Spray Theory and Applications
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Lecture - 34
Multiphase Modeling

Good morning. We will continue our discussion of sprays as multiphase flows.

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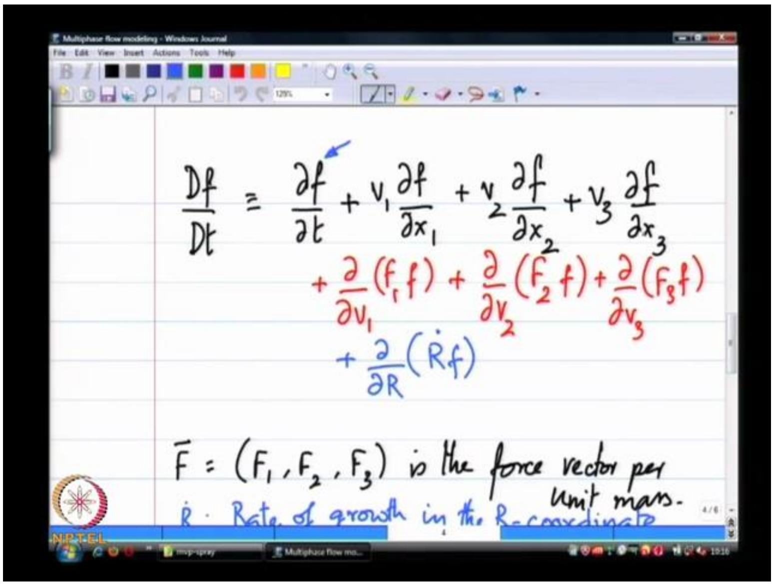

$$\frac{Df}{Dt} = \frac{\partial f}{\partial t} + v_1\frac{\partial f}{\partial x_1} + v_2\frac{\partial f}{\partial x_2} + v_3\frac{\partial f}{\partial x_3} + \frac{\partial}{\partial v_1}(F_1 f) + \frac{\partial}{\partial v_2}(F_2 f) + \frac{\partial}{\partial v_3}(F_3 f) + \frac{\partial}{\partial R}(\dot{R} f)$$

$\bar{F} = (F_1, F_2, F_3)$ is the force vector per unit mass.

$\dot{R}$ · Rate of growth in the R-coordinate

Towards the end of the last class, we had derived a commoving derivative in a slightly general formulation involving not just advection through a special coordinates x 1, x 2, x 3, but also through velocity coordinate V 1, V 2, V 3. As we said F 1, F 2, F 3 would have to be the force vector per unit mass for this advection through the velocity coordinates. The simplest of such force vector that you think of let us say is gravitational force. So, I have a an ensemble particles, that are setting with no interaction and let us say the I just remaining at rest and F 1 and F 3 are 0 and F 3 are some minus g.

So, that would cause particles that were at rest at some time t equal to 0 to begin to accelerate and acquire of velocity and if I was to study this in the context of the probability density function of these particles, it would be were the initial velocity V 0, which in this particular example is 0 would have becomes V 1, at some later point in time following the rule that V 1 is V 0 plus a dt, a in the case minus g. So, the advection through the velocity coordinate happens due to an external force, not due to forces that may originate due to interaction between these particles.

So, let us been clear about what F 1 F 2 F 3 are I will mark this in red, is this is the external force per unit mass or acting on the ensemble of particles on this population of particles. If I look at what happens due to the interaction between the particles.

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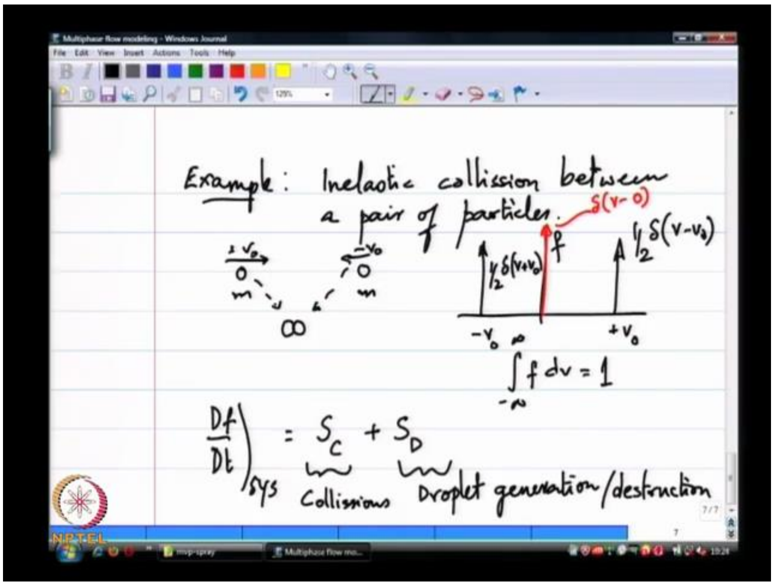

