Multiphase Flows
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Lecture - 16
KTGF and Euler-Lagrangian Model

So, welcome back. In the last class what we were discussing is about the equation of the two-fluid model.

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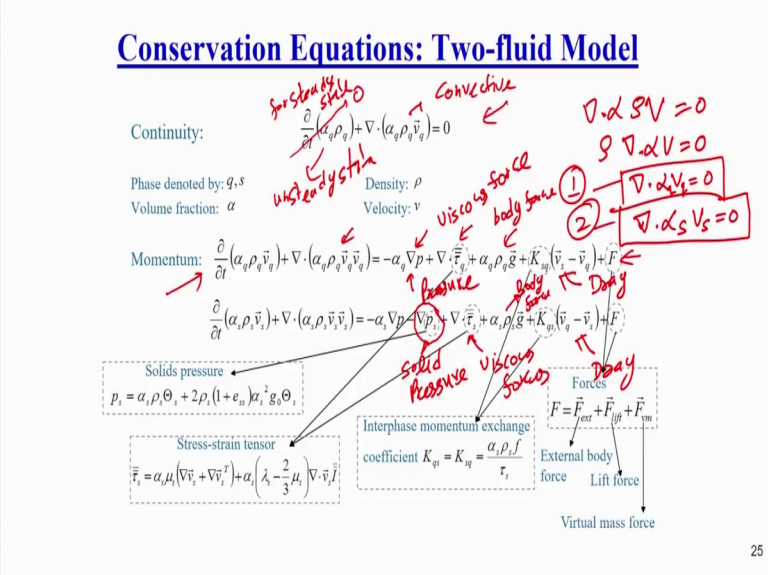

And we have discussed those equations so; I will just briefly revise it again that what are the equations we have discussed. So, we said that in two fluid model what you do you solve individual equations for continuity, and momentum equation for each phases. So, it means suppose if you have two phase, you solve two continuity equation and two momentum equation.

So, if both the phases are continuous, what we do we solve continuity equation which is given by this is dou by dou t of alpha rho q plus del dot alpha rho qv v q equal to 0. This is the transient term, on a steady state mass transfer term or transient term or the steady state term state and this is convective term; So, convective transport so, that is equal to 0 and if suppose there is some generation this will be actually equal to some generation.

But if we are not talking about any reactive system then it will be equal to 0. And for a steady state system, what will happen that this two this term will be 0 for a steady state , state this term will be 0. So, you will be getting this del dot alpha rho qv will be equal to 0 ok. So, that is whatever the way you write this equation if rho is constant.

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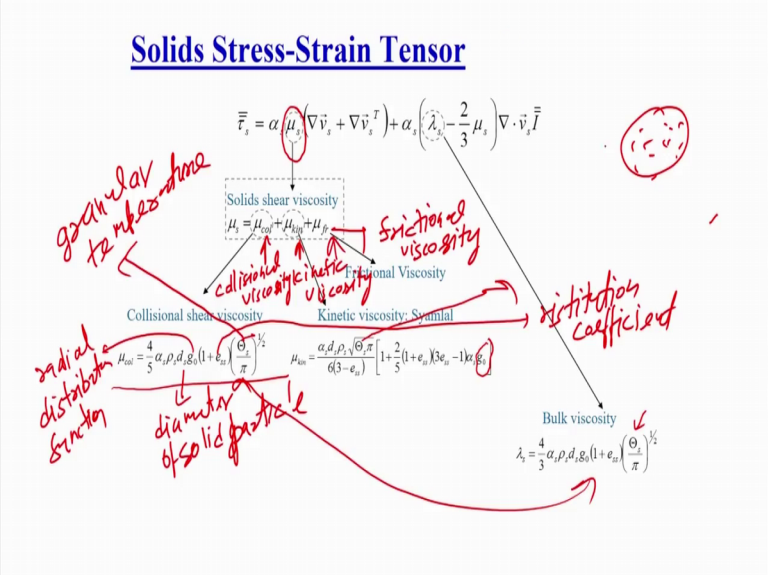

You can put it again for incompressible rho you can pull it out. So, this equation will be rho del dot alpha v and that will be equal to 0, and this will be rho will be 0.

So, finally, you will have a term del dot alpha into v will be equal to 0 for incompressible steady state flow so, this way it will be simplified. Now you solve the same equation for the both the phases. So, say I solved this for the q phase here the similar equation you have to write for the s phase. So, it will be two continuity equation ok. So, one will be for this alpha q this will be alpha q v q another equation will be del dot alpha s vs that will be equal to 0. So, that is the one stage that will be the second.

So, one continuity equation one, continuity equation two, this two-continuity equation you have to solve ok. Now, for momentum again you have to solve the two-momentum equation, now this momentum equation is very close to the Navier-Stokes equation ok. We have assumed that mu is constant if you assume mu and rho is constant Navier-Stokes equation or you basically write a general momentum equation in terms of the tau. So, it is very close to that momentum equation the only thing is, what we have done we

have multiplied the each term with alpha. It means the fraction volume fraction of that phase, and then you will do the same thing for the second phase.

So, we will multiply it is a by alpha s which will be the volume fraction of the that phase. So, again this is the term this is the momentum equation. The first term is under steady state acceleration or local acceleration. This is convective acceleration term ok, this is pressure term which is multiplied by alpha q it means that kind of contribution from that phase. Then tau del, dot tau; now because the tau we are taking the velocity of that phase only, this is not multiplied with the alpha.

Then the overall body force term, which is being because of that phase. So, this is alpha q rho into g. So, this is body force, let me write it again for the sake of simplicity. This will be body force, viscous force, force, this is pressure and this is drag. And we have already discussed that why the drag is written it in this way, and the Ks q value will be written for the different drag closures, the way we have already discussed in the during the drag force discussion. And any issue of force if you multiply here.

Now, this is convective term, this is the local acceleration term. All the terms is being multiplied with the alpha that in the viscous force term, because that will take care of the velocity of that phase only. So, ideally speaking, if you write in terms of the superficial velocity, again that alpha q term will be there. So, this is the way we write, and if suppose the second phase is liquid or continuous fluid.

Suppose, if you are solving the two-fluid model for bubble column, where both the phases are actually a fluid whether it is a water and air both are fluid, you solve the exactly same equation for the gas phase also. So, the same equation you will solve for the gas, which same equation you will sell for the liquid phase.

So, you both are fluid continuous fluid you solve it in this way; however, the equation modified slightly, if the one phase is solid ok. It means discontinuous by nature itself. So, for the solid the equation will be modified. If you will see that all the other terms are the same, only thing is you introduce a new term of del ps which is the solid pressure term ok, solid pressure.

This term you include, viscous forces because of the solid, forces body force again same body force, this is drag, any additional force this is the local acceleration of the solid convective acceleration. So, this is the acceleration completely so, local plus convective. So, in that way you write for the solid the only thing you have to introduce a solid pressure term extra. If there is continuous flow this term will not be there rest every term will be there. As it is instead of the tau del dot tau s you will be writing that del dot tau l say for the liquid or tau a for the air ok, or for the gas.

So, that is the way we write the equation into fluid model, and the basic assumption is both the phases are assumed to be continuum interpenetrating. So, even if it is a solid, we are assuming it to be continuous, and that actually bring lot of a junction in this model. The very advantage of the model as discussed that you are solving only 4 equation ok, if you do not solve other interactions. So, you are just solving 4 equations, and with the 4 equations you are getting the whole solution for the whole geometry, whole body or kind of whole domain.

Now, it is computationally much cheaper compared to the other model which we are going to discuss. The only disadvantage is even the continuous phase you make it interpenetrating continuum, even the discrete phase sorry you make it interpenetrating continuum. And that is the major assumptions of this model. So, this solid pressure and all those terms we will discuss, and as I said that the major problem comes with the solid pressure, because solid do not put any pressure while flowing.

And the major problem is with this tau s, because the tau in the basic basic notion has been defined as if this is proportional to dou v by dou x say or velocity gradient and the proportionality constant is viscosity mu. Now, the way the very notion that tau has been defined cannot be do cannot be used here, because solid do not have any viscosity or you can say solid has not finite viscosity. So, you have to write several equation which will be written in terms of how the tau will be defined for the continuous phase, how the tau will be defined for the solid phase.

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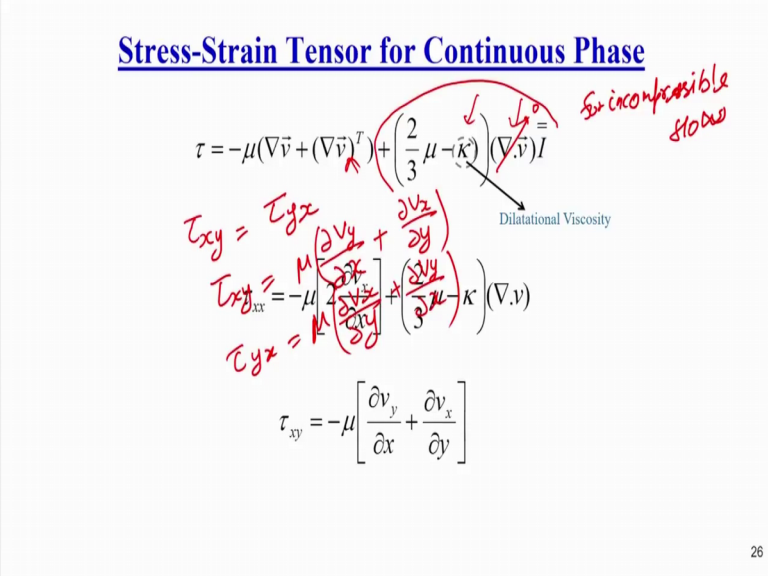

Now, for continuous phase, this equation is pretty much same whatever you have done in your undergraduate courses or the lower level courses of transport phenomena, the tau is nothing but mu dou v del v plus del v transpose plus 2 by 3 mu minus k del dot v into I. Now, this term is basically dilatational viscosity, and that dilatation is viscosity comes into the picture, once there is any change in the volume. So, for the incompressible flow, the change in volume will not be there, anyway for incompressible flow from continuity equation del dot v equal to 0 for incompressible flow this term is going to be 0, it means whole this term will be removed.

