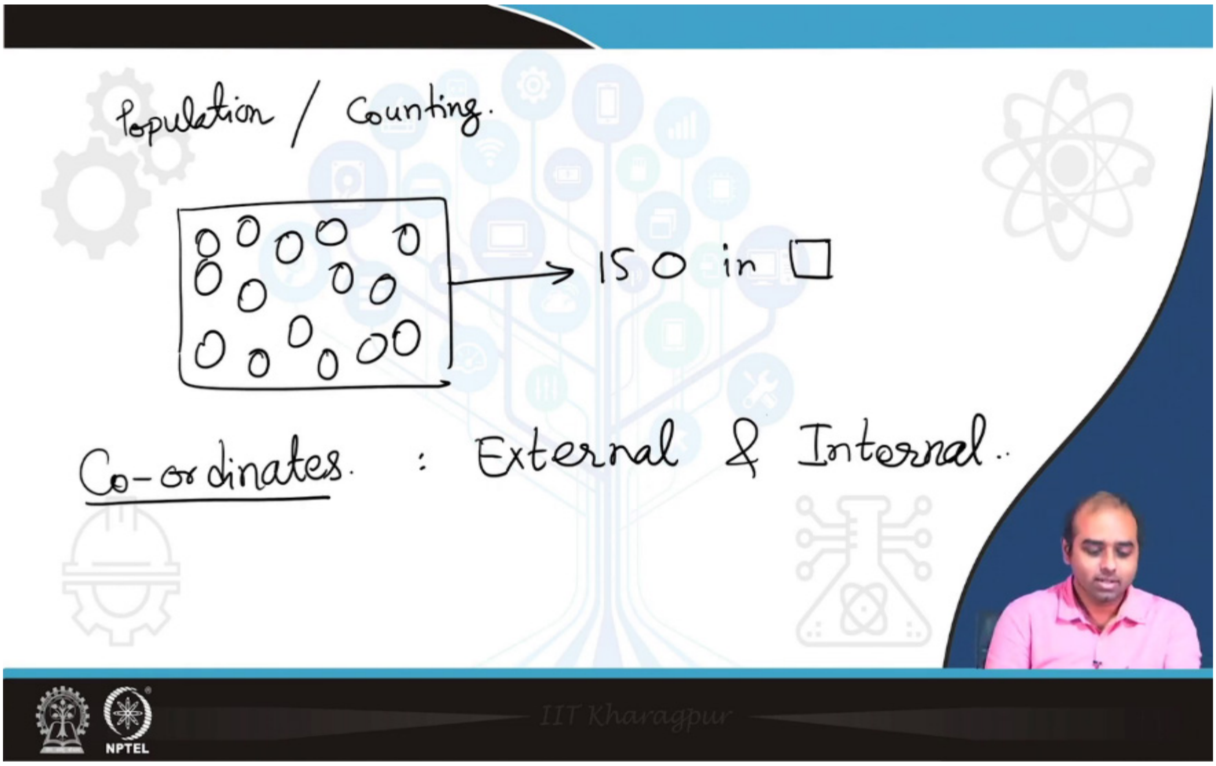

Population / Counting.

Co-ordinates : External & Internal..

So, we talk about a population in this case here. So, population or essentially counting, so it is all about counting and determining discretely what are the how many the number of particles or entities are present in my system. So, if I have a system as my box, and let us say I have certain number of particles in the system, so it is about counting, so I say that there are 1, 2, 3, 4, 5, 6, 6 plus 4, 10, 12 or let us add one more, one more one, so I can say that there are 15 particles in my box.

So, it is about counting, so population or determining the population or determining the dispersed phase is about counting. So, counting the number of particles or the number of entities present in the system, so instead of grossly talking about the concentration that we are used to in talking about Continuum system, where we say that this, these solutes or these particles are homogeneously distributed and we talk about or even though if they are heterogeneous distribution at the molecular level or at the particulate level, it is essentially, they are sort of uniform, so we can talk about or bring in this concept of concentration.

