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Lecture – 38 Multiphase modelling – Governing equations

Welcome back, we will continue our discussion of multiphase modeling of sprays. Towards the end of the last class, we had sort of arrived at a taxonomy of multiphase models, to see possible way by which you could based on the physics of your given problem choose an appropriate model - whether you should be using a Lagrangian model or whether you should be using an Eulerian multiphase or a mixture model or the exact model that we discussed as our choice number one.

So, will start from there and look at the mathematics of some of these models and see what underlies the mathematics.

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So, we said based on the particle relaxation time and the mean free path, these are the two parameters we defined based on which you could chose between the different models, and in the gray area of course you have to there is some room for engineering judgment apart from that, of course we said the exact model would be applicable in all these situations.

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Mixture model governing equations ✓ The balance of mass and momentum for the mixture phase is given by Johnne $\frac{\partial}{\partial t}(\rho_m \vec{v}_m) + \nabla .(\rho_m \vec{v}_m \vec{v}_m) = -\nabla p_m$ $\frac{\partial}{\partial t}(\alpha_i \rho_m) + \nabla .(\alpha_i \rho_m \vec{v}_m) = 0$ Conservation of
Michael velocity field

So, let us look at the governing equations for the mixture model. If you recall the mixture model is essentially a single phased version of a multi phase model, that is in reality we have drops laid an in air that are spray, but we believe due to certain physical laws that the spray seems to obey that we are able to make a simplification and look at a third equivalent fluid which is a mixture and we will only write our balance laws for the mixture. We are not at this level going to be concerned about individual droplets or air as being separate only going to write balance law for the mixture.

So, the first balance law is the Conservation of mass; that you will see here, but before I go to the conservation of mass we need to be clear about our definition of alpha. Alpha is called the volume fraction and this is the fraction of a given infinitesimal spatial region that is occupied by either phase one or by alpha i is the volume fraction of the ith phase in the mixture, where a certain volume of an given infinitesimal volume is occupied by the ith phase and that fraction is given as alpha i.

So, remember this is a field property that is it is a function of x y z and time in general, which means that at every point I am looking at a tiny infinitesimal volume surrounding that point and I envision alpha i as being the fraction of that infinitesimal volume, that is occupied by the ith phase. So, we already we sort of touched upon this, that the idea of our infinitesimal volume now is not our old calculus mathematical infinitesimal volume,

but it is a volume small enough in comparison to the rate of variation of alpha i, but big enough in comparison to individual drop sizes.

So, we cannot be talking about an infinitesimal volume that is on the order of the drop size, we are looking at an infinitesimal volume that is bigger than the drop size, so I can talk of a smudged out volume fraction. So, the first constrain that, is we have from that is this fact that the sum of all volume fractions has to equal 1. So, this is essentially what you might call Occupancy of space, I cannot have empty space. In a continuum formulation there is no such thing as emptiness. So, I have essentially all the space occupied by either air or my drop phase, we are not talking drops we are talking drop phase that is ours. So, if I was to only talk of a two phase problem, in the two phase case, M would be equal to 2 and then I can define alpha 1 and alpha 2 and alpha 1 plus alpha 2 has to equal 1.

Now, based on the local alpha i, I can define a Mixture density, and alpha and rho i is what we will call the Material density. So, that is the actual physical density of the liquid I am spraying and actual physical density of air the material, those are my rho is. Rho m is the local mixture density, that is the density of the constituent the mixture phase that is made up of these two materials.

So, now I have my mixture density. So, will come back and define our conservation of mass, which looks very similar to our single phase conservation of mass equation, that we usually have accompanying a Navier-stokes equations, that the partial derivative of alpha i rho m with respect to time, plus the gradient of alpha i rho m V m is equal to 0, V m is the mixture velocity field. This mixture velocity field is basically based upon the idea that locally at that point both the air and drop phase are moving with the same velocity V m this is a velocity field of course, so, it could be a function in general x y z and time and alpha i rho m V m gradient of that quantity, plus the rate of change with respect to time of alpha i rho m is equal to 0. Now notice how I still have the subscript I, which means that this is an equation that we write for each of the two phases.

