CFD APPLICATIONS IN CHEMICAL PROCESSES

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Week-08

Lecture 40: Modeling Multiphase Systems

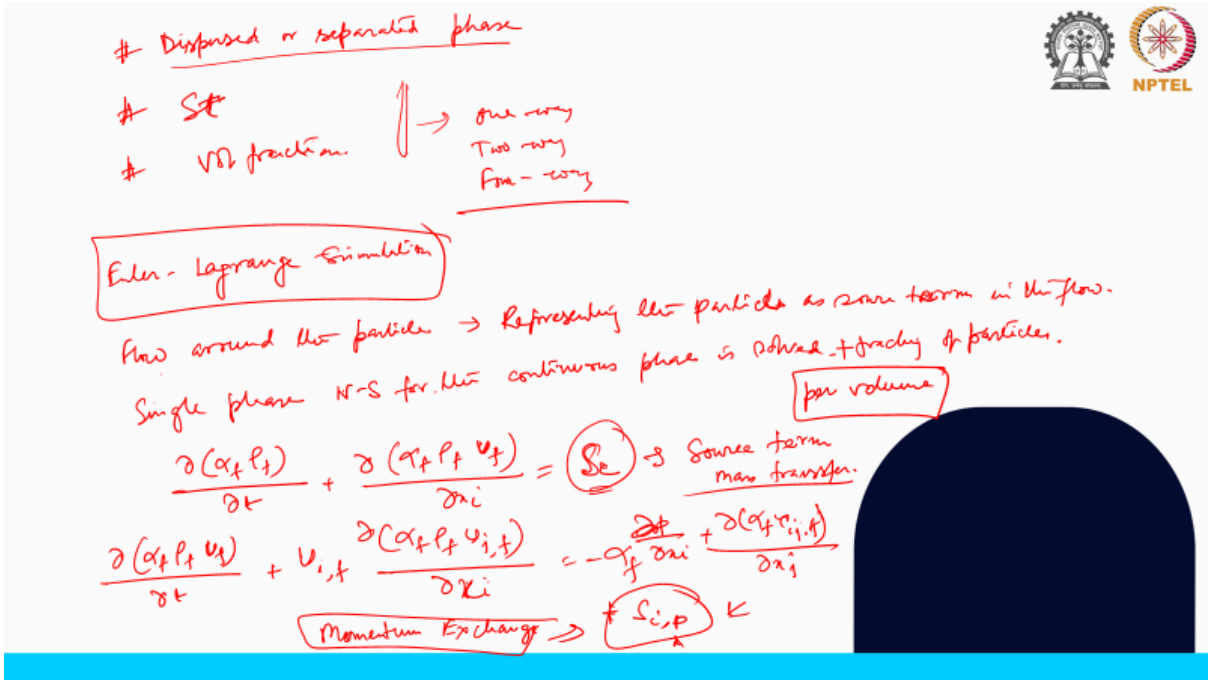
Welcome back, everyone, to another lecture on modeling multiphase systems in the CFD applications of chemical processes. So, we are discussing in detail what the modeling strategies are. And before that, we also discussed the necessity of modeling multiphase systems, but when choosing a multiphase system, we briefly touched on the criteria we have to consider, and that was also broadly based on the dilute or dense dispersed system. Now, in the last class, we saw an overview of the different modeling strategies.

That is the Euler-Lagrangian, Euler-Euler, and in Euler-Euler, the subsets are the volume of fluid method, mixture model, and also the porous bed model. Now, the point is, before choosing any model for the multiphase system, we must have a clear understanding of our objective, okay? And also, we have to be clear on certain things, and those are, first of all, is it necessary to model the system as dispersed or separated? So, in a multiphase system, is that multiphase system a dispersed system or separated?

Now, there is a technical difference that I would like to highlight here. That separated is also closely related to the dispersed phase. But from the standpoint of a multiphase system, the point that I told you earlier is that, depending on the flow regime, one phase may be dispersed in another phase, but at a different flow regime, two phases can flow together with a clear interface. Such a kind of flow we call stratified flow.

Or say we have a clear separation between the two phases or multiple phases. So the point is, again, that means that leads to a certain divergence in the choice of multiphase model. If we have a dispersed system where I am not that interested in looking into the droplet or say the particle shapes, structures and et cetera, and interface tracking is not my objective, then we can choose the Euler Lagrange method. But if the interface is critical, interface deformation, its evolution, etc., then I have to choose the VUF model or any interface tracking model.