But here instead of talking about the concentration, it is essentially the number concentration, you can think of or the number of particles that we are talking about in this particular system. And also, these distribution of these particles, distribution of these particles in the spatial domain may not be uniform or homogeneous always, so that brings us to the idea of the coordinate system. So, there are two types of coordinates, there are two types of coordinate system, in dispersed phase process systems, so what are these two types of coordinates, one is known as external, and one is known as internal.

So, external are the coordinates which specify their spatial location, so the spatial location is essentially the dimensional coordinates that we are talking about of individual particles is the external coordinate in this system or is the external coordinate for the problem the normal. The dimensional coordinate of the system or of the particles, that we are also used to in writing, the dimensional coordinates is the normal spatial location is the external coordinate.

But the interesting part is the internal coordinate, so what is this internal coordinate? Internal coordinate is nothing to do with inside of the particle, it is not at all a spatial Dimension, let me clarify this. And often it becomes quite confusing as we move into the details of the dispersed phase systems. Internal coordinates are something which is related to the particles or it is about the particle.

It could be the particle size or the diameter or its mass or its age, if a particle is disintegrating, so what is the age of the particle or the average age of the particle, so these are the internal coordinate. So, you can we can assume that these internal coordinates are sort of the particle or the this entity characteristics in themselves, rather they are they are dimensional position or the spatial location. So, this is what we refer as the internal coordinate or the sort of the intrinsic property of the system. We are all used to this thermodynamic concept of the intrinsic properties, so, sorry, not the intrinsic properties, it is the extrinsic properties of the system, so which something like mass, volume, its size, these are the internal coordinates of the system, molecular weights for polymers may be, number of monomer units, these are sort of the internal coordinates.

So, any property, any property dispersed phase property, we will add or every dispersed phase property, which is not assumed constant or its not changing or is changing not changing no, adds one dimension to the problem. So, the same way how we treat the spatial dimension or the external coordinates, for example, the same way you also treat the internal coordinates, so it is added dimensionality to the problem.

So, the mass or the size of the system or the particles adds one extra dimension to the dispersed phase system. And of course, adding one extra dimension increases the calculation complexity as well as the coordinates. So, you have we have to choose these coordinates very carefully, whether it is internal or external, whatever it is, but these coordinates add, I mean coordinates are nothing but the dimensions to the problem. And internal coordinate is not the physical dimensions of the locations or their xyz values, it is the property of the system, the extrinsic property of the system which are referred to as the internal coordinates of the system. So, I hope I could make some sense about these internal coordinates in this dispersed phase.

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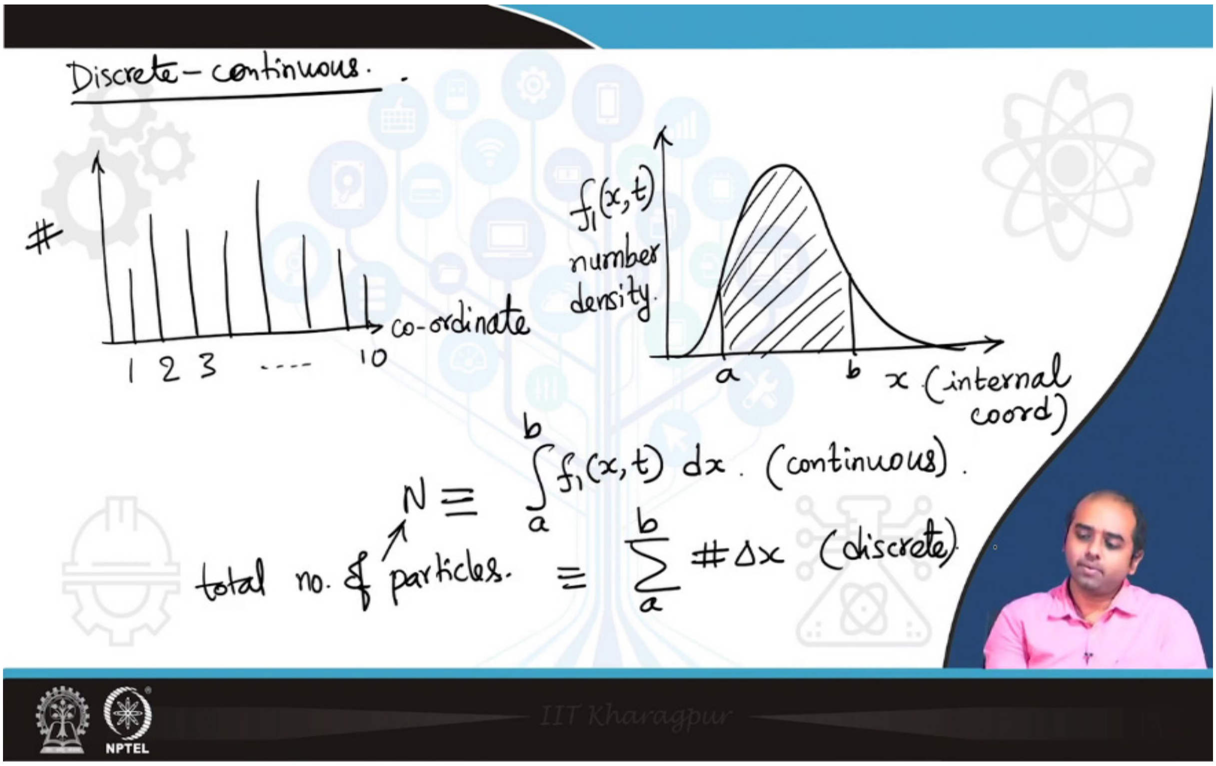

