Mathematical Modelling and Simulation of Chemical Engineering Process
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Lecture 51
Dispersed phase modelling - aggregation

Hello everyone, in this class we are going to talk about and discuss about the aggregation process. So, there are several you know examples of where you find a aggregation prevalent in dispersed phase system for example, formation of the clouds, aggregation of particulate metal it has the nanoparticles then aggregation of you know, cells in the biological process sintering of catalyst or porous material surfaces, aerosols formation of aerosols, there are several such engineering processes where aggregation is an important dispersed phase, I mean aggregation involves dispersed knowledge of the dispersed phase.

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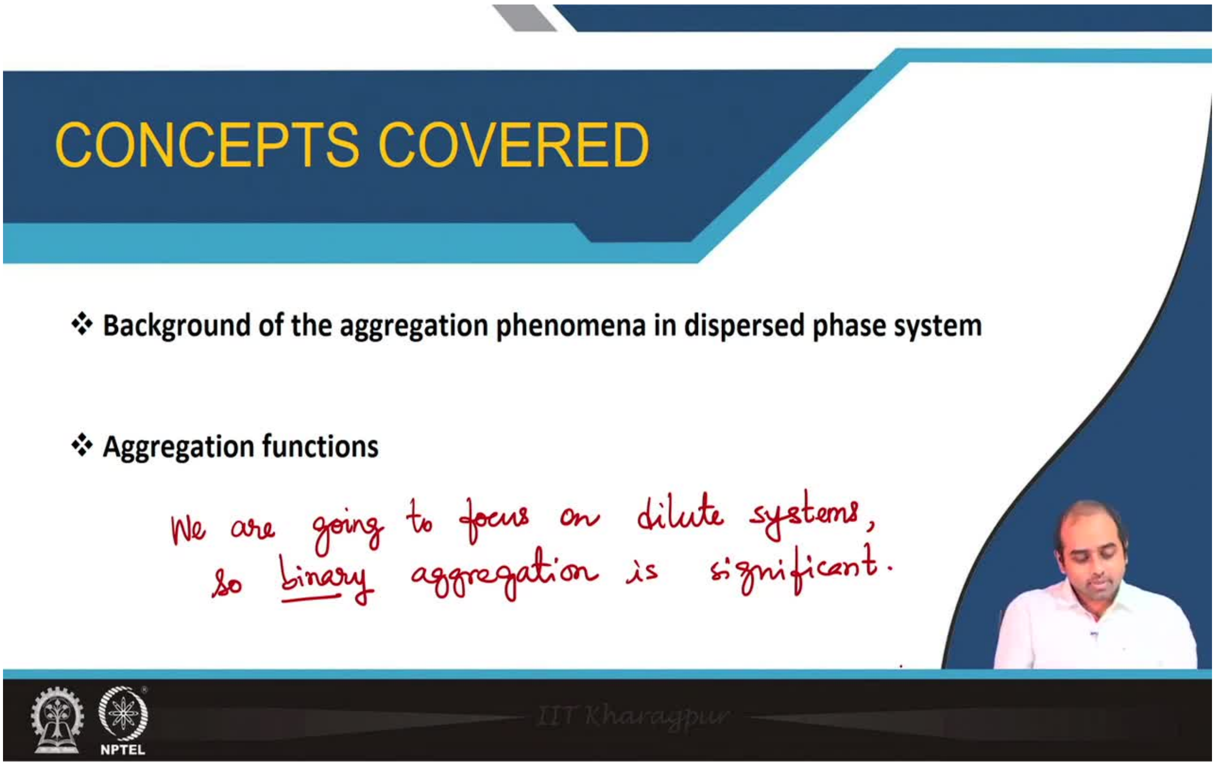

CONCEPTS COVERED

- Background of the aggregation phenomena in dispersed phase system
- Aggregation functions

We are going to focus on dilute systems, so binary aggregation is significant.

So, in this case we are going to talk about the aggregation and try to know more about its background what are the, I mean in this class particularly, we are going to talk about the aggregation and the different types of aggregation functions and how do we write the source and the sink term of the population balance equation for aggregation, I mean for aggregating systems let us put it this way.

So, we I must say here that aggregation is actually a very complex if you think more deeply, so, in this case that we have this new course, we are only going to focus on dilute systems aggregation of, must write it here. So, we are going to focus on dilutes systems and aggregation in dilute systems. So, in this case binary aggregation or aggregation of a pair of particles or molecule is the most significant point.