And for compressible flow yes there can be change in the volume dilatational viscosity will be there. So, this term will also be playing the role. But most of the time the flow we deal with generally in chemical engineering the most of the fluid are incompressible in nature rather than the gases. So, you can neglect this term easily. Then this is the mu del v plus del v tau and I do not want to do go in detail of that, but just to revise it a little bit, it has been done because tau has been found out asymmetric tensors, symmetric second order tensor. So, that is why it will give the symmetric nature we write this in this form.

So, suppose if I write now tau xy, ideally if they are symmetric tau xy will be equal to tau y x, it means, tau xy if you remember will be defined as mu dou v y up on dou x and tau yx will be defined at mu dou z x upon the y. So, they are not actually equal, but they are

symmetric matrix they will be equal. And that is why the another term has been added which is the transpose so, if I do the transpose of this I will write it this, dou vx upon the y here it will be dou vy upon dou x.

Now, this becomes a transpose, it now this 2 becomes equal. So, that is why we write the tau it it in this way it is a 100 year of research I do not want to go in detail of that, but if you want more on this, we can discuss it in the forum or we can discuss it you can drop me a mail, and you can also go through your transport phenomena books. So, that is the way it has been defined and as I said that this will be like this, it will be defined it it in this way and it this will come it in this form.

So, once this is tau x x actually this will be 2 because dou vx plus dou v x will be there, tau xy it will be mu dou v upon dou x plus dou v x upon dou y. So, that is the way continuous phase shear stress has been defined.

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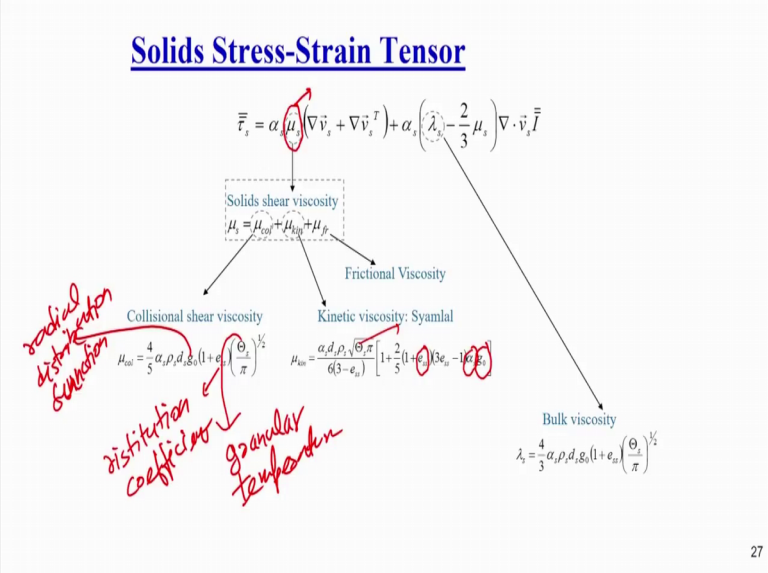

Now, coming to the solid shear stress; so, as I said this is very critical and will kind of left our discussion last time in this place only, because what you need to do now you have to define mu of solid. Now, as I said that solid actually do not deform if you put it in the strain. So, if I put it like this if I rub my hand like this, I am not deforming. So, that is the first definition.

So, it means there is no viscosity in this, or in other way you can say that in finite viscosity (Refer Time: 10:22) huge resistance and any stress or any strain rate is not going to change. Anything ideally the mu is definition itself is pretty much critical, and if you want to use in the two-phase model in this form, you need to define the mu s, and there the problem starts and many people like the drag different researcher has different different relation.

Here also different researcher has given different relation and different kind of correlation for the mu s calculation. And most of those mu s calculation which has been said is actually the mu s is going to be the part of the 3-mu collision, mu kinetic and mu friction.

So, in that way the mu s has been breaking, that why you are going to see why the solid will see a resistance in their motion, because the mu is nothing but has been defined, it is a resistance in their motion. Now, the resistance in the motion can be because of for the solids, it can be because of the collision because they are having collision with one other particle their motion is waiting restricted. Then this kinetic energy because of that there is kind of motion is random and if their motion will be random there again they can hit the other particle, their motion can be restricted and definitely the friction will restrict the motion of the solid.

So, this is the 3 way the mu as said that the mu of solid is actually the summation of these 3 resistances. And now this resistances are actually being defined by the different researcher, and given the different correlation, that collisional shear stress has been given by this 4 by 5, alpha s rho s d s g 1 plus epsilon and this s into phi s theta s upon pi; where theta is nothing but the granular temperature. This is nothing but the granular temperature and we will discuss about that what is granular temperature.

Later on, this is restitution coefficient, again we will discuss about the restitution coefficient after sometime. This is radial distribution function, rho s is the density of this solid, alpha s is the fraction of the solid which is present, ds is the diameter of the solid. So, in this way it has been defined, but this is not the only correlation several correlation is available Lun et al, Syamlal, Gidaspow lot of correlation you will if you go and see the

books, you see the literature you will see all these names will be featured that different correlations are there by the different researcher.

But what is the notion if you see? The notion is how well the particles are flat packed, how close the particles are there that is why the alpha s is being taken into the account. Then your gravitational acceleration of the particle is being taken into the account, that how the particle is accelerating, how the particles are packed near about, that is why the radial distribution function has been there how they are readily distributed.

The restitution coefficient which says that after this the collision whether the collision is elastic or un elastic, elastic means they have they will hit each other and they will go back to the same place. Completely inelastic they will hit each other the velocity will be dead. So, they will not move or if the restitution coefficient value between the 0 to 1, if one means completely elastic 0, completely inelastic in between they will move certain distance.

You can find it out what will be the probability of the collision, and after each collision how far they will move, that will define the probability of the other collision, theta s is the granular temperature, it is being defined as a function of kinetic energy of the fluctuations it means how much kinetic energy it tells how fast it is moving or fluctuating from it is location. So, those all combined together define that what is the mean collision. So, these parameters remain same only the powers and the empirical coefficient values used to be changed for the different correlation.

Similarly, the kinetic viscosity has been defined again, if you will see that this is the function of granular temperature, this is the function of e s which is the restitution coefficient, this is function of g naught which is the radial distribution function and the volume fraction also. These are our empirically developed correlation based on several experiments this has been developed, and they found that how this coefficients or this the kinetic energy viscosity will be correlated, or how you can define the viscosity for the solids.

Similarly, the friction viscosity the frictional viscosity is also being defined, and that this very close to the collisional viscosity in the way is bulk viscosity has been defined

similarly, and that is also very close to the collisional viscosity. Only the power differences are there. So, overall the viscosities has been defined for the solid, and this viscosity is being used actually for the solids calculation of the solid viscosity all these individuals as being used, and then you calculate mu s by summing of all these 3. So, you get that mu s value, and you define all these 3.

Now, the problem is if you are using it for the solid, the accuracy of your prediction is going to depend that how accurately you are choosing these models. So, what you are doing? You are increasing more and more modeling part and modeling which is based on the coefficients are calculated based on some empirically developed correlations. So, drag was already there now we have introduced more models ok, more empirically developed models or more models. Now, that actually make the model use of the model little bit complicated or tricky, and one need to be very careful while using the two fluid model, you should understand that what are the closures which you are using.

What are the equations you are using, what is the limitation of each equation, and if you use this equation how your predictability will be there. And because there are lot of undefined function, if you get the solution your experimental validation becomes a must. If you are not validating experimentally, these models are not matured enough to give you the right solution particularly for multi-phase flow. So, what you need to do?

The experimental validation becomes must. So, all this simulation at least you need to experimentally validate to find that all the closures parameter all these equations or all this the closure equations which we have used, you have used correctly and has a validity for this the experimental law for the setup or you have used or for the condition for which you are operating.

And that validation should not be at a one label it should be a different label for different operating conditions, it should not be only volume fraction, it should not be only mean velocity, because everywhere the kinetic energy kind of a granular temperature is taking play a role, it should also be validated at the fluctuation label. We discuss how the granular temperature is being defined we have already discussed it earlier we will discuss the equation of the granular temperature completely.

But because everything is a function of granular temperature, you need to also validate it with the fluctuation velocity. So, if you are using two fluid model, you are using algebraic slip model, you are using lot of empirical correlation or assumed values, and because of that the experimental validation becomes very, very must very necessary, and it should not be just validated at the mean velocity level or mean condition level, it should be validated at mean level and at least at the fluctuation level. You should match the fluctuation velocities too or you should match the kinetic energy of the fluctuations.

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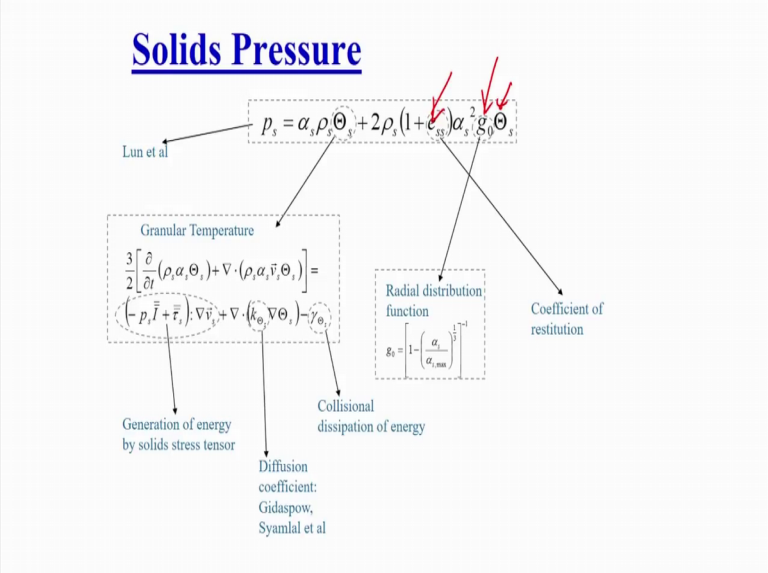

So, that is the way it has been defined similarly the solid pressure has been defined again if you will see, it is a function of theta s which is the granular temperature, restitution coefficient and radial distribution function. All this is the function of that and if you will see this is nothing but the way it has been defined is exactly same way as the pressure has been defined how the pressure is being defined in the kinetic theory of gases, that once the particle of molecules goes and hit the walls.

So, number of collisions per unit time and based on that we define that how much force will be acting on that wall per unit area, we calculate the pressure. Exactly same way it has been defined here that how many number of particles are available, what is their probability of hitting towards any wall or hitting towards the each other, in that way it has been defined here also solid pressure is also being defined. Over all this the solid

pressure is there this is again one of the equation which is given by Lun et al, but this is not the only equation several other equation is there, but all will be the function of granular temperature radial distribution function and the restitution coefficient.