So, alpha i rho m for each i you have a conservation mass equation. So, just to be clear about that fact, I will say this is a conservation of mass equation for phases i. Now if I take the simple two phase formulation and I take an equation just like this with i being equal to 0 and i being equal to 1 and i being equal to 2 and add them up let see what we find.

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7.1.9.94 Mixture model discus $\frac{\partial}{\partial t}(\mathbf{f}_{m}) + \nabla \cdot (\mathbf{f}_{m} \, \overline{\mathbf{v}}_{m}) = 0$

If I take summation over all I, what I find is that I have rho m summation alpha I, plus gradient of rho m V m summation alpha i is equal to 0. You already know summation alpha is equal to 1, so I can write this as gradient of the mixture density plus, sorry derivative of mixture density with respect to time, plus the divergence of rho m V m is equal to 0. In fact, this is exactly the mass conservation equation for a compressible fluid; which means all we are saying in the mixture model is that, this effective fluid is a compressible fluid and the constituent of the compressible fluid these alphas and this rho m being equal to alpha i rho i summation is like my equation of state.

Remember we need an equation of state for the compressible fluid to close the set of equations. So, essentially this rho m being equal to summation alpha i rho i is like my equation of state, it is not to at completely formulated as the equation of state, because I need another property that says, rho i itself is a constant. So, if i know that rho i itself is constant. So, if I treat my air and my liquid as individually being in compressible in the material sense, rho m being equal to alpha 1 rho 1, plus alpha 2 rho 2 is an equation of state that relates the density of this mixture to a property a field variable called alpha 1. Remember I do really only alpha 1 is an independent variable; alpha 2 has to be 1 minus alpha 1, in the 2 phase description.

So, rho m is equal to alpha 1, let us write this out and just we clear about it. So, rho m is equal to alpha 1 rho 1 plus 1 minus alpha 1 rho 2. If I let this be accompany by rho 1 equal to constant and rho 2. So, if I say rho 1 rho 2 are individually constants, this is saying both the individual phases are themselves in compressible, then rho m equals alpha 1 rho 1, plus 1 minus alpha 1 rho 2, is the mixture density and this is essentially sufficient to be called an equation of state because I am relating the mixture density to a field property called alpha.

So, far as this mixture conservation equation is concerned, this mixture conservation equation, the mixture is a compressible fluid in this is a conservation equation for that compressible fluid. The property of that mixture is related to another field variable called alpha 1, for which this is my transport equation this is my conservation equation for that alpha 1.

So, this is now as far as conservation of mass is concerned, the way defines what the fluid is looking like. Now in the momentum sense, this is essentially my conservation of momentum equation partial derivative with. So, this is again familiar, there is 2 parts to this, I have a now a mixture pressure and the mixture stress field shear stress field these have to be related to my field properties. So, the pressure let us just quickly think of what this pressure is. This is the pressure in the mixture that is arising out of the stress field in the air phase plus some super post stress field in the drop phase.

That is if I now separate the two phases, the stress field in the air phase is easy to understand that is the (Refer Time: 15:09) traditionally understood as the hydrostatic static pressure field in a single phase. The stress field in the drop phase is what we talked about earlier, this is a result of the coalitional process is that occur between the individual drops. So it is like it is a stress that arises, it could be a normal stress that arises out of drop being in some sense crowded in one place or drops being agitated locally in some point.

So, I have to have a model to relate this drop phase stress field to some other drop phase properties such as for example, alpha gradients. So, gradient of the velocity field I could even define sort of a temperature which is a measure of this agitation level in the drop phase. So, I could locally have a very high even though the mean velocity may be 0, so I have a locally very high movement within the drops this is like a granular temperature or

a dispersed phase temperature that you could define, that is very often defined in granular phase's granular flows as a matter of fact.

So, I could define all these field variables and come up with relationship between the mixture pressure and these other properties, mind you the hydrostatic pressure. So, if I was do the exact model, the actual hydrostatic pressure in the air is only one component of this mixture pressure and then there is also a stress field that has to be related to some argument list and these are called Constitutive relationships. So, these relate you know you will recognize the mixture shear stress being related to the gradient of the velocity field is like our Newtonian viscosity model.