So, if you have, if you do not have you know dilute systems if you have concentrated systems that it may happen that more than 2 or you know 3, 4 multiple particles actually try to aggregate and form a big lump right, but in the case of dilute system generally aggregation of 2 particles is the most dominating one there is because there is no inter particle attraction. So, whatever aggregation happens is because of a pair of particles only or a binary aggregation that happens and this what we will be restricting ourselves into this class.

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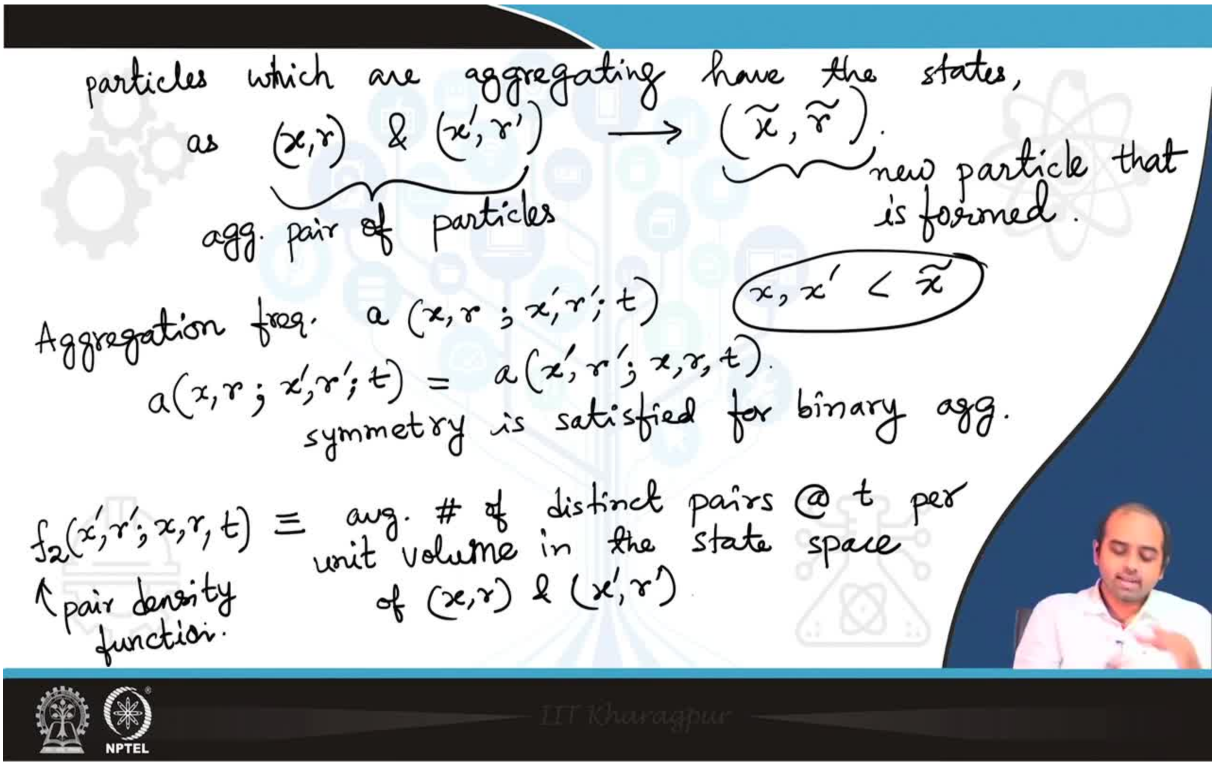

particles which are aggregating have the states,

$$\text{as } \underbrace{(x,r)\ \&\ (x',r')}_{\text{agg. pair of particles}} \longrightarrow \underbrace{(\tilde{x},\tilde{r})}_{\text{new particle that is formed}}.$$

$$\boxed{x, x' < \tilde{x}}$$

Aggregation freq. $a(x,r\,;x',r';t)$

$$a(x,r\,;x',r';t) = a(x',r';x,r,t).$$

symmetry is satisfied for binary agg.

$f_2(x',r';x,r,t) \equiv$ avg. # of distinct pairs @ t per unit volume in the state space of (x,r) & (x',r')

↑ pair density function.