Example: Inelaotic collission between a pair of particles.

$$\int_{-\infty}^{\infty} f \, dv = 1$$

$$\left.\frac{Df}{Dt}\right)_{sys} = \underbrace{S_C}_{\text{Collissions}} + \underbrace{S_D}_{\text{Droplet generation/destruction}}$$

So, we started look at in other example between a pair of particles. So, let us say take particle at of some mass m and another particle of mass m and my system, now is this 2 particle system. And if I allow this 2 particle to come collide in elastically, the momentum is destroyed due to these forces that may originate at the point of collision and all the kinetic energy in these 2 particles is converted to heat, that is our classical mechanics understanding of this kind of collision.

Now when I look at this in the probability density space, I have one direct delta function at plus v this is actually half direct delta function, because the sum total f dv going minus infinity to infinity; if I am only looking at 1 velocity coordinate, then f dv would have equal 1. So, this would be half direct delta function at v, I will call this v 0 just distinguished from the coordinate v and this would be half v minus minus v 0. If I was defined f 2 summation of these two that would ensure that the probability density function have integrate out over its appropriate limit to 1.

So, when this collision happens, this probability density function which I have indicated in black becomes 1 probability density function given by delta v minus 0. The sum total area under the distribution of course remains the same, but it has adverted from this 2 peak probability density function towards this 1 peak at 0. What is the cause of this advection? For go back to the formulation I had for the total derivative, none of these terms can be responsible for this because it was entirely an internal force. So, essentially this total derivative of f, is has an effect due to coalitions and any other systemic effects.

So, if I rewrite this system equivalent of this, it has to equal some contributions due to collisions, plus any contributions due to changes at the system level. That is if I had ensemble of droplets that were let us you know of total mass m, if I was to draw a system boundary, by definition system boundary is where you do not allow mass transfer across it. What sort of effects can cause the system mass to go up, if I do not allow mass transfer across a system boundary? One such effect if I have nucleation of droplets inside due to condensation process. So, I had some vapor inside and the vapor condense to give me droplets.

So, now as far as the droplet face is concerned, there is an increase in the mass due to this nucleation and condensation process. So, I could have some droplet generation, can I say generation, but it could also mean destruction due to evaporation. So, these are all the effects that can happen at the system level, these are all the reasons by which the probability density function of these droplets in the size velocity space, can move can change. So, if I combine the system level equation with version we had before from the advection form we find.

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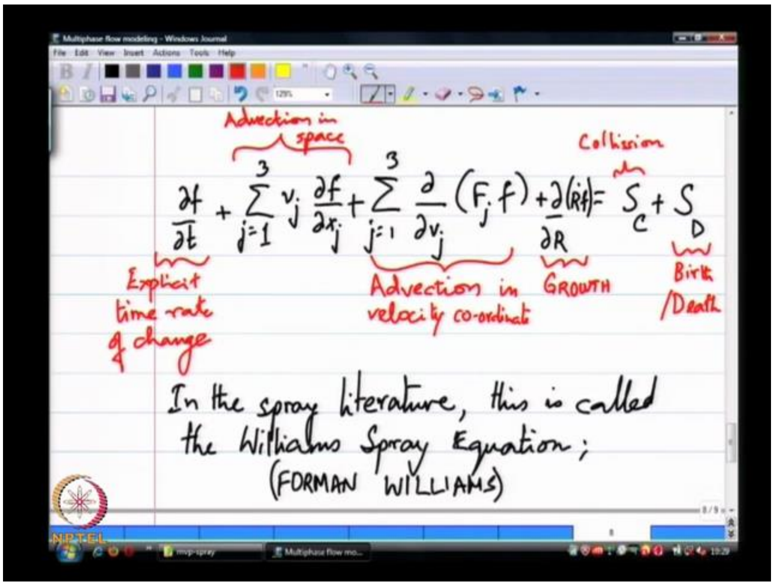