Discrete - continuous.

$$N = \int_a^b f_1(x,t)\, dx \quad \text{(continuous)}.$$

total no. of particles $= \sum_a^b \# \Delta x$ (discrete)

Now, this since everything in the dispersed phase world is about counting and calculating the number of the particles, so things are very discrete here. So, if we try to write down the number density or the number, it is always a sort of this discrete histograms. I think all of you know about these histograms in the statistics, so this this plot is about the number with respect to a coordinate. It could be an internal coordinate, it could be external coordinate, whatever let us say these coordinates are size and I denote that size as 1, 2, 3, 4, like that to 10.

So, these histograms mean number of particles having size 1, number of particles having size 2, this is the representation. And so, this is like the discrete, so say the same thing can also be represented in the sort of the continuous form that I can say a function which is nothing but the number density function, this is the number density function. Generally, it is a function of one coordinate and time, and this coordinate could be the size, so x here is an internal coordinate, let us refer to as the internal coordinate.

This is normally the case and we can draw a curve like this, so it suggests that in between from 0 to Infinity of different sizes, there is a particular Peak value or a particular size, where the number density is more of the number of the counting of the, these particle are maximum.

So, similarly I can also write a number density function with respect to the coordinates and even not having, so discrete sizes there is a continuous size range, so I can also plot a continuous curve I can also make discrete if there are only certain distinct sizes, then it is always preferable to draw this discrete type of histogram, but if there is a very small difference between the sizes and there is a huge range of size, then it is preferred to draw this sort of continuous number density function.

So, the total number of particles, the total number of particles, let us say this number of particles N we are talking about, so the total number of particles or entities. Across any domain or across any size range a to b is the integration of this number density function, so let us say a is here and b is here, so in between this range, if I do the area under the curve, I will get what is the total number of molecules that is present in between the size range, similarly if I want to calculate, so this is for the case of when you have a continuous distribution of the internal coordinate.

And when you have discrete coordinate system you can have a summation, summation is a more preferable technique, so it is like this number density there, multiplied with delta x from a to b discrete, so this is the discrete domain. So, this f1, f1 is essentially the number of particles per unit volume, that is what we represent by the number density. Similarly, this number density for the discrete that is written as hash, is also means the same. It is the number of particles present in unit volume or in a big volume whatever in your system, whatever you have, but it is essentially the number of particles in unit volume, that is what this number density function talks about.

Now, depending on whether there is a continuous distribution of your internal coordinates, for example size or you are having only certain discrete values that are possible accordingly you draw a discrete curve or you have a continuous curve, you can draw histogram if it is discrete if you have a continuous function, it is essentially a smooth curve.