Again, you have to validation becomes must, and validation in which you cannot you cannot only validate at mean level you have to also validate at fluctuation level. And this granular temperature will discuss that how it has been done, these kind of discuss all this the radial distribution function is being defined, in this way that this is 1 minus alpha s volume fraction at that place divided by the maximum volume fraction which is possible raised to the power 1 by 3 whole inverse.

So, that is the way the radial distribution function g naught has been defined.

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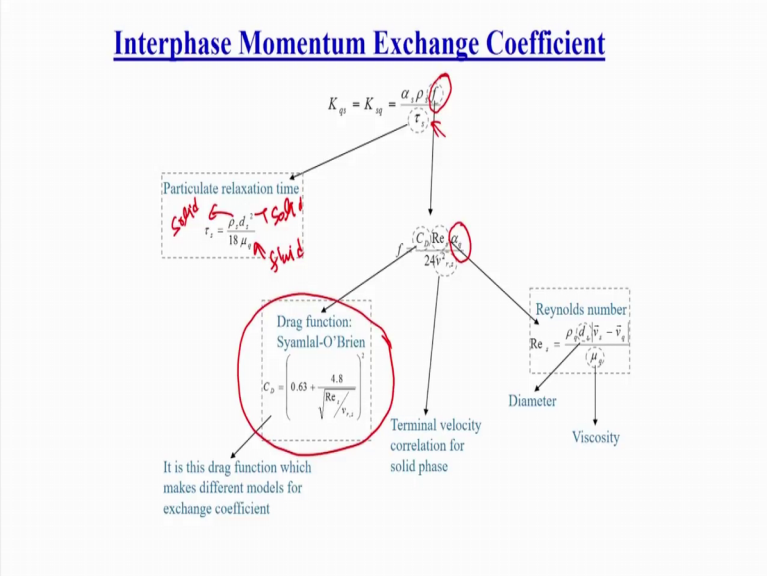

Now, we have used drag coefficient to solve it, we have discussed about the drag a lot during our previous discussion, but what we have done instead of writing in terms of the fd, we have written in terms of the Ks q and multiplied by the slip velocity. Now, if this is two way coupling the particle will the kind of particle will put a drag, on fluid will put a drag on particle the equation will be same.

So, Ks q will be equal to Kq s, it means both drag will be equal only the directions will be different, and that will be defined at alpha s rho into friction factor upon tau s, in that

way it will be defined. And then this tau s is nothing but the particle relaxation times we have already discussed that way earlier also, that once you write it in terms of the f the only change is we are writing in terms of the particle relaxation time also. So, tau s is being defined as rho dp square upon 18 mu, that we have already discussed. The mu will be for the continuous phase. D s will and rho will be for the discrete feature.

So, this is for discrete phase say solid, this will be for solid, and this will be for fluid. So, that is the way this particle relaxation time has been defined, f is the drag factor which is nothing but c d upon 24 upon re the only thing we have done, we are multiplied with the volume fraction because, we know that the fraction of the solid present is going to play a role. So, volume fraction we have multiplied of that phase, and then divided by v square.

Then again one of the typical drag correlations Syamlal, O'Brien; we have discussed several drag correlation, I am not going to use discuss all these things here again, but these are certain correlation you can use Syamlal, you can use Gidaspow, you can use Ergun, you can use Wen-Yu any correlation depending upon what is valid, which drag coefficient is valid in your case.

So, you can use these equations there. V square r is nothing but the terminal velocity of the solid it has been defined with that and terminal velocity of the solid can be calculated the way we have already learned that how to calculate the terminal velocity or settling velocity of the solid. So, that is what we can calculate here.

Reynolds number is always based on the slip velocity as I already discussed in the running the discussion of the drag, that once we talk about the drag Reynolds number we always define based on the slip velocity. We did it here also in the slip velocity, these diameter rho is the density of the fluid, mu is the density of the fluid, d is the diameter of the solid and it will be the slip velocity.

So, that is the way Reynolds number has been defined. And you can calculate the drag coefficient. So, you can calculate all these parameters, again in the drag what you need to do these are the correlation which are empirically developed. And because these are correlations which are empirically developed their validation is necessary their use is limited; their accuracy is limited and again your accuracy of the prediction is going to

depend on the accuracy of the models or the closure equations you are using to predict the flow.

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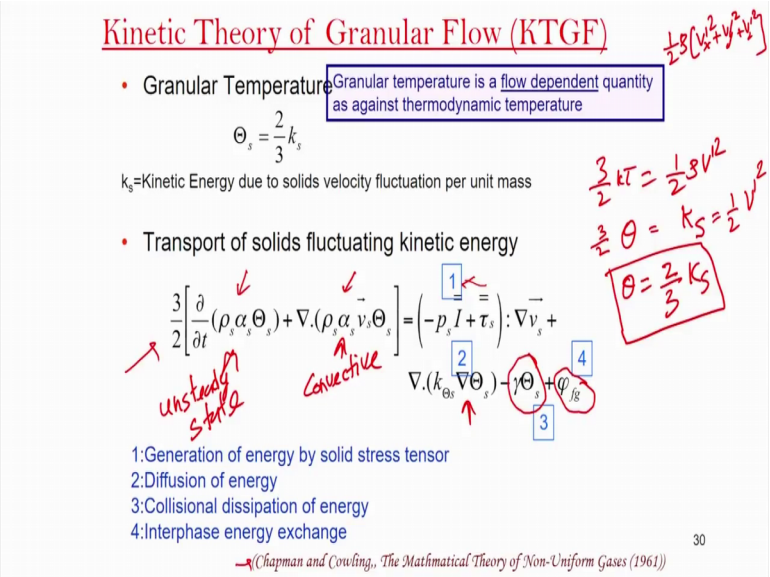

So, that is the way it has been defined granular temperature I have discussed a lot earlier also, that what is the granular temperature it is actually a quantity which is analogous to the thermodynamic temperature, and that comes because of the fluctuation motion, fluctuation motion of the solid, and that is being actually validated this will be equal to the kinetic energy of the solid is equivalent is being validated with the analogous temperature that is actually 3 by 2 k t and this tk is k and t, this will be equivalent to half rho v square and from there, you actually calculate that what will be your kinetic in your temperature or your grandeur temperature.

So, it means if you just remember 3 by 2 is equal to half rho v square, half rho v square, it means 3 by 2 kt is half rho v square, that is the way the molecular in the any gas kinetic theory of gases we use that t is the thermodynamic temperature k is the constants Boltzmann constant, and rho and v square is the particle velocities or particle fluctuating velocities. So, this half rho v square, we can write it in terms of the kinetic energy of the fluctuation if you are writing in terms of the fluctuation velocities, this is called Ks and actually it is being calculated as half rho v x prime square, plus v y prime square, plus v z

prime square. It means kinetic energy of fluctuation in the x direction fluctuation in the y direction fluctuation in the z direction all the kinetic energy.

You add together, and that is what is the k s is the total kinetic energy of the solids. Now, that we are representing with the solids, this is Ks half rho v square, now instead of mv square because it is a continuous fluid we are writing in terms of the rho in not in terms of the m; so, it will be per unit volume. So, that is what we are going to do, and we will do it into the terms of per unit mass. So, that the rho will go out and we will do it per unit mass and volume we will see that for each cell if you do it, then Ks will be defined as if you are writing per unit mass that will be half v prime square.

Once I came v prime square it is v x prime square plus v y prime square plus vz prime square. So, Ks is kinetic energy of the solid fluctuation per unit mass because we have divided it by rho. So, this will be becomes now per unit watts, if you multiply with the rho, it will be per unit volume if you divide by the rho it will be per unit mass. That is the way we define the kinetic energy of fluctuations this will be Ks. Now this is equivalent to the granular temperature, kt which is proportional to the kt a quantity we have given theta, which is analogous to the thermodynamic temperature.

So, if you write it 3 by 2 theta will be equal to ks. So, theta is nothing but 2 by 3 of Ks. That is the way we define, we use the fluctuation we calculate the fluctuation motion we calculate the motion fluctuation in all the three directions, and then the summit together multiply it by 2 by 3, we get the granular temperature quantity which is analogous to the thermodynamic temperature. We have already discussed about this in the previous classes that how that granular temperature is being done.

With the kinetic theory of granular flow, you can actually derive the transport of the solid, and then you can find that the transport equation for the solid fluctuation kinetic energy. And that transport equation for the solid fluctuation kinetic energy can be converted in terms of the granular temperature equation, I am not going in detail of this, but if you want you can go and see this discussion, this is a kind of derivation this is Chapman-Cowling book is there where this derivation is being given you can find it out that how this things has been derived.

So, you can do that derivation. So, this is if you do that, you will find that, this is actually the granular temperature equation is being very close to the momentum equation. The only thing is the momentum equation you take velocity, in the granular temperature you take the temperature and again please remember, that is nothing but the kinetic energy of fluctuation, it means it is nothing but the summation of fluctuation in all the 3 directions. So, that is the way it comes and then this equation if you want you can derive, we can also discuss over the forum if you have any question about this.

So, if you see this this is 3 by 2, dou by dou t, del rho alphas in to theta s. So, if you see this term then plus del dot rho alpha s vs into theta s. So, this is the local unsteady state term, this is the convective fluctuation term. So, this is un steady state this is the convective way how the flux whole fluctuation is being transferred from one location to another location that is the convective term. So, you can say convective acceleration term of the fluctuation, this is the unsteady state term, the first term is del ps into I and ps into I is the generation of energy by the solid stress tensor.

So, this is the first term which is being earned with all of the solid stress tensor, that how much energy is being kind of generated because of this. So, viscous dissipation because of that the solid stress term, how much energy is generated. So, that is the term is being given here. So, this is actually we are doing the complete energy balance. So, how much energy under steady state term is there, how much energy has been transported. So, total energy acceleration fluctuation energy, then how it is being consumed.

So, it can be because of the energy dissipation or generation how much generation will be there because of the viscous dissipation. So, this is this term is being given. Now the second term is actually going to talk about the energy diffusion. So, whatever energy has been transported, how it is diffusing out, and then the third term is actually the collision dissipation, that how much is the collisional dissipation of the solid is there. And the 4th term is the interface energy exchange.