$$\underbrace{\frac{\partial f}{\partial t}}_{\text{Explicit time-rate of change}} + \overbrace{\sum_{j=1}^{3} v_j \frac{\partial f}{\partial x_j}}^{\text{Advection in space}} + \underbrace{\sum_{j=1}^{3} \frac{\partial}{\partial v_j}(F_j f)}_{\text{Advection in velocity co-ordinate}} + \underbrace{\frac{\partial (\dot{R} f)}{\partial R}}_{\text{GROWTH}} = \overset{\text{Collision}}{S_C} + \underbrace{S_D}_{\text{Birth /Death}}$$

In the spray literature, this is called the Williams Spray Equation;
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And I will write in a slightly compact fashion; this is in the spray literature, this is called the Williams Spray Equation due to a man name Forman Williams. And we must also mention that this is very similar in fact, has a very strong connection to the Boltzmann equation that fussiest used study gases. So, you can think of gases which is made of molecules, which are made of molecules and we can write a probability density function for the ensemble of particles, it is not I mean for an ensemble of particles in the size velocity space and that advect through the velocity coordinate, size coordinate due to respective forces and is altered due to the collision terms. So, this is also has connections to the Boltzmann equation, which is used in kinetic theory.

So now, we started to define this f has being probability being our density function, we now have an equation that tells us how f changes in the spray. If I go back to what f is for a moment, we said f is a probability density function we did not quit pressingly define if it was number probability density or mass probability density, we can define f to be either of two and it worth just as well nothing in the equation would be different, if we make this mass probability density function as suppose to a number probability density function.

Now if you look at this has mass probability density function.

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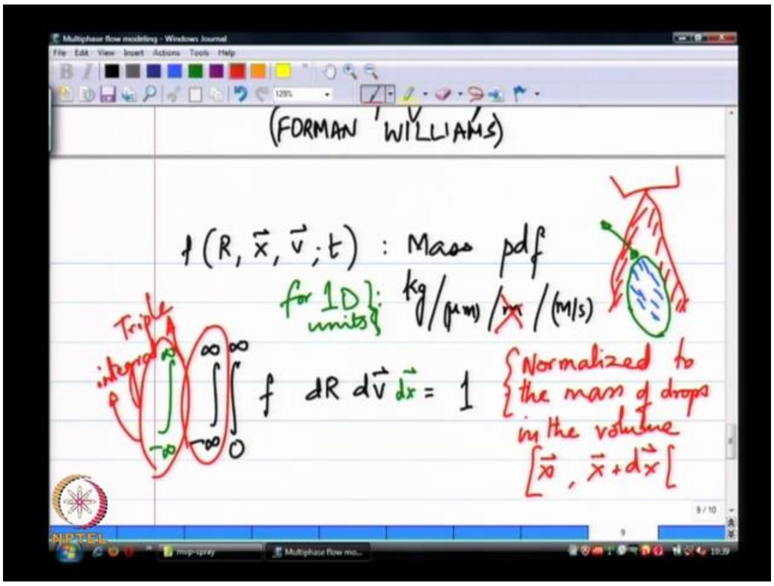

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$f(R, \vec{x}, \vec{v}; t)$: Mass pdf

for 1D units: $kg/(\mu m)/\cancel{m}/(m/s)$

Triple integral

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{0}^{\infty} f \; dR \, d\vec{v} \, d\vec{x} = 1$$

Normalized to the mass of drops in the volume $[\vec{x}, \vec{x}+d\vec{x}[$

So, I am now going to define f of R; of course I forgot writes my r terms let me include that. So, I will describe what each is this is basically due to growth of droplets, this is due to collisions, this is due to birth of droplet or death, this is advection in the velocity coordinate, this is the explicit time rate of change.

So, if I now continue on and look at what the forms, if I define f has mass probability density function and the use of vector notation just too; so this is just to be clear it has units of kilograms per micrometer of the drop size, per meter of physical space, per meter per second of velocity. So, this is the units of this probability density function. If I integrate this over the appropriate limits of r let us say. So, I will take this equation.

So, f is a probability density and I will just quickly write out the integral condition that we have in explicit form that is the probability of finding a drop in the size 0 to infinity with velocity components. So really this first integral is a triple integral. At a given point the probability of finding a drop from 0 to infinity and components minus infinity to infinity is 1. Now this is a little different from that I developed earlier, that I have written down here were the normalization factor for this probability is the total ensemble of drops in the volume x to x plus dx.