Now, the factors are the functions that is there that plays a major role in this aggregation is first is the aggregation frequency, but before we talk about the aggregation functions or the factor is very important to note down that we are talking about a pair of states. So, for particle let me put it this way, particles which are aggregating have the states as so, I am writing one internal and one external coordinate.

So, this is the pair of particles which are aggregating right and the new particle or the aggregated particle have state like this. So, this is the most generating most generic framework or the how we describe the coordinates of the aggregation or aggregating particles and the aggregated particle. So, this is like the new particle that is formed. So, these are the pair of the particles which are aggregating as I said we are only considering you know a binary aggregation, only a pair of particles that can aggregate and not more than 2 particles which were aligned aggregate and this is true for dilute system.

So, now, let us define the aggregation frequency. So, in the above example x comma r x represent the internal coordinate and r presents that external coordinate or the spatial dimensions essentially so, aggregation frequency is given by a, let us write there as a x r x prime comma r prime t this is aggregation frequency is actually valid for the case of this pair of particles only.

So, also I must say here that this x and x prime is less than x bar this has to satisfy. So, the particles that we are considering as aggregating cannot be larger than the aggregated particle size right same as the case of the breakage the particles that is formed after the breakage cannot be larger than the main particles, here also the particle or the aggregated particle or the larger particle that is formed.

So, from the you know this what should I say the starting pair of particles their size cannot be larger than the final aggregated particle size. So, this is also another condition that I should say and then also there are something that we see here in terms of the aggregation frequency since this is binary aggregation, so, aggregation of I mean this is a symmetric function always for binary aggregation.

So, this is equal to this so, aggregations are always this symmetry exist for the frequency of in the case of symmetries satisfied for binary aggregation and this (aggregation) as I have already said the aggregating pairs you know this x and x prime are the locations are x comma r and x prime comma r and the number density function of the new particle that is formed is generally marked as f 2 so instead of f 1 here we try to denote this number density function of the aggregated particle that is formed as x 2. So, x 2 depends on the pair of coordinates of the pair of the particle that is formed from the states x and x prime.

So, this is the average number of particles. So, distinct pair, distinct pairs at time t per unit so, this is like the aggregating pair, that is what we denote the number density function as f 2 instead of f 1 per unit volume in the state space of x r. So, this is something like the pair density function you can talk about right instead of the number density function this is more relevant in this case f 2 represents the pair density function.

So, the aggregation frequency a denotes the probability or the you know these particles are probability per unit time of the pair of particles which is aggregating and this is dependent on the particle coordinates both internal and external next we also mark this pair density function f 2 as the average number of distinct pairs at time t, which essentially can you know aggregate together that is how we define these f 2. So, this is these are the two important definitions here.

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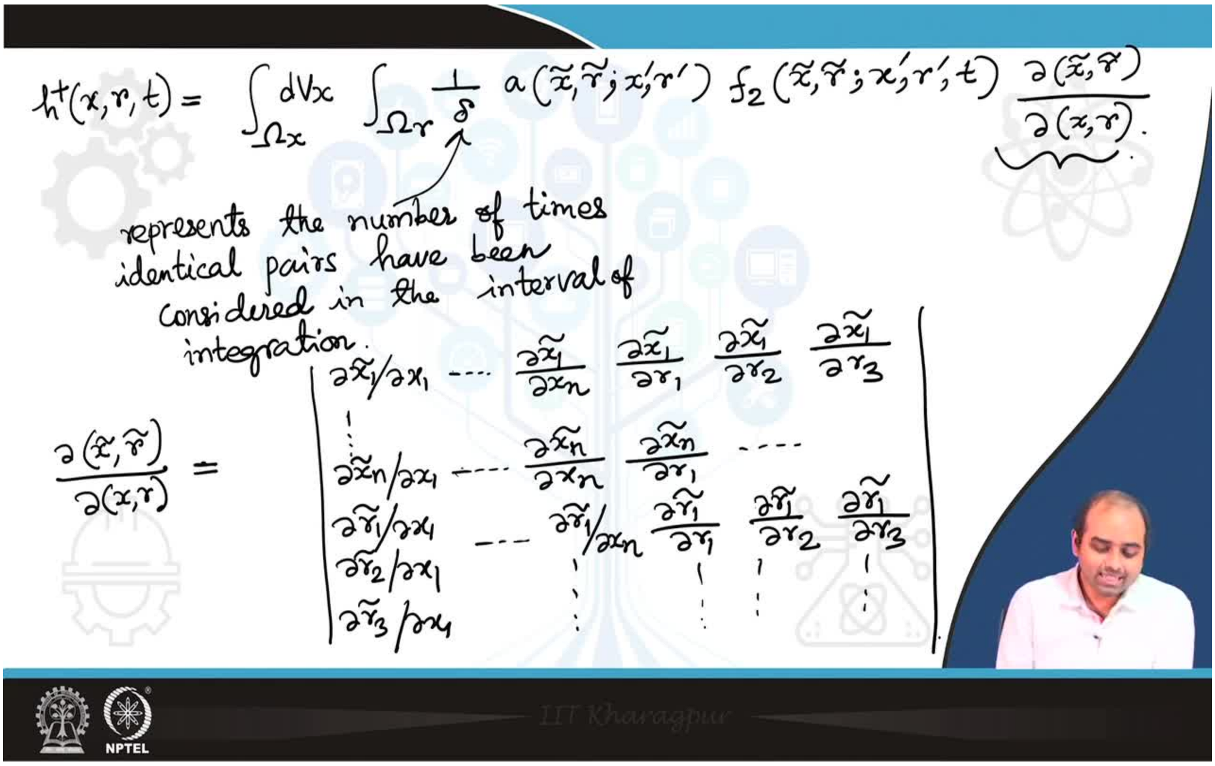