So, how much energy is being exchanged between the interfaces. That is the way the kinetic theory of the granular flow is being defined. This is a big derivation, I am not doing in detail of this, because that is not the scope of this course we want to just show you the equation. So, that I can just tell you this or know that once we are solving the

kinetic theory of granular flow, momentum equation with the kinetic theory of granular flow what equation, you are solving then you are solving actually this equation.

So, what we do? For the gas solid flow in 2, fluid model equation or Euler equations once you solve for the gas solid flow, generally we solve the kinetic theory of granular flow; So, two fluid model or Euler equation with kinetic theory of granular flow. So, once you solve with the kinetic theory of granular flow, you actually solve this equation. And for theta s calculation you do 2 by 3 Ks, for the ps and tau I again you use the correlation which we have discussed earlier, just before one or two slides.

The way we saw. So now, if you solve the kinetic theory of granular flow the two-fluid model with the kinetic theory of granular flow what you are going to solve, you are going to solve now 5 equation, 2 equation for the continuity of individual phases; 2 for momentum of individual phases and one for the kinetic theory of the granular flow. So, 5 equation now you are going to solve together. I am not counting any other closure equation definitely you have to solve to get this solution.

But majorly you are solving this 5 equation. And that is the way the kinetic theory of granular flow has been defined and has been derivated, that this is the way it has come out. So, you solve along with all these equations, and that is called two fluid model or Euler approach. Now the major advantage of the approach again I am saying that, you are just solving even if you solve the kinetic theory of granular flow which is being used against a closure to model a mean motion of the solids to the fluctuation motion of the solid, it gives the correlation in that way.

So, what we are doing? If you solve the using drag, both way drag, it means you are using the drag in both the equation individually, like if you are using the drag in both the equation, let me go back quickly, let me go quickly back. So, if you are solving this equation drag equation, there in both the equation it means now you are using the we are coupling one fluid is affecting the motion of another, and solid or discrete phase is affecting the motion of the fluid phase is affecting the motion of the discrete phase, your solving two way coupling and you are joining it with the drag.

If you are solving the kt gf also, it means what? You are solving how the mean motion of the discrete phase or solid phase is correlated with the fluctuating motion of the solid phase, you are solving that coupling to, and if you want to solving in the fluid phase how the mean motion of the fluid phase is correlated with the mean with fluctuating motion of the fluid phase, you have to solve any turbulence model, like k epsilon model r ng model. So, all these things you have to or k mean model any of these models you have to use. And I am not going in detail of those turbulence models because that is not the scope of this course. That is more towards the turbulence course.

So, you can solve 3-way coupling, all the 3-way coupling. The only thing which we have not discussed in solving this is that, how the fluctuating motion of the solid is correlated with the fluctuating motion of the fluid. So, that equation we are not solving here, but all other 3 way coupling we can easily solve. What you need to do you have to just keep on adding the equation. So, if it is of only one way coupling or two way coupling your you have to just solve 4 equation, if you want a 3-way coupling you have to solve the kinetic theory of granular flow also equations so, it means 5 equation.

If you want that all the turbulence also, the turbulence for the continuous phase you have to solve one more equation say k epsilon equation or k omega equation for the continuous load. So, you will have to solve the 6 equations. I am not again telling you not talking about the drag closures and all they were definitely several closures equation you have to solve.

But majorly you are solving this 6 equation and that is the major advantage because, you are increasing you are reducing the amount of computational power which is required to get the solution. You are not doing any inherent assumptions like the slip velocity you are not using any algebraic equation and all, which is restricting the use of the ASM model, for very low volume fraction and volume with the co current flow all those assumptions we have removed.

And what we have found, we have found the equation which can be have a very wide applicability. So, that is the major advantage the applicability is very wide, you can use it for co current you can use it for counter current cross flow, for high volume fraction system for low volume fraction system anything you can use it. The only thing is you are

assuming discrete phase also as a continuous phase, you are assuming solid as interpenetrating continuum, and you are using several closure equations which are empirically developed and therefore, the accuracy of your model is limited to the accuracy of those closure equations which you are going to use or the constants in the closure equation which you are going to use.

And therefore, it requires serious validation. Experimental validation becomes must at least at the current state of the art whatever it is. Maybe a day will come when we will use the multi scale modeling approach the way I discussed that you define the drag from the Euler LaGrange you develop the close other closure equations from other equations, and then you use those equations which is developed based on the fundamental here and maybe then the validation requirement will not be that much serious.

But at current state or that validation is must in two fluid model, if you are using two fluid model equation, definitely you need to validate your simulation data. So, with this we have completed the other leg also of the two-fluid model or continuum model. Now, the next of modeling technique is Euler LaGrange model or we will say DPM model discrete phase model or discrete element model, now discrete element model is one of the model of the discrete phase.

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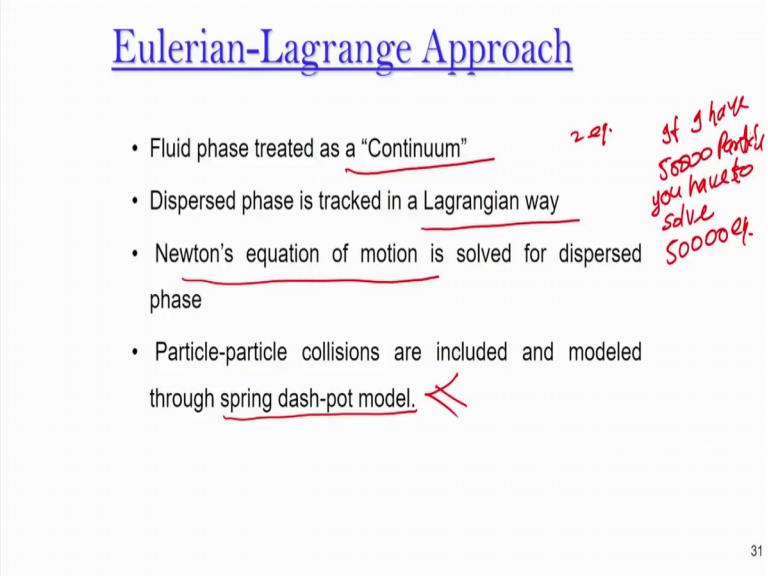

So, what the Euler LaGrange approach says. As I said that one phase is Euler continuum, another phase is LaGrange discrete. And you are solving continuous equation or continuum equation for the fluid phase, you are solving discrete phase equation you stand with the LaGrange way, what is the LaGrange way of tracking we have already discussed that in the module 3, that Lagrangain way of tracking means you are solving Newton's second law of motion for individual particles, we have done it for one particle.

Now, what you need to do if you are solving for a multi-phase say fluidized bed or bubble column, you have to solve the Newton's second law of motion for each bubble. And you have to also see that how they are interacting with each other. While solving the module phase 3 module 3 where we solve the interaction equations, model for acting we were not taking we said that, we are not solving it for when you are solving it for only one particle, and interaction between the two particles or two this bubbles is missing.

We are not solving that we are not solving the collisional thing. We are not solving the interaction that two particles are interacting also with each other. We have not thought that that is one particle which is moving or multiple particle moving, but they are not interacting with each other. That is a very ideal case.

In the real case of the reactor scale definitely the fluidized bed the particles will be interacting with each other. So, we have to also solve the interaction between the particles. So, that is what we do in the Euler LaGrange. For the fluid phase we call the continuum equation which is nothing but the momentum equation, we have discussed earlier for the dispersed phase tracking we do it in the LaGrange way, it means you solve the Newton's second law of motion for the discrete phase, that is what it is given here. Then particle collisions are included and model through a spring dashpot model.

Now, this is not necessary you can use any other collisional model also, but this is the most famous model which is a spring dashpot model. That is what is the Eulerian LaGrange approach is there it means what you are going to solve, you are going to solve one continuum equation. It mean one continuum equation for the fluid phase, it means one continuity one momentum equation for the fluid phase. This will be the two equations, here LaGrange way you are solving the Newton second law of motion for each particle, and that please mind it each particle.

It means, suppose, if I have 50,000 particle, then you will have to solve 50,000 equation. and that enormously increase your computational line, why? Because you are now solving huge number of equations, even with the 3-way coupling you are solving only 6, now you are solving even without having any coupling any collisional equation, I have not included that, you have to solve say if you have 50,000 particle 50,002. And then on top of that we have solved the collisional equations so that you can model that how the particles are having collision.

And based on the collisional equation, we will discuss that it has been further divided in the different classes. So, that is called Euler LaGrange model, and in the approach definitely it is more accurate, because you are solving very fundamental equations without having any assumption that the solid is becomes continuum, they are interpenetrating we are neglected all those assumptions. So, it is more towards the real model or real physics, but the computational time requirement is enormous in this case. And that is the major drawback major advantages your move towards the reality.

Definitely the prediction accuracies are much better, but still we will discuss we use lot of empirical correlation and therefore, experimental validation again is must in this case also.

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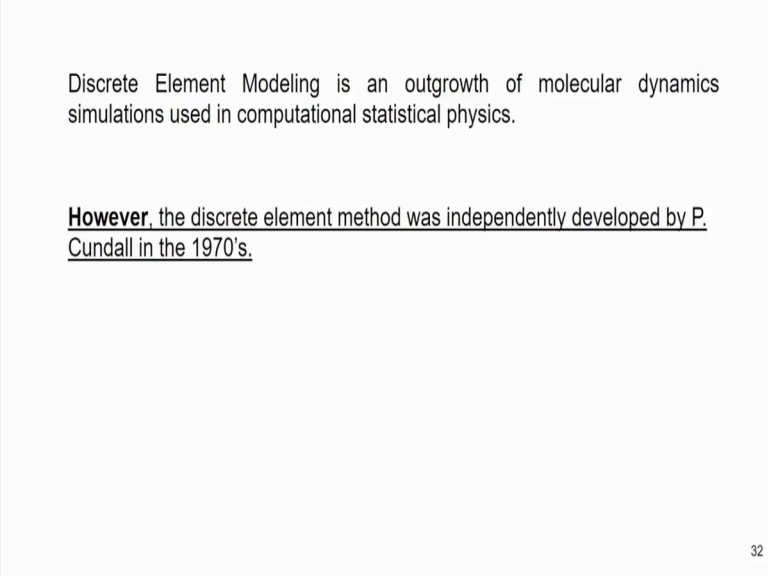

So, discrete element model actually how it has been developed, it has been developed as an outgrowth of a molecular dynamics simulation used in computational statistics physics. So, it comes actually with the molecular dynamics simulation, that how the molecules are moving together how they are interacting with each other.