So, in another words, the probability if I take the normalization factor has been the total set of drops in the entire spray, then I have a probability of finding a drop in volume of x to x plus dx. So, probability of finding any drop in my volume x to x plus dx, itself being less than one, if my normalization condition is the total set of drops in the entire spray, then the probability of finding set of finding any drop in the volume x to x plus dx is some number less than one of that count this integral minus infinity to plus infinity and 0 infinity f, d R dv is a smaller this is the total number of drops found at that point in the volume x to x plus dx. So, really speaking this is normalized to the mass of drops to the volume x to x plus dx.

So, if I take the normalization the denominator in my normalization condition, as been the total mass of drops in the volume x to x plus dx, then you know that is how you get this integral to V 1, in fact this is the total mass of drops. So, the units of this f or not same as the written here, you would not have this per meter; oh sorry that per meter is a probability density function in the special coordinates. So, I if I want ask the question I have a spray, I want to ask the question what is the distribution in the droplets in the spray? I do not care what they are size is I do not care what there velocity is, how is the mass distributed in this spray? Which is f is a mass pdf, if I ask the question how is the mass distributed, I may find that there is a more mass here in the edges and that there is less mass somewhere here in the middle let us say.

So, in a contour sense I might say, there is a contour inside which there is low mass density, outside which there is high mass density, this is a special mass pdf. If I take this special mass pdf and if I take a small point and I look at what the special mass what the distribution is within the mass that is concentrated at this point. So, I am now not concerned that there is less mass here, if I took the mass concentrated at this point and I want to see how is this mass distributed in the size and velocity coordinates I can create a pdf and that pdf is given by this integral. So, if I now say just mass pdf is defined point wise.

So the difference is, if I treat x as a pdf variable that is as variable in which I am also accounting for the probability density, then I get this per meter actually is if I am only dealing with special dimension, but per meter cube if I am dealing with 3 special dimensions, just like this would be per meter per second, if I am only dealing with one dimensions. So, this is for a 1D case, this is the units are this. If I am not dealing with space with a special coordinate, explicitly as being part of my pdf that is I am not interested in how this pdf, how the mass is distributed probability density of mass distribution specially, but I will treats space just like time and take a snapshots this is how we did earlier discussion.

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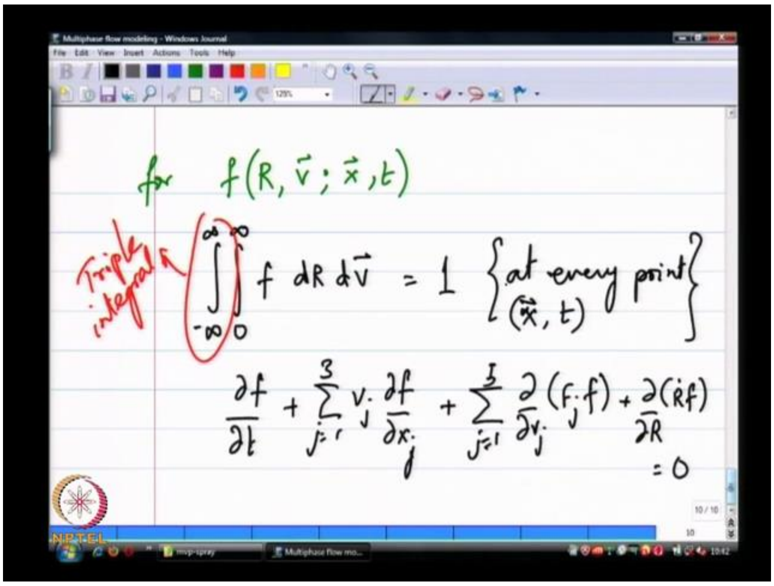

for $f(R, \vec{v}; \vec{x}, t)$

$$\underbrace{\int_{-\infty}^{\infty}}_{\text{Triple integral}}\int_{0}^{\infty} f \, dR \, d\vec{v} = 1 \quad \left\{ \begin{array}{l} \text{at every point} \\ (\vec{x}, t) \end{array} \right\}$$

$$\frac{\partial f}{\partial t} + \sum_{j=1}^{3} v_j \frac{\partial f}{\partial x_j} + \sum_{j=1}^{3} \frac{\partial}{\partial v_j}(F_j f) + \frac{\partial (\dot{R} f)}{\partial R} = 0$$