So, if I make that viscosity be a function of the local volume fraction of alpha 1, let us say in the simple two phase formulation, that is an extension of our Newtonian viscosity model to a mixture level. Now these constitutive relationships are required before I can close the set of equations, because if you look at just these I have p equations in to unknowns, I have my unknowns are alpha 1, alpha 2 V m P m and tau m and I only have 3 equations in the conservation form these are my as conservation equations, these are my conservation of mass for alpha phase, alpha phase 1 phase 2 and the conservation of momentum for the whole mixture. If you look at the mixture conservation of momentum equation, that does not have any subscript i. So, we are only writing one momentum equation, one balance of momentum for the whole mixture.

So, we have to have to more relationships which are my constitutive relationships to complete to close the set of equations and have p m related to some other fields, alpha i gradient of v m etcetera. So, this part is an area of active research even today, if I want to use mixture model you if you look if you look at the literature there is lots of papers that use mixture models to study sprays or bubbly flows. If this, lots of different multiphase flows that use mixture model, but you will see the level of simplicity that goes in to these constitutive relationships and if you begin to question the physical reasons for such simplistic arguments, you will find yourself in an area where, you will find yourself in unsorted territory. Because the reason such simple forms are employed is because that is the best we can do as far as trying to employ our intuition from single phase flows, we are basically in the process of extending our intuition from single phase flows to multi phase flows.

Now, how do I get these constitutive relationships, really one way usually is experiments, but in this case experimentally to get these kinds of relationships experimentally is very difficult. So, the other way is to go to the exact model and do like fully resolve droplet level simulations and extract the local pressure field as a function of some other arguments and that is of tractable approach and is quite widely being use today. To extract realistic constitutive relationships that relates the stress field to some other field variables.

This is the simplest of multiphase models, so if I take the constitutive relationships and say my P m is independent of the simplest of constitutive relationships, could be that P m is dependent of all alpha and gradients. So, it is just like my hydrostatic pressure field in the air phase or I could relate tau m to i simplest forms of the relating P i P m to only alphas and relating tau ms to only gradient of the m, just like a Newtonian fluid would behave.

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So, let us move on and we look at the next level of complexity, which is my Eulerian multi phase model. The Eulerian multiphase model again starts by writing a conservation of mass equation for each of the. So, this is for the i equal to 0 phase, there is a particular reason I have written this in this form, but really it does not matter, I could have let this i go from 0 to m and it would not make any difference.

So, now I have this conservation of mass for each of the phases constituted constituting the mixture, but the difference now is that we are going to write a separate conservation of momentum equation for each of the phases. What have we done in this process let us look at our list of depended variables, if I simply take M equal to 1, here m equal to 1 would mean a 2 phase flow, because i equal to 0 is one phase, and i equal to 1 is another phase. So, I write an equation like the top two here for my I equal to 0 and an equation like this for i equal to 1 and i have alpha 0 is one of my unknowns, rho 0 is just the material density of the fluid, V 0 is the velocity field that is unknown for the phase 0 likewise I have a alpha 1 V 1, I have P 0 P 1, tau 0 tau 1 these are my unknowns.

I can come up with a relationship or we will have to come up with the relationship between P 0 tau 0 and alpha 1 alpha 0 in the gradients of the velocities that is what we called are constitutive relationship. We also know that alpha 0 plus alpha 1 has to equal 1 that is occupancy of space relationship.

So, we essentially created as suppose the mixture model, we now have one more new velocity field here which is my V 1 which is new. So, we have in three dimensions, we have three velocity components and alpha for each of the 2 phases. So, this is I have 8 unknowns at every point in space, apart from the 2 pressures. So, once I relate the pressures to some other field variables, I have 2 pressures, 6 velocity components in all and 2 volume fractions, that is my complete list of unknown variables as suppose to the mixture where mixture formulation, where we had 2 volume fractions, 3 velocity components and 1 pressure.

So, we essentially added 4 more unknowns to the list. The problem is not just at the addition of 4 more unknowns, it is the numerical complexity and the solution complexity that comes with it that in that process some convergence challenges, for this kind of a model formulation the simplest assumption made. So, now, look at the pressures for a moment, we are able to postulate an individual pressure field in each of the 2 phases in this kind of a formulation, but they are not really completely independent of each other and so the list of unknowns become smaller through algebraic relationship that exist between these kinds of other variables.