One of the examples is the volume of fluid method. The point is the other consideration once you say segregate your problem that it is a dispersed phase system. Now, there the question you have to ask that whether the particles would follow the continuous phase which means you are asking whether how many couplings are there or what kind of particle-particle coupling or particle-particle interaction you have to resolve. That means what is your Stokes number.



So that would help you to decide whether it is a dense dispersed system or it is a dilute dispersed system. And accordingly you have to go for the modeling strategy because the dense dispersed system again cannot be modeled with the conventional Euler Lagrange method. Even your commercial CFD solvers have limitations in using the Euler Lagrange modeling strategy implementation for a problem that has, say, this dispersed phase volume fraction more than 10%. So this is also the question that you have to ask yourself.

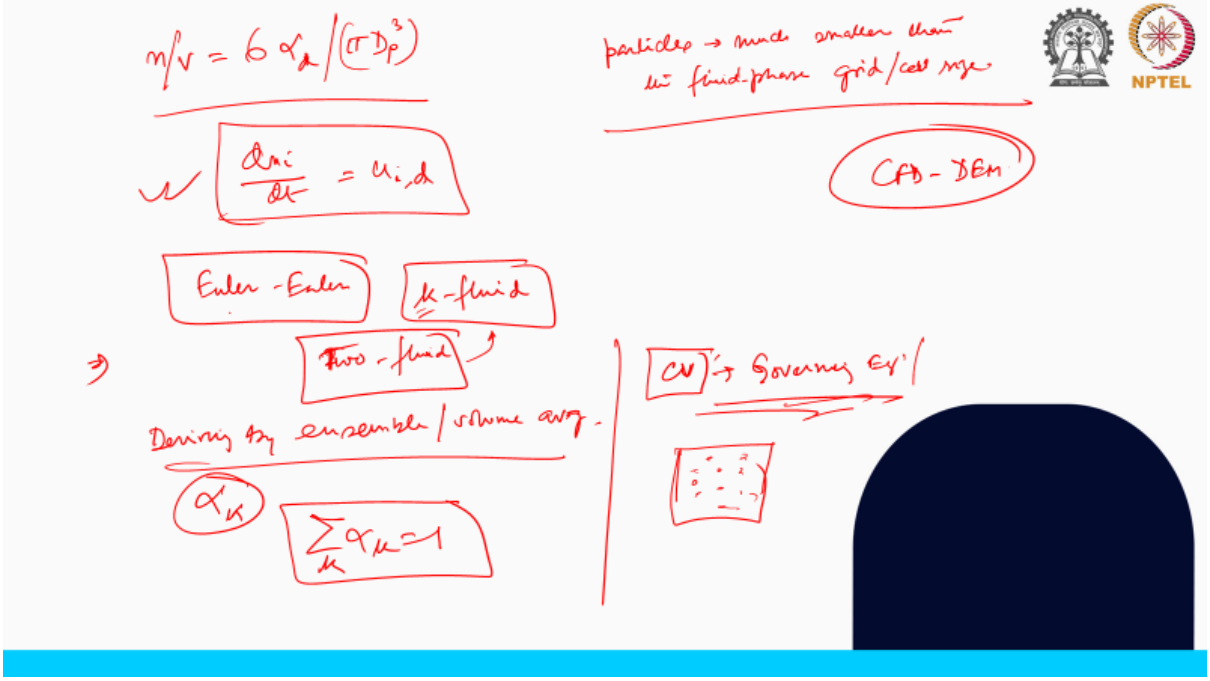
And similarly, how much does that also indirectly answer what the volume fraction is? How much is the volume fraction of the dispersed phase or the local volume fraction? How many particles are there? Because those number of particles, whether you can resolve them for the problem or it is necessary to resolve such a problem. And these also collectively answer the necessity of whether you require one-way coupling, two-way coupling, or four-way coupling.

So, which kind of interaction are you trying to understand, okay? So, if you have to go for individual particle tracking, then you should choose the Euler-Lagrange simulation or the MOD model. So, Euler-Lagrange simulation is also sometimes called the point-particle approach, okay? Because here it is done by resolving the flow around the particles, okay?