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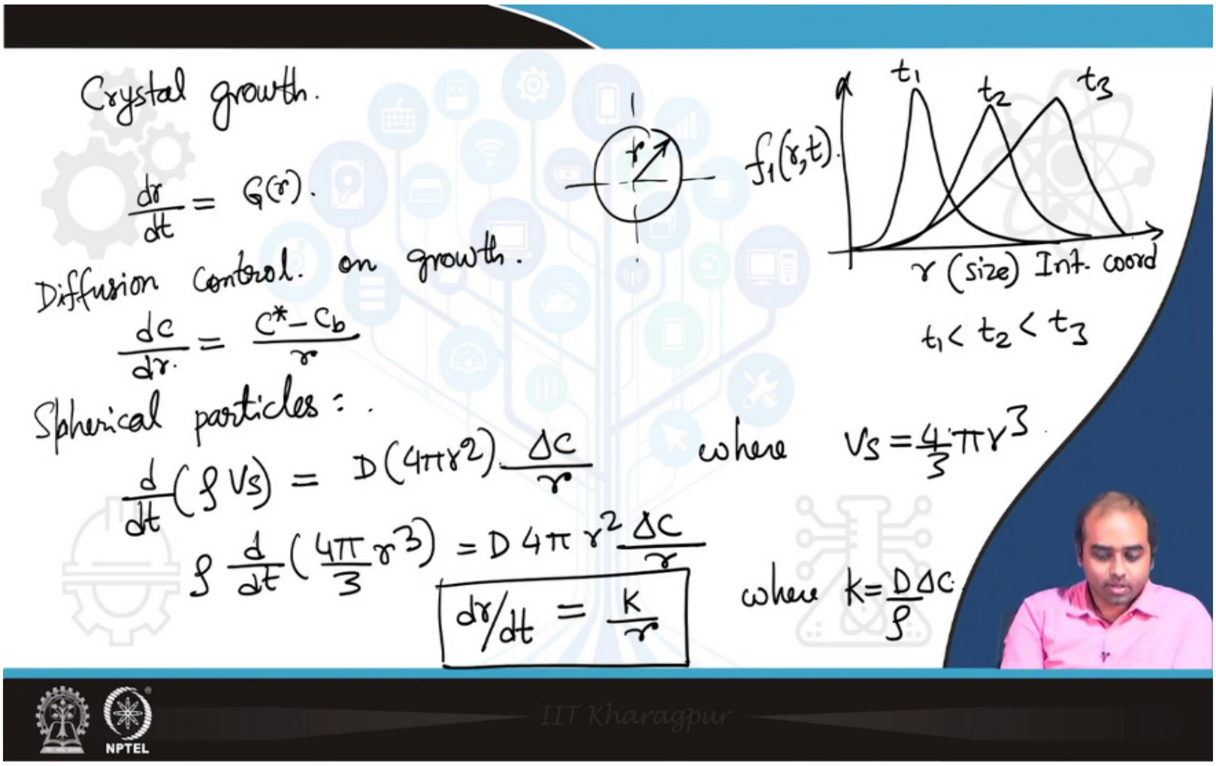

Crystal growth.

$$\frac{dr}{dt} = G(r).$$

Diffusion Control. on growth.

$$\frac{dc}{dr} = \frac{C^{*} - C_b}{r}$$

Spherical particles:

$$\frac{d}{dt}(\rho V_s) = D(4\pi r^2)\frac{\Delta C}{r} \quad \text{where} \quad V_s = \frac{4}{3}\pi r^3$$

$$\rho \frac{d}{dt}\left(\frac{4\pi}{3} r^3\right) = D\,4\pi r^2 \frac{\Delta C}{r}$$

$$\boxed{dr/dt = \frac{K}{r}} \quad \text{where} \quad K = \frac{D\Delta C}{\rho}$$

Let us talk about a crystal growth process in this context. So, typically in the crystal growth, this is the kind of number density function that we see with time. So, in crystals growth there is never a, so here it is r, which is the size, right, so it is the internal coordinate. So, in crystal growth essentially you do not get only particular size, you always get a size range. You do not get only one particular size of the crystals at any point of time, there will be a series of or there is will be a distribution of different size particles, and these distributions will continue to grow.