That is the way discrete element model has been developed. Later on, in the Cundall and Strack, what they have done? They have actually clubbed this discrete element model, with the fluid phase, the discrete element model originally developed is only for the granular phase there was no fluid involved they clubbed it with the fluid phase, and that is become Euler LaGrange model, that how the flow both the continuous place and the discrete phase are moving together. And he has developed it independently not as a molecular dynamic suggest.

But independently developed in 1970's that how the dm model will be working with the fluid phase. So, that is the history of the fluid this model, some people get confused that it is very close to the molecular simulation. Yes, it is really close to molecular simulation, but then the fluid part we will have to add here. And definitely the collisional way we model collision is little bit different whatever you do in the molecular dynamics.

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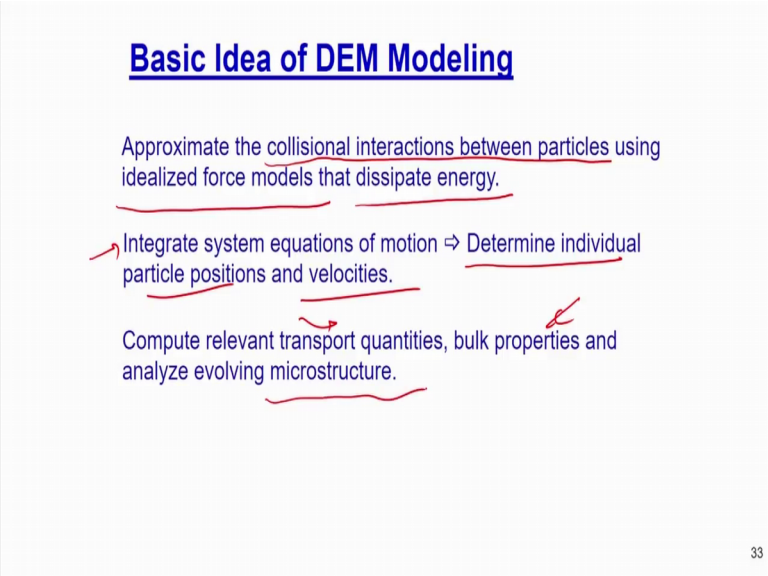

So, what is the basic idea of the DEM simulation? That has been given here, that approximate the collisional interactions between the particles using idealized force

model that dissipate energy. And we will come that why the experimental this things is needed, and why the DEM is still not matured enough to give the production on it is own. So, what you need to first do? We approximate collisional interactions, that how the particles will interact with each other by idolizing the force field we say that this will be the force field around the particle, and how the energy will dissipate because of the collisional collision.

We try to have a approximate this and we find the collisional interactions. Then we integrate the equation of motion with it is the first we see that how the collisional interactions will be there, then we integrate the equation system equation of motion, that equation of motion we actually add, now even to do the equation of motion it determines the individual position of the particle And the velocity, once you add the equation of motion means Newton's second law of motion once you are solving. It will give you the position, and the velocity as we have done in the particle tracking earlier.

Then you calculate the relevant transport quantities, bulk properties and analyze the microstructure. So, that is the basic DEM formulation. It means first what you do? You take a distribution of the solids; you will try to find it out that what are the interaction forces is going to be there what are the attraction model which you need to incorporate.

How the energy dissipation will take place, then you add Newton's second law of motion or equation of motion into it, and try to find it out how the particle position, and velocity is changing with the time, and with the location. And then based on that once you know this you can calculate the transport quantities like you can calculate this velocity. You can calculate your kind of fluctuation, you can calculate your diffusion all those quantities the transport quantities.

The bulk properties all those things you can calculate, because you are tracking the individual motion of the discrete phase if any structures are forming like if suppose some of the group of the particle is coming together, you can get that if the particle Are getting agglomerate, you can get that although the structures you can easily get. So, that is the basic idea of the DEM modeling in which there is no fluid in wall.

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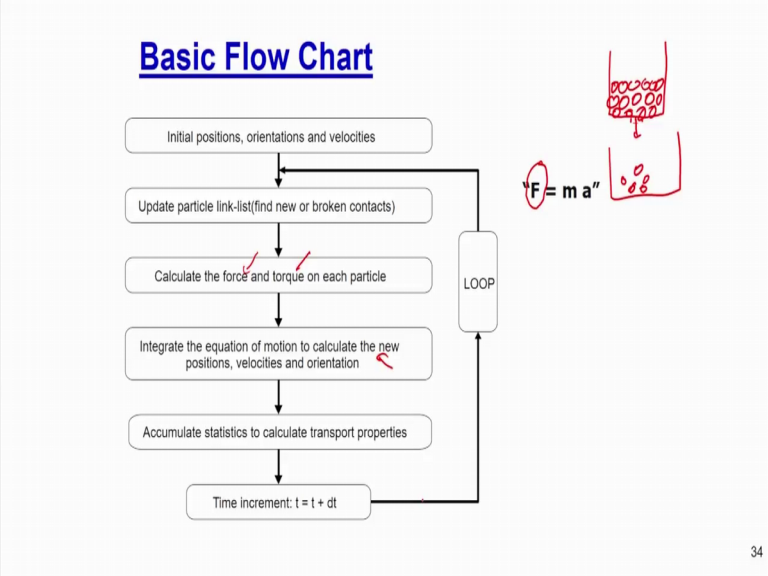

So, the basic flow chart of the DEM modeling. We have already discussed that is why I am going quicker, because most of the things whatever we have done we have already discussed, said while discussing the tracking the path of a single particle. Now, what we are going here? We are doing we are solving that equation along with the fluid phase equation now you are going to solve. So, we are going to kind of see that how the particle is affecting the motion of the fluid is affecting the motion of the particle And how the particle collision is affecting the motion of each other.

So, again we are solving the 3-way coupling. In this way in that way if you see this the initial position and orientation of the velocity, first what we do we define a geometry in the basic flow chart if I discuss. We define that what is the geometry of my geometry, how the particle is initially fitted. So, suppose this is a pad bed we define that how the particle has been placed inside the column of interest. Once it is done, what we do? We update the particle link list and find a new broken context.

Now, what we do suppose if this is say a granular flow, where we are saying that this is my initial position of the particle, and the particle is falling down and filling in a time. At time t equal to 0, I will give a position of the particle. So, earlier all the particle was there suppose in a hopper. At t equal to 1 what I did? I suppose, I put a small plate and I opened that opening at time t equal to 0. So, what will happen? The particle will start

falling and they are filling in this bottom tank, what will happen? Because this moved the particle the position will be changed. They will be broken the contacts will be broken.

And then what you do because the context has been broken the particle will start moving. Now the particle is start moving you calculate the force and torque acting on each particle. How you can calculate force? You know the mass of the particle you know the velocity dv by dt, you calculate the acceleration, you calculate the force acting on the particle. Once you know the forces, you can also calculate the toque.

So, you calculate the force and torque on the particle, then what you do? You integrate the motion of the motion of Newton's second law of motion, and then you calculate that what is the position of the particle.

So, we know that how the particle has been broken. Now they start moving we use the second law of motion, Newton's second law of motion and we try to find it out what will be the next position of the particle. So, you get the next position of the particle we get the velocity of the particle, even we can get the orientation of the particle ok. That if suppose this is not a spherical particle this is a particle which has certain l by d ratio say 2. You can also get that how it will be oriented, because you can calculate the torque based on the torque you can find it out what is the alignment of the particle.

So, you can get that then again what you do you accumulate the statistics and calculate the transport properties like velocity fluctuations force field all those things you calculate, and then what you do you increment it to the next time. So, earlier we were doing say t equal to 0 plus delta t you again do delta t plus delta t it means 2 delta t you actually do that and then again you start you update the particle position. You again calculate the forces, you again include the integrate the equations of motion and calculate the properties like position and velocity then again you calculate the transport properties and again update it.

So, in this way you keep on doing this calculation, and this is the basic flow chart and you find that how the particles are moving, or dumping into the next part into the next reservoir. That way you can do this discrete particle simulation DEM simulation to see that how the particle is moving. So, that is the flow chart of the DEM simulation.

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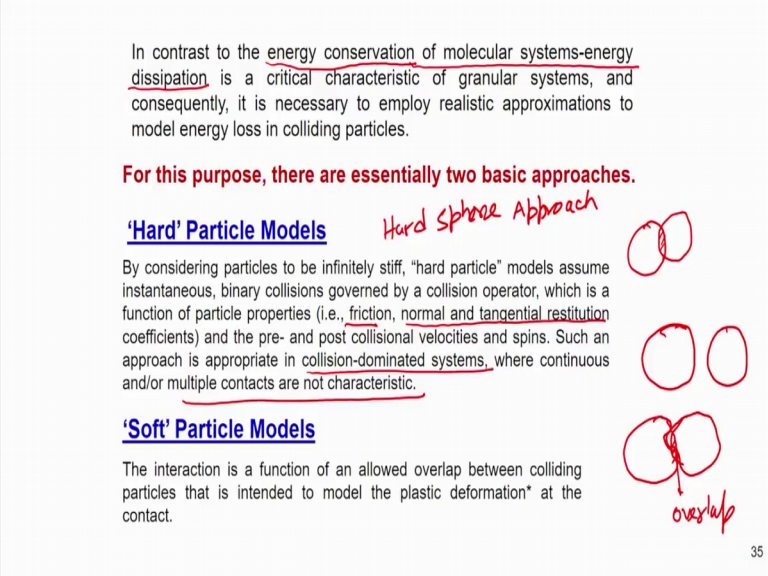

Now, what we do here, actually if you see that this is actually that we are trying to do the energy conservation.

So, what we will solve? We are trying to solve the energy conservation of molecular system energy, and instead of the energy dissipation. So, in the molecular dynamics what we do we solve the energy conservation for the molecular system energy and with energy dissipation. We say that how the energy is being calculated; while in the granule at temperature granular flow what we do we calculate the energy dissipation.

So, that is the difference in the molecular dynamics simulation and the DEM simulation. In molecular dynamics we solve the energy conservation equation for the system, and here we solve the energy dissipation; which is becomes a very critical characteristics of the granular flow, that how the energy is being dissipated. And then from there we actually find that the realistic of this approximation we do and we found that how the energy dissipation is going through by the collision of the particles.