Or indirectly, you can say by representing the particle or particles here, a bunch of particles as a source term in the continuous flow or the continuous So, in this kind of simulation, if there are two phases present, one is the continuous phase, and one is the dispersed phase. So, the single-phase Navier-Stokes equation For the continuous phase is solved, and while solving it, it is clubbed or augmented with tracking of particles.

So if we use this Lagrangian notation, the equation would look like if this is the continuous phase, the F, subscript F, then alpha is the volume fraction that we have seen earlier as well. All has its conventional form. is the S c where S c is essentially the source term for mass transfer if that is happening between the phases, ok. This is the continuity equation and your momentum equation would be rho f u j f x j this is beta i equals to minus alpha f

del x i tau ij for the fluid phase f xj plus the source term. Now, here this source term is actually the momentum exchange. Momentum exchange between particles and the fluid. So, the expression if you remember the BVO equation that we have seen earlier where all the forces, the generic expression of the forces were shown in the previous class. So, all the forces there would essentially be part of this momentum exchange source term that would appear here and those forces.

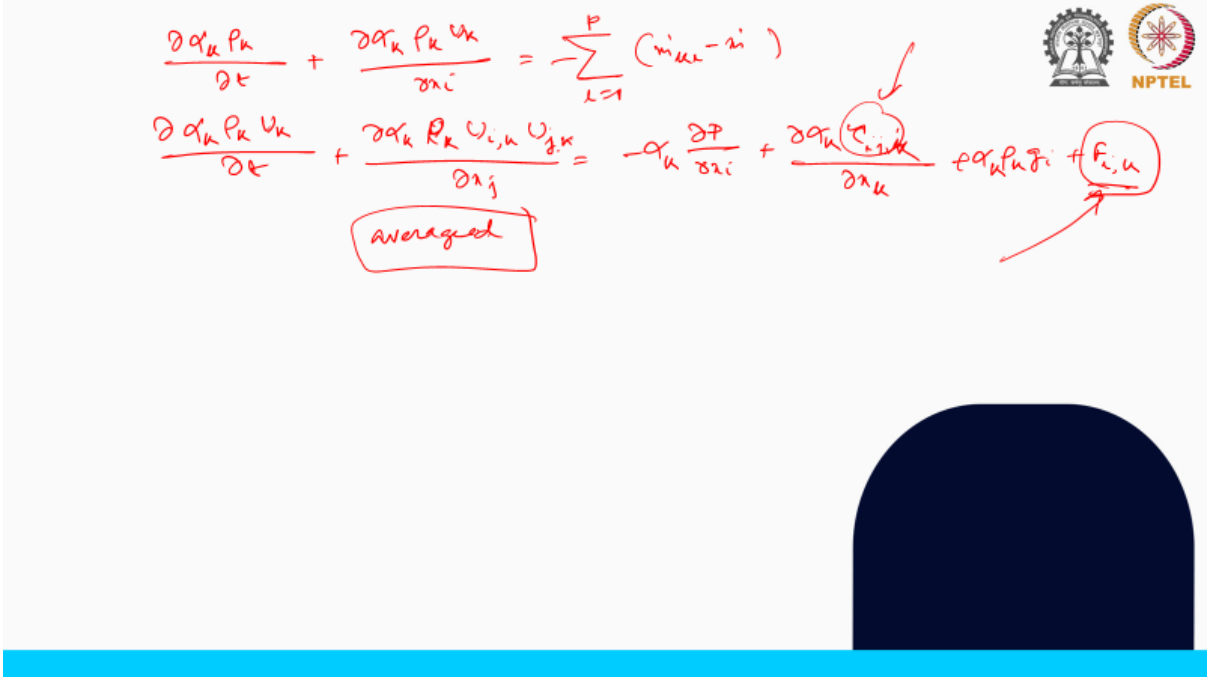


Now, all the terms that are written here are per volume. All these expressions, the variables or the properties that are written, are per unit volume or on a per volume basis. But those forces are for the individual particle. So, those have to be integrated over the number of particles and also the particles that would be there per individual volume, the per volume. So, the point is, this number of particles by the total volume is essentially the alpha d if we consider pi dp cube.