I mean it the peaks can be wider or peaks can be sharper, whatever but this will continue to grow, I mean the particles will continue to grow with time, so essentially t1 like this, right. So, with time, these peaks will be shifting, but always there will be a distribution. Generally, what we see is that always there is a distribution of the particles, okay. So, now in a crystal growth let us, so this r is nothing, but the thus, size of the crystals assuming they are spherical, the radius of the crystals, so the crystal growth rate, dr dt can be written down as G which is also could be a function of r or the size.

So, if there is a diffusion control on the growth, we generally write dc dr is equal to C star minus C b by r. So, C star is the saturation concentration, and C b is the concentration of the, so C b is the bulk concentration and C star is the saturation concentration. So, that is how we generally write if diffusion controls the growth parameter.

So, for spherical particles, we can write something like this, change of mass is equal to the diffusion multiplied with the surface area of the particles, delta C by r this is something we can write for spherical particles. If it is a diffusion-controlled process, where Vs is equal to 4 by 3, the volume of the sphere pi r cube, now if you consider the density to be constant, you get d dt of 4 by 3. So, what we see that dr by dt turns out to be something K by r right from here, so where K is equal to D by rho grad C, isn't it? So, if I try to relate the crystal growth process with respect to this dr.

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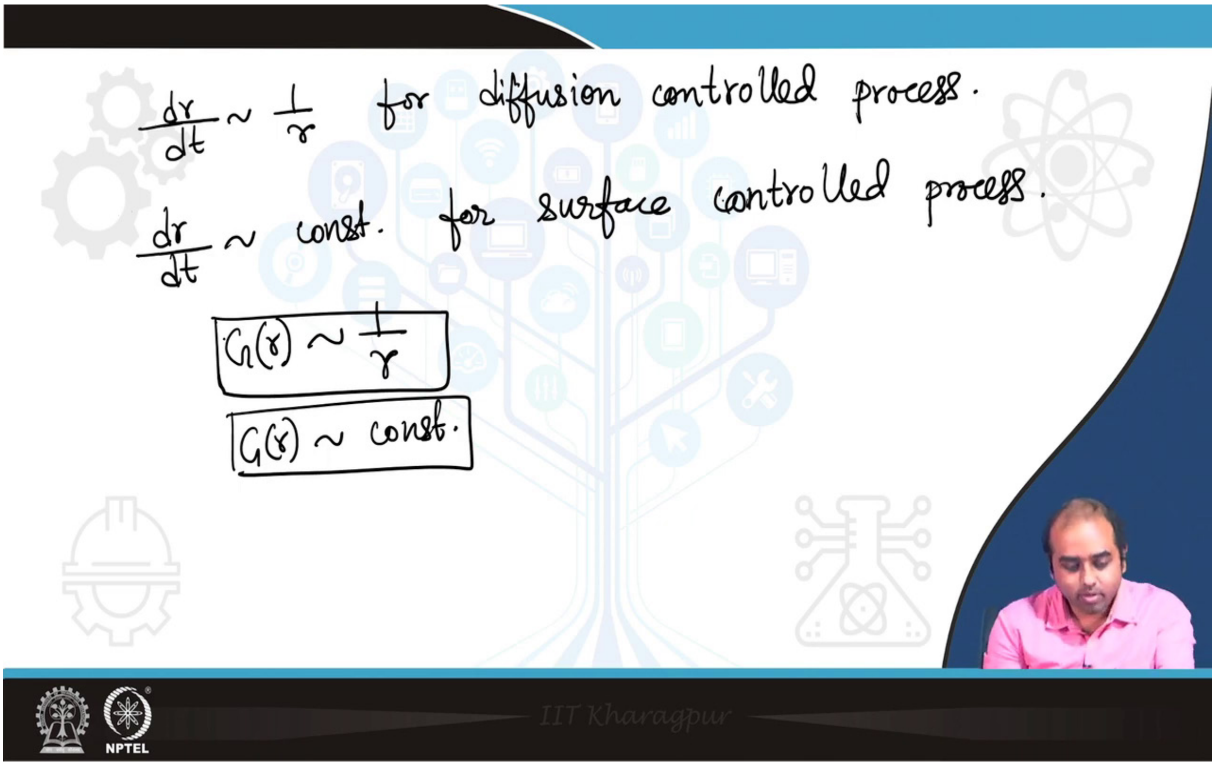

$\frac{dr}{dt} \sim \frac{1}{r}$ for diffusion controlled process.