So, f is function of R and v with x and t as parameters. So, if this is a case then only r and v are my parameters, where as if this is a case then I have another triple integral minus infinity to infinity of dx, if have to normalize, if x is also part of my pdf independent variable list, then this is a condition that I have to satisfy this will also be a triple integral. If on the other hand I want to treat x is only a parameter. So, at every point I create a pdf of only size and velocity, this is how let us say we do a p d p a data set, we are not doing a p d p a data set treating x as a depend as one of the independent variable list in the pdf. Because p d p a definition is a point measurement instrument, where as I am looking at something that measures specially I may be able to do the x, I may be able to find x as part of my independent variable list.

So, if I now write revolution equation for this f not revolution equation, a normalization condition for this f then and this is true at every point, again this is a triple integral. If I take my William spray equation, I am going to take the case of dilute spray with no evaporation condensation. So, the S C and S D are 0 in this is what we called a dilute spray, Dilute non-evaporating spray. Dilute essentially means no chance of collisions happening. So, collisions are so rare in occurrence that I can ignore that effect. So, if I said this equal to 0 on the right hand side and perform this integration over the size coordinates.

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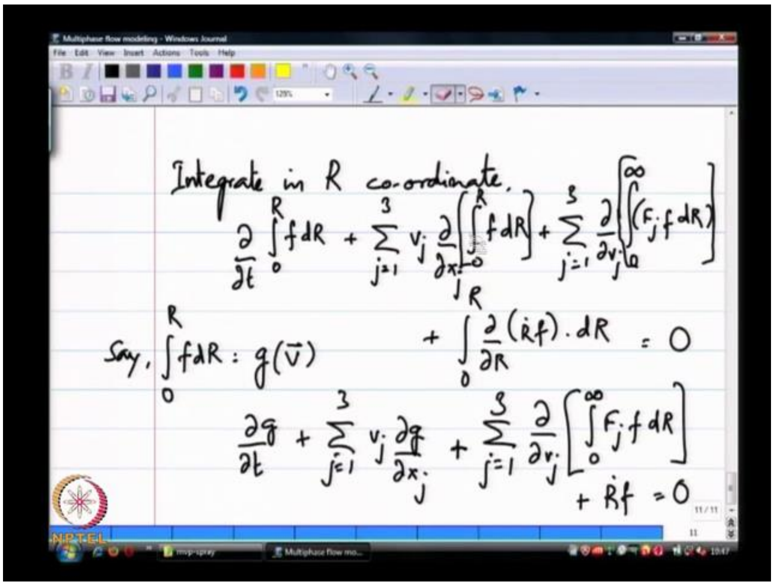

Integrate in R co-ordinate.

$$\frac{\partial}{\partial t}\int_0^R f\,dR + \sum_{j=1}^{3} v_j \frac{\partial}{\partial x_j}\left[\int_0^R f\,dR\right] + \sum_{j=1}^{3}\frac{\partial}{\partial v_j}\left[\int_0^\infty (F_j f\,dR)\right] + \int_0^R \frac{\partial}{\partial R}(\dot{R}f).\,dR = 0$$

Say, $\int_0^R f\,dR = g(\vec{v})$

$$\frac{\partial g}{\partial t} + \sum_{j=1}^{3} v_j \frac{\partial g}{\partial x_j} + \sum_{j=1}^{3}\frac{\partial}{\partial v_j}\left[\int_0^\infty F_j f\,dR\right] + \dot{R}f = 0$$

So, I want to now see if I only integrate this equation, in the R coordinate, we saw from our discussion of multivariate probability of densities, that this will also be probability density in only the velocity coordinate. Because whatever this function is a function of only the velocity v and that will also probability density because integral of that over the appropriate limits of velocity would become 1. We saw that in an example earlier, notice how some instances brought the integral inside the integration and in an other instances I did not, the reason for this just understand that, in this case integral integration O R and time derivation are commuted. So, I can exchange to operation in order.