Like for example, alpha 0 plus alpha 1 has to equal 1. So, through relationship between these individual field variables, the total number of independent unknowns comes downs

slightly. But we have into a touched upon this term here that did not exist in the previous formulation. So, now, that I have 2 phases, let us just take i equal to 0 and equal to 1 and the 2 phases are moving with different velocities, they become sources and sinks of momentum to each other

So, I can have inter phase momentum transfer, that now becomes important; notice the form of this term K 0i is like a drag coefficient and that coefficient multiplied by the differential velocity, the relative velocity between the two phases, is a simple constitutive model for a force a drag force that exist between the 2. So, drag is the simplest of these inter phase momentum transfer terms, now again if I assume i equal to 1, there is a K 01 which is depended on the relative velocity between the 2 phases that takes on a positive sign in one equation and the negative sign in the other.

This is basically saying the force acting on 1 phase is equal and opposite of the force acting on the other. And if I take all the equations, all the balance laws for each of the different phases and add them up that gives me the even in this formulation I can derive a mixture level balance law, but that would have the individual velocity components (Refer Time: 29:24). So, I could still define sort of a velocity of the center of mass of the mixture, I know now that the 0 th phase i equal to 0 is moving with 1 velocity V 0, i equal to 1 is moving with a different velocity V 1, but based on the relative volume fractions and mixture densities, we can define what is called a Barycentric velocity of the mixture.

And we can write a formulation for the bar centric velocities of the mixture and in that formulation these inter phase drag terms vanish. So, inter phase drag cannot effect the Barycentric velocity of the mixture because it is a force internal to the whole mixture, but it does effect the individual physic movement, velocity fields in the individual phases. So, let us for a moment look at this shear stress terms tau 0 and tau I, tau i is specifically what is tau i? Tau i is basically the shear stress field that exist in the drop phase.

So, if I take a collection of drops with no air in between, if I try to put a hook on one of the drops and drag it, does this drag other drops with it that is the basic definition of shearing; So, if I pull one drop with me or a you know small group of drops, what does it due to the other drops? If there is no effect on the other drops that means, the effective

viscosity of this collection of drops is 0, there is shear stress that can be sustained in this mix in that collection of drops.

So, if i now take this collection of how do I now find the viscosity of this collection of drops, one would have to do or the effective viscosity of this collection of drops, one would have to do fully resolve simulations to look at the effect of collision between drops, which is basically responsible for this effective viscosity and derive from sort of an inverse from a regression these kinds of constitutive relationships and this is like I said an active area of research in itself that would be (Refer Time: 31:52) pursuing to complete to bring these model formulations up to some level of applicability, where they are more realistic for dens sprays.

So, why do I say dens sprays, if I look at real fight sprays and do this same thought experiment of putting a hook on a small group of drops and dragging them, because they are a very high Knudsen number collection of drops, the effective viscosity of something like that would be basically 0. Whereas if you are in the dens spray reason, where collisions are more frequent then if I try to do this thought experiment in the dens spray region, you can imagine that the effective viscosity of this mixture would be nonzero.

So, this shear stress term sustains itself in the den spray region, while it goes to nearly 0 in the rarified region.



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I want to look at, I want to pause here for a moment and show you one possible way by which you could look at modeling what use are these kinds of models, in a real spray. What use are these Eulerian models in a real spray.

So one of the areas of applicability of these Eulerian multiphase models in sprays, especially when you have breakup and coalescence is to look at population balance modeling, we look at what population balance modeling is for a moment; let us say I have a little box with lots of different drops and this for the sake of convenience I am going to derive divide these drops in to different bins. So, I have let us say drops spanning from some d min to some d max, I am going to divide this into different bins. So, this is my ith bin, this i plus 1 th bin, this is i plus 2.

So, if I want to look at how to model breakup let us say. So, initially all the drops are of this large size and these some process that is causing these drops to breakup.

So, if I take the number of drops in the ith bin and that is sum n i why would n i change. N i changes because of two reasons, because drops in the ith bin are breaking up, so if gamma i which is often call the a breakage frequency, so if the ith drops are breaking up at, if the drops in the ith bin are breaking up at some rate. So, gamma i is a rate of breakup of drops, then gamma i times n i with the negative sign is the rate of breakup of drops and that is essentially with the negative sign taking drops out of the ith bin.