$\frac{dr}{dt} \sim$ const. for surface controlled process.

$\boxed{G(r) \sim \frac{1}{r}}$

$\boxed{G(r) \sim \text{const.}}$

So, for what is something we see that dr, dr by dt is 1 by r for diffusion-controlled process. And for surface-controlled process, dr dt is generally constant for surface control process. So, you can realize that the growth rate for diffusion control process is 1 by r, and for surface-controlled process this growth rate is essentially constant. So, depending on looking into the evolution of the particle size distribution with respect to time, you can essentially confer or you can understand that, whether the growth rate is diffusion controlled or whether it is surface controlled.

So, this is how looking into the particle size distribution data you with respect to time, you can say whether what sort of growth-controlled mechanism it is exhibiting. So, next we are going to talk about the framework of the population balance equation.

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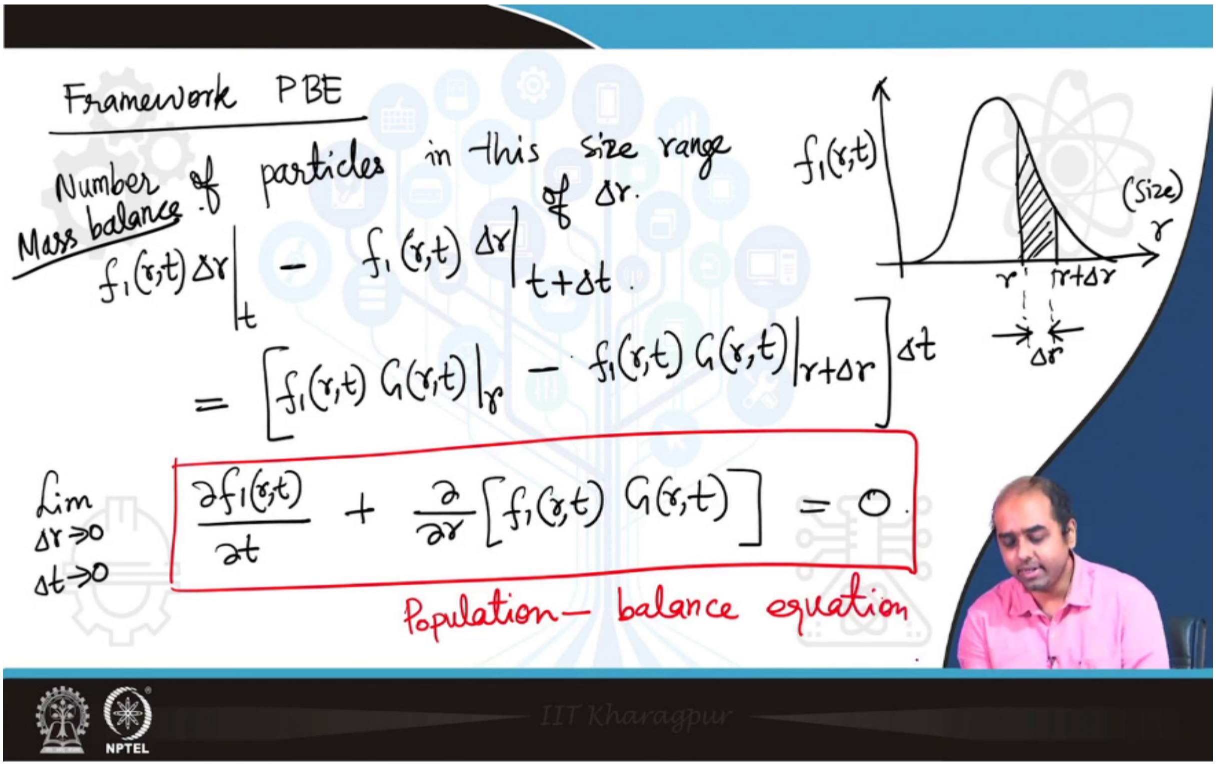
Framework PBE

Number of particles in this size range of Δr.