$$h^+(x,r,t) = \int_{\Omega_x} dV_x \int_{\Omega_r} \frac{1}{\delta}\, a(\tilde{x},\tilde{r};x',r')\, f_2(\tilde{x},\tilde{r};x',r',t)\, \underbrace{\frac{\partial(\tilde{x},\tilde{r})}{\partial(x,r)}}.$$

represents the number of times identical pairs have been considered in the interval of integration.

$$\frac{\partial(\tilde{x},\tilde{r})}{\partial(x,r)} = \begin{vmatrix} \partial\tilde{x}_1/\partial x_1 & \cdots & \frac{\partial\tilde{x}_1}{\partial x_n} & \frac{\partial\tilde{x}_1}{\partial r_1} & \frac{\partial\tilde{x}_1}{\partial r_2} & \frac{\partial\tilde{x}_1}{\partial r_3} \\ \vdots & & & & & \\ \partial\tilde{x}_n/\partial x_1 & \cdots & \frac{\partial\tilde{x}_n}{\partial x_n} & \frac{\partial\tilde{x}_n}{\partial r_1} & \cdots & \\ \partial\tilde{r}_1/\partial x_1 & \cdots & \partial\tilde{r}_1/\partial x_n & \frac{\partial\tilde{r}_1}{\partial r_1} & \frac{\partial\tilde{r}_1}{\partial r_2} & \frac{\partial\tilde{r}_1}{\partial r_3} \\ \partial\tilde{r}_2/\partial x_1 & & \vdots & \vdots & \vdots & \vdots \\ \partial\tilde{r}_3/\partial x_1 & & \vdots & \vdots & \vdots & \vdots \end{vmatrix}.$$

Now, let us try to write the h plus and the h minus terms. So, first let us write the h plus term the new particle that is generated by aggregation. So, this is actually across the coordinate spaces first we have a x this is the aggregating pair or the number density function, this is the Jacobian. So, here this delta is sort of the redundancy factor. So, delta represents, this represents the number of times so, this is like the redundancy factor 1 by delta accounts for the redundancy, the number of times identical pairs have been counted, identical pairs have been considered in the integration or in the interval of the integration.

So, this is sort of accounting for the redundancy factor and this a represents the aggregation frequency of the particles that are aggregating and that is multiplied with f 2 the pair density function the important is this Jacobian. So, this Jacobian represents the determinant and this this represents essentially the determinant of the Jacobian.

So, let us write it down and how does this term looks like so, this is the determinant with all the possible x coordinates and with also the r coordinates so there are only 3 r coordinates in this system are x y z coordinates and there could be several internal coordinates like this is goes on up to del x sorry x n delta x 1 delta r 1 then you have del r 1 with respect to delta x 1 and delta r 2 with respect to delta x and delta r 3 with respect to delta x 1 and then delta so, this is the Jacobian determinant of this Jacobian is contributed here in this integration as the relative (de) you know differential of this new aggregating frequency with new aggregated state with respect to the original state of x comma r.