So, we calculate the energy dissipation energy dissipation we say that how much energy will be lost, because of some realistic approximation we use some correlations we will discuss about the correlation later, we use some correlation to see that how this energy is actually dissipating. And that dissipation generally occurs because of the particle collision, and therefore, the particle collision solution solving is the most critical part of

any DEM simulation. And to do that, what we need to do? We have to have some model of some basic or kind of realistic approximation we need to do which can solve the particle collisional equation. And that becomes a heart of any dm simulation, that how you are modeling the particle collisional equation for collision will be heavier.

And to model that these two-basic approach has been used in literature one is hard sphere approach one is softest sphere approach. So, again I am coming back that how though I said that very people confused that this is very close to the molecular dynamics simulation, yes, it is close to the molecular dynamics simulation. If you are just solving the granular phase flow, you are not solving the fluid phase at all. Then it is very close, but the molecular simulation the approach is energy conservation the model.

Here we model the energy dissipation and we try to find it out that how the energy dissipation is taking place through the collision of the particles. And based on the collision how you are modeling the collision the DEM approach has been further divided in two part. One is the hard particles model or we say it hard sphere approach some book also follow it. I say particle because the particle can be of any shape, but some people say is hardest sphere and softest sphere approach or you can say hardest sphere model and softest sphere model.

In the hardest sphere model what we do? We actually consider the particle to be infinitely stiff it means they are very stiff they are very hard particles. Say, you think about two iron particles which are very, very hard very stiff and the model assuming instantaneous and binary collisions. So, we assume that there is two particles which are very hard, very stiff they are not going to deform at any cost.

They will hit other each other instantaneous hitting will be there, and the collision will be binary. So, that is the way we model the collisional equation by using some operator collisional operator and that collisional operator will be the function of friction normal and tangential restitution coefficients and pre and post collisional velocity and a spins, even the mass of the particles.

So, that is the hardest sphere model has been used we will discuss it then you will understand it in more detail such an approach is approximately collisional dominating

system, where the continuous and multiple contexts are not the characteristics. So, that is the major limitation that the continuous collision or multiple contexts at the same time should not be the characteristic of the flow. So, what it says? It says that suppose what is how it will be going on, I have suppose two spheres of made of say iron ore ss.

They are various tests they have very hard particles it means they are not going to deform, they are moving together they will be moving together they will be interacting if they will interacting they will hit each other. Now once they will hit each other, what will happen? The collisional parameters will be governed or will be found by using first that what is the friction; between the particles which is acting once they are interacting with each other in presence of some fluid or something.

Then what are their normal and continual restitution coefficient, now what is the restitutional coefficient I said that this is e value, if the collusion is completely elastic the value is going to be one, if collisional is completely inelastic it means after collision the velocity becomes 0, the value will be going to 0, or if this is between the between the elastic and inelastic this value will be equal to between 0 and 1, it means, this co elastic the value will be between 0 and 1 bar.

So, you model this you model see the property, now this things depends on the properties, like this properties particle properties what is the non-friction normal and tangential restitution coefficient is also depends that, what is the velocity at which they were approaching towards each other before the collision what is the mass of the particles which you are interacting with each other before the collision if suppose there is no mass change, then before the collision and after the collision mass will going to be the same.

And then what is the velocity of the system after the collision? That is the way the collisional parameters in hard sphere model is being developed a hard particle model is being developed. And generally, these models are used for the flow condition there the collisional dominating flow is there, but the continuous and multiple interactions are not the characteristics of the system. It means, it should not be multi particle collision, it should not be multi particle collision at the same time, it should not be that phase this model is being used. That is called hard sphere model.

The use of this model because of this limitation that it should not be the collisional dominating flow, or the context should not be a kind of context dominating flow, this limits the application of hard sphere in most of the chemical engineering equipment of chemical engineering reactor which we use like fluidized bed and all. And most of the time what we use is called soft particle model. So, in the soft particle model what we do? We allow as the name suggests the particle is soft.

Now, we are not assuming that infinite stiff particle, it is very hard particle you are not assuming that, we are assuming that particles are soft let us say a rubber ball, which can deform little bit it means if suppose two rubber ball are interacting with each other, what will happen like this is a step body. If I am interacting there is no deformation it is not like I am going inside here, but if two rubber ball will be there what they will do? They will actually change the shape and they will allow the overlap. It means one ball say it was this like this before the collision.

During the collision, it may be like this, it have a small overlap because of this. So, what we can do? We can assume this is a spherical we can assume this is a physical and I can say that this is small overlap is possible. This is called overlap. This is the particle Again, and this is after the collision the assume both the particle two means and we say that, a small deformation is being accommodated overlap is being given. So, that is the major advantage of this that the soft particle Also it can be used, and you assume that you model this part is that there is a scope is available for the particle deformation.

And then, use the particle deformation theory to model the contacting in between. So, that is the softest fear model again we will discuss. Now, that what how you model the collision in the hard particle, and you model the collision in the soft particle. But this is the basic approach of the hardest sphere model and the softest sphere model. And the hardest sphere model is basically being used where the multiple characteristics multiple contexts are not the characteristics of the flow. If that is not their hardest sphere particle model can also be used soft sphere model is have a widely accepted, it can be used for any system.

Now, what we need to do we need to model the contacting. As we said that in DEM the contacting is the most important part. And that is what it is kind of differentiating the dm

simulation with the LaGrange track which we have done earlier. Where the single particle was removed, and we have assumed that the single particle motion is not getting the one particle motion is not getting effect between the other particle, and they are not contacting with each other. So, even there multiple particle flowing there in the LaGrange interact whatever we solved earlier, they are not interacting with each other.

But here, we assume in DEM that they are interacting with each other, the flow is collisional dominating, we model the collision, that is what we say that we model we first assume the force field if you go for the dm flow chart. We first assume the flow field force field, we model the contacting, and then we impose the recursion of motion to find the new particle position and velocity, and again we calculate the transport properties again we model the flow through collisions.

So, that is the way we solve it. So, the collisional equations is modeled properly need to be modeled properly, and then based on that collisional equation model, we define the approach DEM model in two part.

One is the hard particles model, another one is the soft particle model. And now what we are going to do? We are going to discuss what is hard particle And what is the soft particle.

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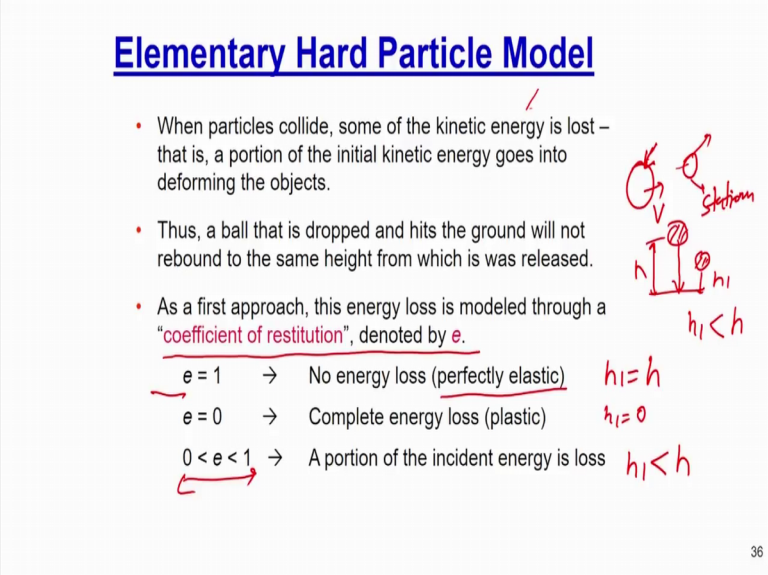

Again, I am not going in detail of this, because if I cover all the things in great detail we will take huge time, you can go through these equations there are several papers available on this, you can go and read the Cundall and Strack paper you can read the papers from DEM papers mostly coming from the Kuipers group, Susy group, many other people group which is being there.

If you have any problem we can discuss over the forum. What is the elementary of the heart particle model? So, what we have said that the two infinitely stiff particles are having collision with each other. When a particle collide, some of the kinetic energy is lost that is proportional to the initial kinetic energy goes into the deforming object. What is happening to particles is having collision? Because one particle and two particle, let us assume one particle is stationary this particle say is stationary, and this particle is moving with a velocity v. Once they will have in the collision, then what will happen? The kinetic energy of this particle will be lost; the kinetic energy of this particle will be lost.

Because it was say moving with the velocity v the kinetic energy will be lost, and how much it will be lost? That will depend that it will transfer some of it is kinetic energy to this and this particle will start moving how much loss in the kinetic energy will be there. That will be actually equal to the deforming the object, that how much object has been deformed how much objects has been moved from that location, how much it has been deformed opposed from that location. That is the first elementary that when a particle collision take place we say that someone will lose it is kinetic energy, and that lose in the kinetic energy will be proportional to the deformation of the object.

Then it means what? If a ball dropped and hits the ground will not rebound to the same height from which it was released. Till the this is not completely elastic. It means suppose this is a ground, we have already did that, there is a ball, if it goes and hit the ground what will happen? The ball will try to come up. If it is a very rigid particles what will happen? Say it started with a height h, it will achieve a new height which will be say h 1, and h 1 will always be less than h. It will not able to achieve the same height ok.

Because of some loss in the energy to the surface, and that loss in the energy what it will do it will try to deform this surface. What we do? We model it we model the collision with the coefficient of restitution. The first approach is there that model the energy loss

by modeling the coefficient of restitution which is denoted by a, and e is equal to 1; means, perfectly elastic no energy loss. No energy loss means h 1 will be equal to h e equal to 0 complete elastic complete plastic flow. It means, complete energy loss will be there. It means, the actual value will be actually 0, it will not move anywhere it will just loss all it is energy to the surface and it will stay there.

And e between 0 and 1, it means what? That h 1 will be less than h it will lose some of it is energy it will never gain that energy more than that, and it will achieve a height which will be smaller than that. The hardest sphere model we use this approach, we model the collision by the coefficient of restitution through the coefficient of restitution. We calculate the value of e, how the is being calculated? Again, you have might have done it in your some undergraduate physics courses.