Mass balance

$$f_1(r,t)\Delta r\Big|_t - f_1(r,t)\Delta r\Big|_{t+\Delta t}$$

$$= \left[f_1(r,t)\,G(r,t)\Big|_r - f_1(r,t)\,G(r,t)\Big|_{r+\Delta r}\right]\Delta t$$

$$\lim_{\substack{\Delta r \to 0\\ \Delta t \to 0}} \boxed{\frac{\partial f_1(r,t)}{\partial t} + \frac{\partial}{\partial r}\left[f_1(r,t)\,G(r,t)\right] = 0}$$

Population-balance equation

So, framework of the population balance, so population balance equation is essentially a mass conservation but in the dispersed phase case. So, this is a very famous equation in this first phase modelling, almost the heart of the dispersed phase systems, so let us say I have this f1, r comma t, and here I am having this in a function of r.

So, let us say I take a region r and r plus delta r, so normally this small size fraction is delta r, so please note that this r is not the radial coordinate right, so r is the size or the internal coordinates. So, I take a small fraction of delta r or it is a small size fraction in this particle distribution. So, the number of particles in this size range of delta r is f1, in r comma t, delta at, sorry, this is the number of particle size that is present in this size range at r.

And now, if I am trying to make a balance with respect to time, so what I am trying to say is that number of particles growing in time is equivalent to the change in the particle size distribution across this time, across this size segment of delta r. So, let us say this is the part I mean particle that I am having at t, and let us say this is the particle distribution that I am having at t, sorry, multiplied with number of particles, I am having at t plus delta t.

This is the change of the number of particles with time of a time interval of delta t, is equal to the particle growth rate, that is why I say this growth rate is very important, at r minus the particle that is growing at r plus delta across, I mean this change across this time delta t, this is the balance. So, the number of particles in the size range of delta is f into delta r, right. So, now we are making a balance, this is essentially a mass balance, where we are saying that whatever is present at time t, and whatever is present at time t plus delta t, this difference can be attributed to the difference of the total particle growth rate, so the number of particle size distribution multiplied with the growth rate, if you multiply the specific growth rate essentially, so this means the number of particle which is growing at r, and the number of particles which is growing in r plus delta are in the time segment of delta t.

So, now if you do the limit delta t tends to be 0 and limit, so if you take these limits delta r tending to 0, and delta t tending to 0, you can write down the appropriate differential. So, I will be getting d, f1, r comma t, dt plus d del r of equal to 0, isn't it? So, this is true for any size coordinate, I mean the easiest since I have taken this internal coordinate as the size, because this is the easiest to understand.

But this is true for any size coordinate, I mean any coordinate, whether it is internal or whether it is external. So, this is the population balance equation, of course here there is no breakage or no additional sourcing functions or aggregation. And we have written down with only one coordinate, so if there are more number of coordinates, I mean internal external this derivative would actually extend to those.