So, essentially the source contribution to this aggregation frequency or this aggregation this aggregation population balance equation of this aggregation process the source contribution is the aggregation frequency multiplied with the number density or the pair density function and then you divided with I mean it is it is multiplied with the redundancy factor because you do not calculate two pairs more.

So, if you are counting x and x prime you do not count in x prime and x has a different quantity that is why this redundancy is there and then finally, it is the factor that the Jacobian and that is the relative you know, this delta with of the new state with respect to the original state that is how we are making this aggregation term and the source contribution to this aggregation.

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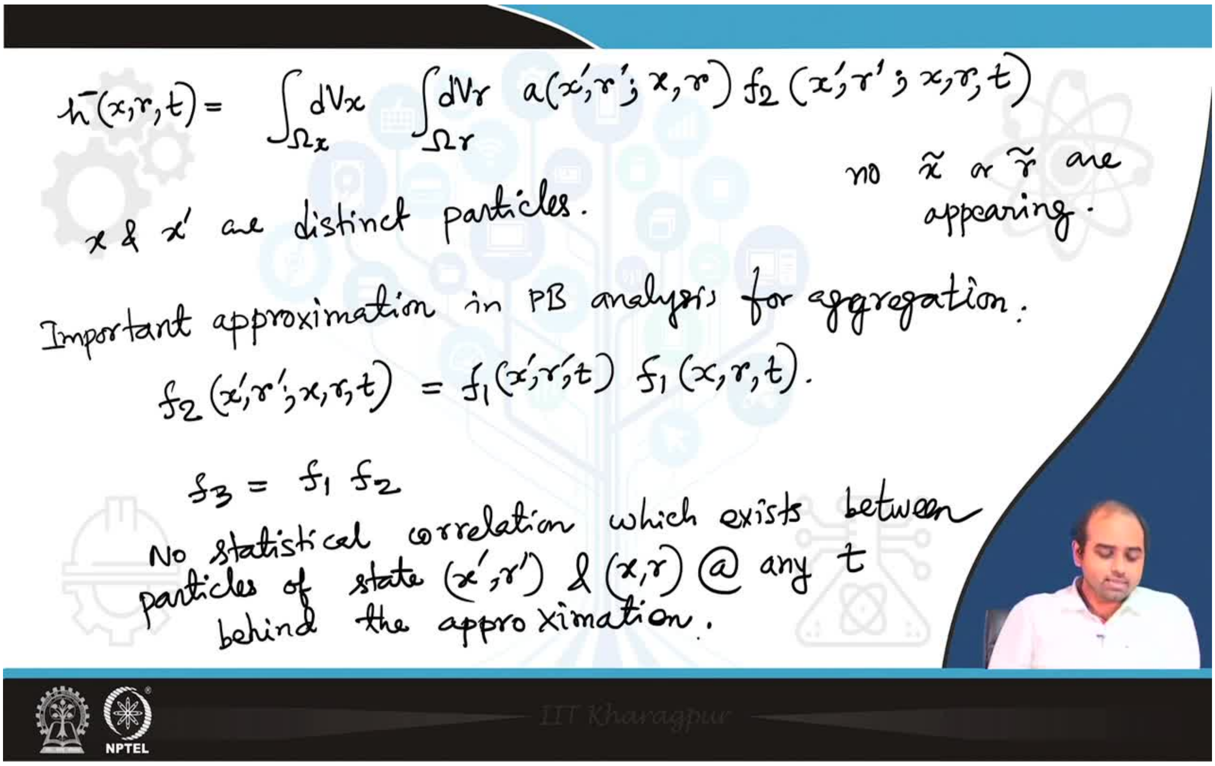

$$h^-(x,r,t) = \int_{\Omega_x} dV_x \int_{\Omega_r} dV_r \; a(x',r';x,r)\, f_2(x',r';x,r,t)$$

no $\tilde{x}$ or $\tilde{r}$ are appearing.

x & x' are distinct particles.

Important approximation in PB analysis for aggregation:

$$f_2(x',r';x,r,t) = f_1(x',r',t)\, f_1(x,r,t).$$

$$f_3 = f_1 f_2$$

No statistical correlation which exists between particles of state (x',r') & (x,r) @ any t behind the approximation.