The other possibility is that I have some drop in the i plus pth bin, breaking up and putting some mass, putting some number of drops in the ith bin. So, when a drop that is larger than the ith size class, breaks up it puts drops in the ith bins. So, i have some other jth size class breaking up at the same rate gamma j N j and a fraction of that gamma j N j which is given by this n i j coming in to the ith bin. And I could have this go over all the drops from i to M, really speaking it should be i plus 1, I cannot have the ith bin breaking up to give drops in the ith bin.

So, at best I could have the i plus 1 th bin breaking up to put drops in the ith bin or I could have the i plus 2 th bin, breaking up put in drops in the ith bin etcetera. So, this n i j is a fraction of drops, that result that end up in the ith bin from a breakage event in the jth bin. So, this n i j is a fraction of drops that end up in the ith bin, originating from a breakage event in the jth bin. Some drop in the jth bin jth bin broke up and it breaks up in

to lots of fragments, it could break up in to 2 equal half, it could break up in to one big drop and one tiny fragment flying of it could break do lots of different things.

And this break up event now puts some fraction of those drops originating from the jth bin in to the ith bin. So, this is a balance of the number of drops in the ith bin, which due to breakup. So, when I have some break up process causing these drops to break up, some physical process we do not know, that physical process has to obey something like this.

Now, this is called a phenomena logical model, notice how I am not yet brought in any physics of what is causing this break up. The physics is essentially hidden in these constitutive coefficients gamma i and n i j, this is my opportunity to bring in the physics. Say for example, I might believe through a physical process that a larger drop is likely to break up more frequently than a smaller drop. So, for example, if I believe that there is a smallest size drop, that just does not break up.

Then I might say that gamma 1 which is the break up frequency of the smallest size class is 0 and I might write a relationship between gamma i and d i the size of the drop or I might write a relationship between gamma i and some other property that is imparting this energy for break up to the drops and n i j is our phenomena la phenomenology of how a given size of drop breaks up.

So, if a drops breaks ups is it likely to break up in to 2 equal halves, in which case my n i j. So, if it is exactly breaking up in to 2 equal halves, then say for example, n 24 would be 1 and all other n i 4 where i is not equal to 2 is 0, so if for the case of j equal to 4. So, i am just looking at drops originating from break up happening in the 4th bin and if let us say for a moment that all the diameters are spaced equally in an arithmetic progression, then a drop breaking up in the 4th bin only puts drops in the second bin because it is breaking up in to 2 equal halves and it cannot put drops in the third bin or the first bin.

A drop breaking up in the 100th bin, puts drops only in the 50th bin and in no other bins. So, this is a phenomenology that is based on some physical understanding of that particular break up process. So, the population balance model that we wrote this part is only a frame work, it is a phenomena logical frame work, the physics comes in the form of these gamma is and n i js and over the course of the last lecture decade or so, the various models have been developed for both gamma i and n i j to accurately capture the physics of a given physical problem. Say for example, we have a multiphase a reactor bubble column, where you have bubbles of some size coming in at the bottom of the column and they may break up and leave and we want to look at the phenomenology of the breakup of these bubbles because that is important to creation of surface area, to creation of surface area is important to mass transfer.

So, if I look at the mass transfer pro process and if I want to model that mass transfer process, I need to model the evolution of the size distribution of let say drops or bubbles or whatever the case may be. So, what we are going to do now is look at how we can take our regular Eulerian multiphase model governing equations and include this population balance a terms. So, essentially we look at drag as been the only coupling between these two. In fact, if I take a 2 phase formulation of this there is only 2 coupling mechanisms between the individual phases, as it is apparent in this case one is through drag and other is through occupancy a volume. So, alpha 0 plus alpha 1 has to equal 1.

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If I now look at what happens if I include population balance, I have these drag terms, but I also have additional coupling in the form of these population balance source terms. So, think of what this means if I have the drops in a box, the left hand side of the drops in a box population balance was just d n i d t. Which is the rate of change of the number of drops in the ith bin as a function of time; when I now have a flow field super imposed

over these drops, I have to go I have to write the material derivative of that of that flowing field.