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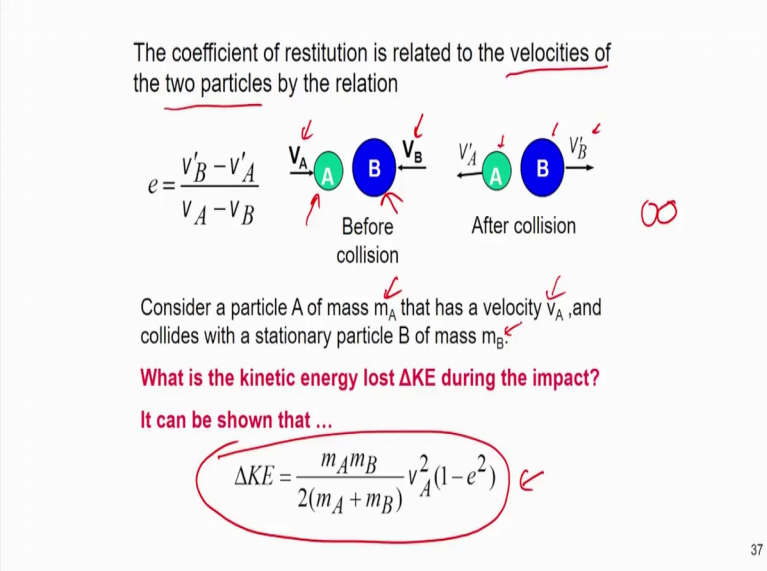

But let me again revise it. So, what we do? The coefficient of correlation is related to the velocity of the two particles which is being hitting each other. And let me tell you it is not only the velocity it is also the mass of the particle. We assume to the velocity, if suppose both the particles are made of the same material definitely the mind the same size mass of the particle is going to be the same. If they are not of the same material, this will be different actually. That before there is two particle A and particle B, before the

collision they were at a certain distance, particle A was moving with the v A particle B was moving with a velocity v, v and they are having a collision.

What will happen? Once they will have a collision, they will hit each other say they are hitting normally, as I said my hand is saying that after hitting normally they will go back to back they will change their direction they will go back to back. And suppose if I assume that the mass of the particle is not changing, because there is no deformation of the particle. So, mass of the particle is not changing, velocity is v A prime for the a. Velocity is v B prime for B after the collision then the restitution coefficient is defined as v B prime minus v A prime upon v A minus v B.

Relative velocity after the collision divided by relative velocity before the collision, and that is what is the restitution coefficient. That is the ratio is called the restitution vision, before collision what was the velocity after collision what was the velocity that relative velocity is being defined with the restitution coefficient e, if suppose one particle is a stationary, say B particle is stationary B, B value will be 0. That way it is being done.

Now, if you see the restitution coefficient value, it is it in cm minus v B and v B minus v A because of the energy transfer. So, that restitution coefficient values does not go in negative, it will always be the positive. That is there and if suppose you consider the mass of the particles is also different you want to add the mass of the particle here, then and you want to find it out that how much total loss in kinetic energy will take place. So, let us assume the mass of the particle A is m A velocity is g A, mass of the particle is m B and let us assume that it is velocity is 0, it is a constant to simplify it you can again derive it for the this equation for the particle mv is also moving.

What is the kinetic energy loss? Delta KE during the impact so, if they will help. So, suppose a particle which is moving with a velocity v A, mass is m A, it is hitting a particle And of mass B mv, but the particle is a stationary. So, what will happen? It will lost it is kinetic energy, how much lost in kinetic energy is there I think this has been derived, when your solid mechanics courses, you will get that it says m A plus m m A into m B upon twice and may plus m B, v A square into 1 minus c square you can revise this you can find this formula.

If you are not able to get it we can derive which it in detail. We can discuss it over the forum many things, I am leaving over the forum the major region is, these are something which we cannot cover in detail in one class or two class, it will require enormous time. So, these are the basics which you have already done in your physics courses or in your mechanics courses, you can revise then, if there is any problem we can discuss over the forum. So, that is the way it is being calculated and kinetic energy loss you can calculate.

Let how much loss in the kinetic energy will be there. That is the hardest sphere model or hard particle model approach is being used which is being used in the DEM simulation, if you are doing that, your collision is being modeled this way, you model there is two you calculate the restitution coefficient you calculate the kinetic energy loss. And from there calculate that how the velocity loss will be there, and how the pollination of the particle will be changing.

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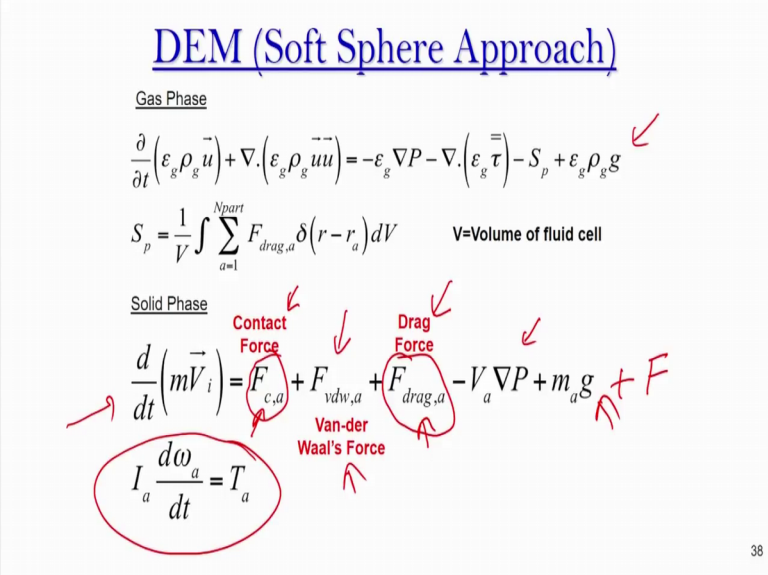

In the first sphere field model, what we do? What we actually solve the equation for the gas phase; you solve the equation for the solid phase. So now, we are solving about the Euler LaGrange model, in the Euler LaGrange DEM model with the soft sphere approach what we do? We solve first the equation for the gas phase we solve the continuity equation, we solve the momentum equation for the gas phase here, and the

continuity equation or momentum equation is same as whatever we solve for the normal cases this is the equation which we have already discussed.

And then we solve in the Newton's second law of motion for tracking the velocity of individual phase individual particle. So, this is the equation you are already familiar, we have solved this equation for the LaGrange tracking, the total force m d by dt m into v is equal to acting on the particle is equal to the total force acting on the particle. So, rate of change of momentum is equal to the total force acting on the particle.

Now, what are the total force acting on the particle? Earlier we have done drag, gravity, buoyancy or any other body forces, say electrical forces or magnetic forces. Now what we do? We are saying that their particle can affect they can have a collision and their motion can be get affected with each other. So, definitely we are saying that the rate of change of momentum is definitely going to equivalent to the drag, it will be the body force, it will be the pressure force that what is the pressure force it is there a pressure gradient in which the body has been kept because now the fluid is moving.

So, what is the pressure gradient the body has been kept. That is also going to see that how the body forces will change, but now what we are adding? We are adding the contact forces that contact forces is F ca we are adding the van der Waal forces which will be acting between the particle, we add these two forces extra compared to what the LaGrange track we were solving. We added the velocity gradient or the pressure gradient field in which the solid has been also added.

But this is the two-major thing which we have added, and these 4 solve the annular motion, we solve the annular equation IA is equal to d omega by dt equal to ta. Again, the rate of change of angular momentum is equal to the force acting or regular force acting that is nothing but equal to the torque.

So, you can calculate the torque, you can solve even the spin of the particles. So, that is the way we are solving the equations for this. Now, what is needed? You needed the contact forces F c, you needed the drag force, you needed the pressure gradient and you needed the van der Waal forces. Now, van der Waal forces, I hope everyone knows how

to calculate the van der Waal forces, you can calculate the van der Waal forces, drag is pretty much same which is going to affect the motion of the fluid also.

So, drag equations are going to be the same; which we have already discussed how to use the drag we have already solved the problem. You can add any body force also if you want say you can add one more force any other force which is acting here. Gravitational force we already know how to model the only thing is in the shortest year how to model the contact forces.

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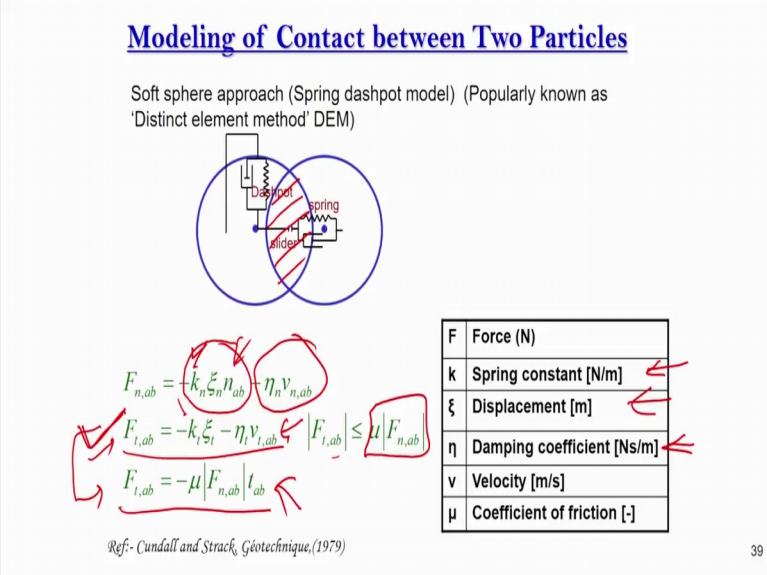

Now as I said in the softest sphere, the two soft particles are being hitting each other, and overlap is allowed it means deformation of the particles is allowed.

What will happen? Once the particles say is having collision, and this is again the Cundall and Strack paper in 1979 from where this approach has been taken, that if the two particles are having collision, what we do? We model the collision by using the spring dashpot model, it means what? If suppose the particle are hitting each other like this, we allow certain overlap we are allowing certain overlaps here. And we are saying that, this one spring and one dashpot is being placed in both normal and tangential direction.

So, this is can be hit it in this way, this can hit it in this way in the tangential direction in the normal direction. So, we are assuming one spring, and one dashpot in the normal direction and tangential direction to model this collision and that is why it is also called a spring dashpot model. Now, why there spring and dashpot model we are using, a spring coefficient will tell me about the restitution coefficient values it means hide the spring coefficient better the elasticity lower the spring coefficient lower the elasticity.

So, it means the spring coefficient values are high, it will go back to the same distance, it is low it will not go back to the same distance. The damping is being used because, it will lost some energy, and this loss in the energy will be model through the damping. So, again we are using the same approach, that if I throw a particle on the solid surface it will not able to achieve the same place, because there will be some loss in the energy.