Now, about what about the sink, so, the sink is term part. So, in the case of the sink or writing down the sink function essentially we see that h minus, this h minus which is the sink contribution for x r and t, this is again integration of all the coordinate spaces we are having a comma x comma r. So, in this case the there is no multiplication of these Jacobian factor, because we do not, I mean we do not need to account for the formation of the new states. So, these you know this sink term whatever we are considering in this case is actually the part that is removed from the system and what is removed states which correspond to x and which correspond to x prime.

So, that is why we multiply with the aggregating frequency with respect to I mean, along with the pair density function, but we do not consider any effect of the new state formation. So, in this equation, know where you see that the terms x that you know, these terms related to x tilde, or x bar or these r bar are appearing. So, no x bar or r bar are appearing in this equation.

So, structurally the equation is same, we are trying to multiply the you know this aggregating frequency multiplied with the pair density function and that multiplication and then integrating over the entire you know this state space gives us the particles or the number of particles or whatever is removed from the system.

But in the case of the aggregation I mean whatever is removed, I mean we have to multiply I mean we have to work the new particles that is formed based on the knowledge of the existing particle which is actually removed. So, that is why we try to write I mean that time when we are writing the particles of h plus term the contribution of the source we take into account of the x bar and the y bar the new particles that are forming.

So, aggregating frequency of the new particles with respect to the old state, that is what something we are trying to write, but in this case, whatever particle that is getting removed, everything is in old state. So, that is why there is the x bar and y r bar does not come in this picture in the sink term.

So, also please note that this redundancy factor also does not appear here. So, whatever particles is removed from the system are x prime and x. So, there is no point of connecting the I mean counting them twice. So, x and x prime both are different and distinct phases, when we are trying to consider So, x and x prime are distinct particles. So, whenever we are trying to calculate the sink term, we are trying to see that when does this x and x prime are removed?

So, there is no question of counting them twice but when we are we trying to estimate the source term from this x and x prime we cannot count it twice. So, if we are counting the aggregating the pair density function with respect to x of the new particle, then you cannot should not count the x prime because x and x prime together from the new particle. So, the new particle whatever we are trying to count or trying to add is based on the old state of x and x prime so, I cannot count it double aggregating particle, aggregated particle is not double and they are not two distinct particles. They are not having states x and x prime both it is only x bar.

That is where the redundancy factor came into play there. One of the important approximation that is often used in these aggregation process or let us say in this population balance analysis for aggregation in population balance analysis for aggregation that is considered is something like this f 2 is equal to f 1 of the individual density functions of state x and x prime.

So, this is like an approximation that we always use in terms of in terms of writing the pair density function of the aggregated particle and this gives some sort of closure to the problem because we do not define our population balance equation with respect to f 2. So, there has to be some correlation of f 2 with respect to f 1 that is like imperative for this problem, and this is the approximation we consider for any instant of time.

And of course, please note that there is no statistical correlation behind this aggregation, sorry behind this approximation. So, this is a sort of hierarchy of approximation that you can consider. So, essentially if I am considering f n or let us say if I am trying to consider f 3, I can consider f 2 be like aggregation of f 1, then f 2, f 1 with f 2 something like that. So, this is sort of a recursive you know the f 3 cannot call a pair density it is like a triplet density function.

So, like this this approximation is generally held, but please note that there is no statistical, no statistical correlation which exist between particles of state x prime r prime and x comma r at any time behind this approximation. So, unless this approximation exist the population balance equation is not closed because as I said that this new pair density function is unknown.

So, without the knowledge of f 2 or without the knowledge of f 3 or whatever any further aggregating function, there would be an infinite hierarchy of functions which would be unknown. So, unless there is a closure approximation on how these functions or the pair or the triplet density functions as related you cannot solve or you cannot make this population balance equations unique. It would be like bit undefined and we do not have closure to the problem.

Now, the question is whether this approximation is reasonable or not is something beyond the scope of this course. So, for that you can go deep into details on the population balance model and its assumption but that is something we will not discuss here and this we will take as it is for now, but with slowly you will realize that this is a very reasonable approximation particularly for large populations.

So, we will stop here for this lecture. In the next class, we are going to talk about the aerosol dynamics as a real world aggregation problem and we will see that how the dispersion of solids or, liquid particles in the continuous gas phase can essentially be modelled and what sort of coalescence behavior we do experience there. I hope all of you found this lecture quite interesting, and we will come with more in the upcoming classes on aggregation. Thank you for your attention.