So, in the Eulerian formulation where I have these drops coming in to a control volume and leaving, while these break up process is are happening; the first thing that you see is that the left hand side is now of the form with the material derivative, where alpha i is the volume fraction of the ith phase and if you look at what you see on the right hand side of these equation you see this alpha i by x i, x i is essentially size of drops in the ith bin, it is actually let us been even more clear it is not just any size, it is the actual volume of a drop in the ith bin.

So, volume of a drop in the ith bin, alpha i is the total volume fraction, alpha i by x i gives me the number fraction of drops at a given point that reside in the ith bin. So, you see that the rest of this equation looks very similar to the population balance form except I have this i have this gamma i n i what looks like n I, when gamma j n j times some n i j which is a fraction of the drops that come over in to the ith bin. And because I am looking at a multi phase formulation, where I say each of the size classes is also allowed to move with its own velocity field.

If we go to that level of generalization of the flow field, then drops breaking up in one phase resulting in showing up in a smaller size class are also bringing in momentum with them because total momentum over the entire mixture has to be conserved. The breakup of drops from a larger size class, putting drops in to a smaller size class is completely internal to the whole air plus drop mixture.

So, whatever momentum exchange process is that happen are suppose to be equal and opposite. So, that is the reason for these 2 terms that you see in the red ellipses, where any momentum leaving the jth phase, accompanying the mass transfer from the jth phase to the ith phase ends up in the ith phase. Likewise any momentum leaving the ith phase due to breakup of drops in the ith phase leaves the ith phase again these are only phenomena logical.

So, this is some break up process this is some process, it is like a balance law that tells me mass coming into the ith phase and mass leaving the ith phase mass and number of drops are sort of related. So, how do I let this mass come in and go, is where the physics of the problem comes in. So, for example, in a general flow situation like this, the actual break up of drops is due to a relative velocity between the air and the drop phase.

So, we could relate the gammas to some kind of a relative velocity in the drop phase and when you do that essentially this is a model of secondary atomization that follows your primary atomization process. So, you have some primary atomization that produces a distribution of drops and from there on you could look at studying the secondary process is using a phenomena logical model like this. This is where you can take multiphase models and apply it to atomizing sprays, without this atomizing part they this red is essentially the atomization part of the multiphase formulation, without the atomization part these are my governing equations, where if I have the balance laws and the appropriate constitutive relationships and I know the size of the particulate phase because these drag coefficient is going to require some information of the size of my disperse phase drops.

So, if I know the size of the disperse phase drops, I have this equations complete that I can look at transport of drops in the spray. I cannot include how the process of these drops breaking up without the help of something like a population balance model. This completes our discussion of multiphase models and you know mixture model Eulerian model, that I just want to leave your cell leave you with the sort of a thought, you went through this process of asking (Refer Time: 49:46) some physics based questions and finding and arriving at a model choice that is appropriate. In reality though most of our models are neither here nor there or they involve both.

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So, I will just take a simple hour glass that is flowing sand, if we look at the Knudsen number which is the distance traveled by a given particle between 2 collisions. If I look at the Knudsen number in this region verses the Knudsen number in this region they have vastly different, this is the case where if you imagine this sand particles are all giggling and this giggling sand particle are going to colloid very frequently. So, this part is right for our kind of a continuum model, this part after you gone pass the constriction is essentially where individual particles are moving with no knowledge of their neighboring particles, there all falling in this same gravitational field with about the same terminal velocity, if they have (Refer Time: 51:07) a terminal velocity.

But the mean free path which is the distance between collisions has gone up significantly during this process. So, if I ask the question what model is appropriate for this? This is actually a very very close representation for real spray, we have a very den spray region where we require a continuum model where I mean because of the frequency of collisions, you either require a model to handle the frequencies of collisions in the individual particle like a in a discreet particle model or you go to a continuum.

And on the other count when you have reached in to the rarified region, you require something that defaults to where individual particles are moving with no knowledge of other particles around. This is an area that is research wise very active. To patch rarified spray models like Lagrangian particle tracking, is a very good choice for rarified spray models, but you requires some kind of an Eulerian model in the discreet in the den spray region. Patching these two together is what real life research these days looks like.

We will continue our discussion in the next class.