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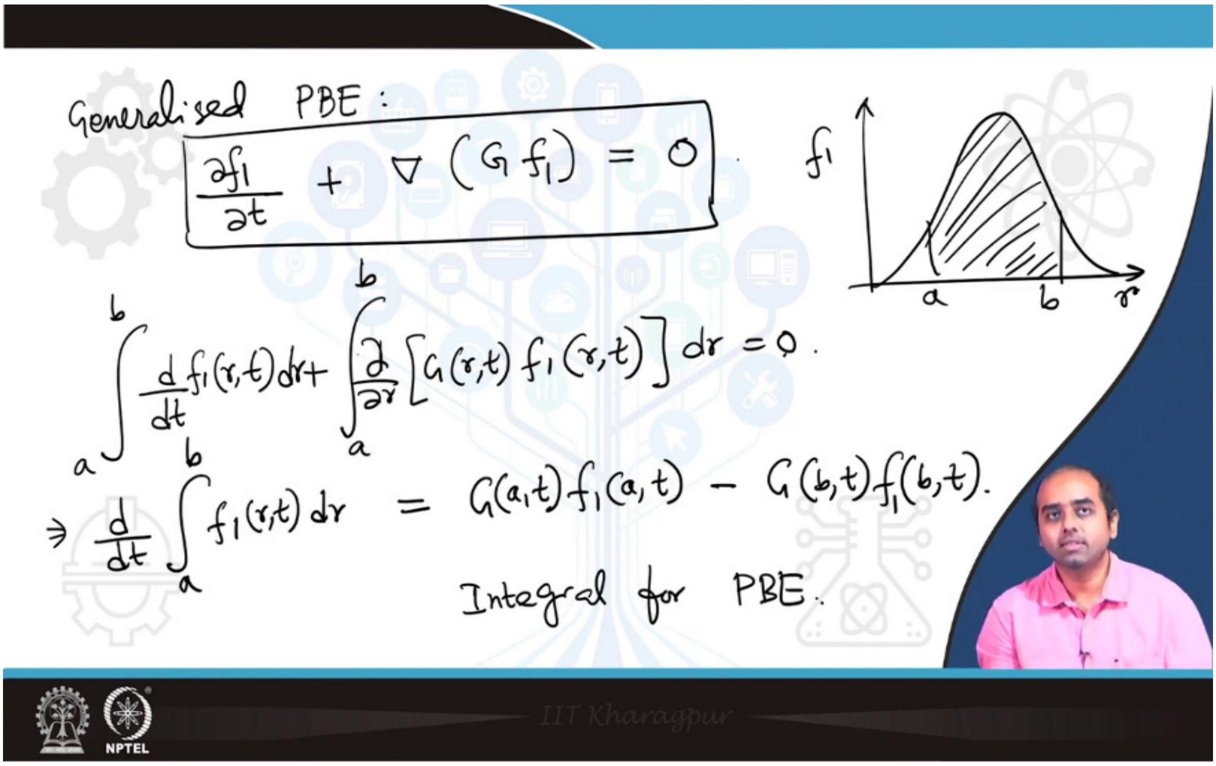

Generalised PBE :

$$\boxed{\frac{\partial f_1}{\partial t} + \nabla (G f_1) = 0}.$$

$$\int_a^b \frac{d}{dt} f_1(r,t)\,dr + \int_a^b \frac{\partial}{\partial r}\left[G(r,t)\, f_1(r,t)\right] dr = 0.$$

$$\Rightarrow \frac{d}{dt}\int_a^b f_1(r,t)\,dr = G(a,t)f_1(a,t) - G(b,t)f_1(b,t).$$

Integral for PBE.

So, the generalized PBE equation would look something like this, the generalized PBE equation would look like f1. So, it could be any coordinates and you take the grad of those many number of coordinates or the grad operator of those functions, of course this G and f are all scalar functions with respect to time, so you take the grade of those functions depending on how many number of the coordinates we are having.

So, across this equation, also holds good, if you want to estimate across any two discrete points. So, let us say these two discrete points is a and b, so across these two discrete points, if I try to find out this, I will apply this PBE equation, so the PBE equation del del t of f1 r comma t is equal to this is the PBE equation we are having del del r of sorry plus, this is the PBE equation.

And I can essentially integrate it out on both sides. So, if I do that first one is the integration with respect to r I am talking about over the limits of a to b, so this is something I can do. So, left hand side I can take out the limit, del del t of this f1 r d with respect to dr, a, b and right-hand side I can apply the Leibniz rule, so I will get z a comma t f1 a comma t, this can work.

So, individually their growth rates are the total, this number of particles multiplied with the growth rate, specific growth rate and the difference can also be contributed by this integral, so this is also another integral form of the PBE you can talk about, integral form of the population balance equation, and we already wrote the generalized differential form of the population balance equation, okay.

So, we will close the class here today for this lecture and in the next lecture we will see a first a simple example of a seeded crystallizer particle crystallizer. And then we will move ahead with the aggregation and the breakage functions. Thank you for your attention, I hope you like this class today.