So, the loss in the energy is being modeled in the damping way, and that damping is being caused mainly because of the fluid which is being placed in between and also particle surface also. That is the way the Cundall and Strack with soft sphere approach collisional things are modeled.

Now, you can see this equation actually if you see this is the spring coefficient equation, typical spring coefficient equation in the normal direction, only the damping factor has been added. That how much it is being going to damp the k is the spring coefficient value epsilon is the displacement. So, if you remember your basic spring coefficient a spring force that is f equal to minus k s. So, that is the spring coefficient value, eta is the damping coefficient, because again as I said that it will damp something it will lose the energy. So, that is why we multiply with the eta in this.

And then you also substrate that how much is the velocity and the damping coefficient is there before after moving. So, that is the way you calculate the contact forces in the normal direction. Similarly, you calculate the contact forces in the tangential direction again if you see this is nothing but the same thing whatever I have written; it is the k zeta t into eta.

Only the damping coefficient in the tangential we have removed because now it is moving it in this way and then to calculate that damping coefficient actually in the

tangential direction two equations are being used. One is being calculated it into the first equation is like this way, second equation is you take the normal forces, you take is the coefficient of the friction into the account multiply the normal forces with the coefficient of the friction, and then you find that what is the F t.

And then if you see that whatever the ft calculated by this way, if the F tab, whatever you have calculated is less than the mu times of F t. Mu times of f and it means this, then you use this equation if it is greater than that you use this equation. It means what we are saying that the tangential collision is going to be lower than the mu times of the normal collision. And mu is the coefficient of friction mu times of this. If it is lower or equal then you use this equation.

If this equation is predicting a value which is lower or equal then mu times of F and yb. You use this equation, if not you use this equation. So, by this way you model the total contact forces, van der Waal forces we know drag we know, and we solve the whole equation for the particle movement, and we couple it with the fluid movement, fluid velocity with the continuity and the momentum equation for the fluid and we found that how the phases are interacting with each other.

How the particles are having collision with each other, and how the collision is changing their motion, how the fluid is changing the motion of the particle all the things you can solve. But the problem again what I am saying again with this approach, this is very close to the physics very accurate towards the real physics. But the problem is the computational time. So, if you just assume 50,000 particles is a very small fluidized bed. Very, very small fluidized bed will have a 50,000 particles, you want to use DEM simulation you have to solve 25, 50,000 equations for your you Newton second law of motion equations. For that 50,000 equation you have to calculate the collisional parameter just spring dashpot models, and then you have to solve two equations other.

So, you have to solve enormous number of equations, and that will take huge time huge computational time to model. Sometimes even in the current era, if you want to model 50,000 particles with a very high accuracy, it will take days to complete that simulation. So, that is the major limitation of DEM simulation, but it is very close to the real-world problem to the real physics. And that is why there is a scope that you can develop even

the collision model from this place, and if we use the multiple kind of modeling approach, this collisional model which has been developed or validated at this scale can be used in the Euler simulation for having better prediction.

So, that is the one way but again DEM model, though it is very close to the physics we are using the basic 6 models. But we are solving actually we have to find the value of k t k d value k n value we have to find the damping coefficient values; these values can be calculated through the Young's modulus experiment there are several correlations are there to calculate all this. But sometimes we use some values, and because of that experimental validation is needed.

Again, you are using drag force, because you are using drag force and drag force is actually being modeled with lot of empirical correlations. Again, if you are using those empirical correlation Gidaspow, Syamlal, Wen-Yu anything, again you need experimental validation. So, even at the current state of the art DEM cannot be said that it is 100 percent correct. You need to validate it with the experimental data to find the validity or accuracy of the DEM simulations. This is the typical DEM simulation fluidized bed simulations.

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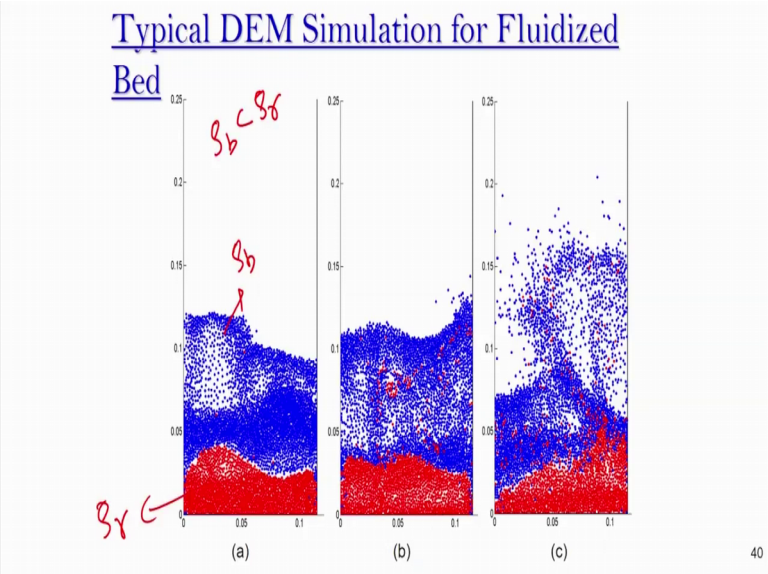

We will discuss the fluidized bed we will again come back to the same, but if you see this is the rate two different particles, the smaller particle smaller density particle is blue

colored, this is say density rho b, this is rho d, rho r and rho b is having the lower density then rho r. So, blue particle is smaller color a smaller density, red particle is are heavier densities, we are fluidizing once we are fluidizing this what is happening the particles are moving blue particles are definitely moving is on the top of the bed because they are lighter. And they are moving faster and we are seeing slowly how the red particle is diffusing and they are moving with each other.

So, we are solving this the whole DEM simulation, we are tracking the motion of all the particles, we are solving the interactions between the blue particles, interaction between the blue particles and the red particles, interaction between the red particles, and interaction of these particles with the fluid we are solving all this together to get this fluid behavior of the fluidized bed. But the problem is to solve this it is computationally very expensive and that is why most of the time we limit ourselves to a very small dimensions of the bed.

So, we call it as a sub bed scale model, we can model it for the very smaller bed dimensions. So, with this our modeling part is over if I will try to conclude some of the model I have not discussed, then I can say the multiphase modeling in divided in two parts. One is for the gas liquid flow; one is for the gas solid flows.

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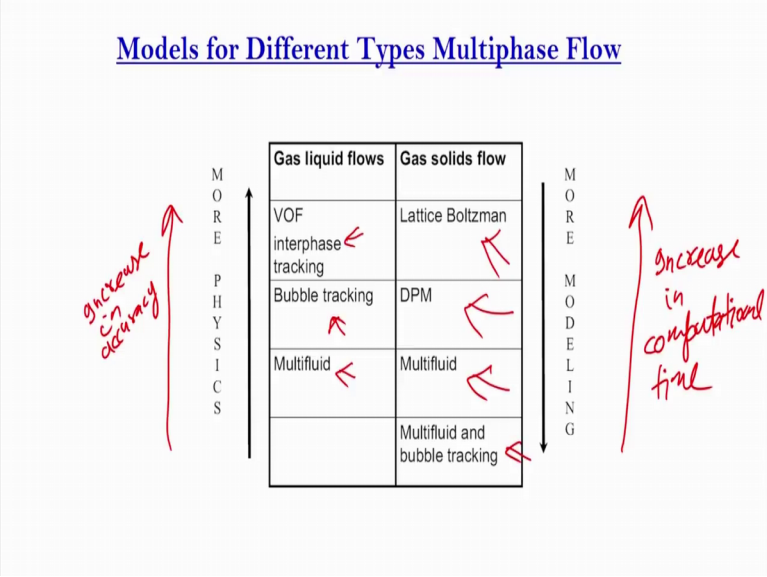

So, in the gas solid flows if you want for the more modeling or more physics, then if you go from the bottom to top, you will be coming very close to the physics, it means 2 fluid model or a multi fluid model will have more modeling, as I am going from the top to bottom it means we are using more modeling because we are using more and more assumptions.

Once you move from the bottom to the top you use more physics, I have not discussed the viewing of modeling that is another class of model, where you actually do the interface tracking to see that how the bubble is moving, or liquid droplet or bubble is moving inside. And not discuss that, but if you go through this, you can solve the multi fluid model, you can solve the bubble tracking model you track the bubbles, and you can solve the vof model.

So, once you go from bottom to the top, your physics is increased, but computational time is also increased, because you are using less model. Your computational time will be enormous, and those models will be restricted to the sub grade scale. You cannot model the whole bubble column by using the vof it is ruled out. You can model a small section. And similarly, you come from the top to the bar this in the gas solid flow. I will say that it is a multi-fluid model with the bubble tracking or you do that. You use the two-fluid model, you use the DPM model, you go to the lattice Boltzmann model.

Again, lattice Boltzmann model, I have not discussed because it is too mathematical and it is very close towards the molecular simulations. I just limited myself in the two voiced popular approach; which has being popularly used in the chemical engineering domain; that is, fluid model medical model or two fluid model and DPM. Again, you go from the bottom to the top, you go for more physics, top to the bottom more modeling.

So, definitely the computational time increases, this is computation increase in computational time. So, if you go there, the increase in the computational time , but increase in the accuracy too. Based upon whatever the flow field you want to use, whatever the system you have, how much accurate system accurately you want to predict your flow, how much kind of you can compromise with the accuracy what label degree of accuracy you need, how much computationally time you can devote, how much of time you can wait for your simulation results, you can choose one of the models.

And we have discussed that what is the limitation of each model, what equation you solve in each model, and what is the accuracy you can think. But as of now none of the model is. So, accurate that none of the experimental validation is needed. The experimental validation is must. The only thing is if you are using the two-fluid model definitely the balance the kind of the experimental validations should not be only at the mean label you should touch to the fluctuation velocities too.

Ideally, it will be good if you validate all your model to the way motion prediction mean predictions as well as the fluctuation prediction. But two fluid model it is almost must to do that. So, that is the whole basics of how the modeling is being done for the multi-phase flow reactors, and now what we are going to do from the next classes. We will discuss about the different multi-phase flow equipments, we will see that what are their basic features, and based on that basic feature, you can see that what is the modeling approach you can use.

What are the equations? You can solve to find the features or to model those multi-phase flow reactor with. This the 6th portion is over, now we will discuss the module 7 and module 8, which will be mainly based on the different multi-phase flow reactors.

Thank you.