So, if I now define this has being some sort of probability density function in velocity. So, since we said this will have all the status of our probability density function, we are able to do this. So, if I rewrite this, what do I get? Sorry, this was 0 to infinity. Notice have I have still left with some f terms I do not have any equation only in g terms, because I know integral 0 to infinity, let us say have replaced integral 0 to infinity, f d R with some g of v, it is like a probability density function in the velocity coordinate and am able to take care of the first two terms, but the last two still have this f part remaining. If you look at especially the third term, I still have f because, if F j the force acting on a set of particles external force is a function of R, then if it is not a function of R, I can take that out and write this as F j times g.

So, if F j is not function of R I can write this as F j times g. if it is function of R then I am in trouble because I have F j from I earlier formulation as a external force per unit mass acting on these particles, and if there is size dependence on it, then this becomes little tricky to write. If we think of an external force per unit mass on a set of droplets, where there is size dependence, the simplest of such forces is drag. When you write the drag on a spear for example, the drag on a spear scales as the size of this spear. So, you essentially have to have I mean this is not something that is out of the ordinary very commonly found in sprays, that this F j is a function of R and as a result I am not able to do this integration right away, this is the start of what is often called the closer problem.

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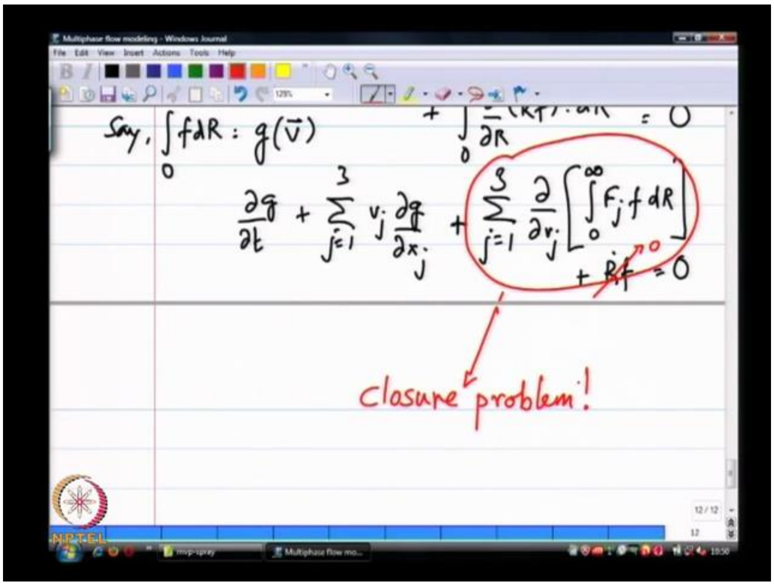

Say, $\int_0 f\,dR = g(\vec{v})$

$$\frac{\partial g}{\partial t} + \sum_{j=1}^{3} v_j \frac{\partial g}{\partial x_j} + \sum_{j=1}^{3} \frac{\partial}{\partial v_j}\left[\int_0^\infty F_j f\,dR\right] + \cancel{\dot{R} f}^{\to 0} = 0$$

Closure problem!

So, this part say for example, I will said R dot 0 will come back look that later, but this part here were I am unable to write F j this integral F j f d r. In terms of g is what is the reason for what we call are closer problem; so, what we will do in a next class is will start from here and the governing equations that we are used to see are our Navier stoke equations. So, we want to see how to go from something that looks like the Boltzmann equation or in this case William spray equation and arrive at a multiphase or even a 2 phase set of equation, 2 sets of equations describing the gas phase and the droplet phase.

So, we going to do that mathematics in the next class, but before that we want to understand what are the phase. So, if I take a spray wave done this many times you know we have air in the interstitial phase between drops. But if I take all the drops with vacuum in between and the air alone, in some sense they look alike; in the sense that drops are macroscopic distinct entities that are separated by emptiness in the case I talked about where the drops are taken out with vacuum in the middle. Now if I really zoom into the air part, the air is also discreet molecules with emptiness in the middle.

So, really the only difference between air and the drop phase is the size of the particles, were molecules of oxygen and nitrogen may be a few tens of angstroms, drops of liquid may be fraction of micron to several hundreds of micrometers, and the interstitial phase also scales. But other than these scaling effects, the nature or morphology is somewhat similar. We will use this argument our building block, to replace the drops with the continuum; just as we replaced as discreet set of oxygen molecules and nitrogen molecules with this continuum idea called air.

We will replace set of drops with the continuum for today we will call it as spray or call it drop fluid. So, this drop fluid plus air put together makes our spray. We will see how to get this far from the Williams Spray Equation in the next class.