Considering the simplest assumption is that these are spherical particles. Now, again, depending on the shape of the particle, you have to introduce sphericity, and accordingly, this formulation has to be redone. But here is the link in the momentum expression, between the forces that are acting on the particle and its interaction with the continuous phase. That is the momentum exchange term.

So, Euler-Lagrange simulation solves only for the continuous phase Navier-Stokes equation. It solves the Navier-Stokes equation for the continuous phase, and the particles are tracked by their force balance, okay. And in order to track those particles, to track their trajectory, one thing you have to make sure, which is very critical, is that the particles have to be smaller than the fluid phase grid. Because you are dividing the domain into a number of cells, as you have to discretize

your Navier-Stokes equations, you have the governing equations. To do that, the grid size that you are having, the particles that you are tracking by the Euler-Lagrange method, should be much smaller than the fluid phase grid size or the cell size. Because the velocity field that you have to calculate from the source term has to be undisturbed by the velocity field. So the point is, once we have this formulation again for the individual particle, that is, T xi, you can consider this for the individual particle.



So you have to integrate it. And then you have to take the trajectory and the force balance of the generic expressions of all the forces that we have seen for all the particles. And quite logically, you can understand the number of particles is limited because it involves solving these differential equations for all the particles. So, the point is the movement of all the particles you have to simulate by integrating the trajectory this equation and the force balance for the individual particle we have earlier seen the complete force balance equation. Now, the point is,

Again, I will reiterate here that if you have several particles, but you have somehow have to capture those or to have the trajectory for such system, can consider a range of particles depending on their size, shape, or other relevant properties; you can combine that. And for that bundle of particles, you can track the trajectories, considering those would behave similarly.

And that limitation of number of particles can possibly be taken into account, but for a dense system when the volume fraction is much larger then implementation of this becomes extremely difficult.

So, with low volume fraction and one- or two-way coupling, the Euler-Lagrange method gives you an accurate solution or, in fact, a much more accurate solution than the Euler-Euler simulation. Because in Euler-Euler simulation, clearly you do not know the particle trajectories. So the point is, there are stochastic models that takes care of these particle-particle interactions, the four-way coupling that I told you earlier is difficult to capture by the simple Euler Lagrange method or the conventional Euler Lagrange method.

Whether the particles are colliding or in which direction it would go, that kind of information is completely, you cannot get. from the Euler Lagrange method. So, and that is why it has to be augmented by some advanced method which we will not discuss here, but specific to the problem of or your research interest you can go into that direction. But I can tell you that the discrete element modeling, the DEM modeling actually gives you that information of the four-way coupling. And that also can be combined with the CFD for the complete flow picture.

That is why you will hear those who are interested in further research on this area can look into this keyword that the CFD-DEM coupling. such CFD gives you this overall information of the flow field and this DEM would give you the individual particle behavior or the collection the behavior of the collection of the particles they are four way coupling. So, I hope this implementation of Euler Lagrange and its limitations are clear to you and now if I move on to say the Euler method. This treats, we have clearly reiterated, I mean, let me again reiterate here that the dispersed multiphase flow as say two or multiple, because do not get confused with the concept here is only Euler-Euler.

If you have three-phase system, it is still called the Euler-Euler modeling, but then it can also be called as K-fluid modeling. where k is the number of phases that you are having. If it is 3 then the 3 fluid modeling, but conventionally it is called the 2 fluid model because this is the Euler Euler. So, 2 fluid or Euler Euler represents the same concept or the same meaning. More generally one can call that as the k fluid model.

So, here is that it is done by deriving the governing equation by ensemble average or volume average. Now, the important parameter or the quantity here is the volume fraction. If I say that is the alpha k, k means the kth phase, the kth phase. Now, here there is no such dispersed phase. All the phases here are continuous phases.

Remember this clear distinction. Here, there is no such concept of a dispersed phase, although we are modeling a dispersed multiphase system. Now, we consider those dispersed phases also as continuous phases, and accordingly, this alpha k is the volume fraction—the alpha is the

volume fraction of the kth phase. So, this is one of the important concepts of the Euler-Lagrange model because this quantity doesn't give you the information of the size, the shape, or the behavior of the dispersed phase. It is just the volume fraction it takes into account.

And that is why, if you try to resolve that information, you have to use some closure model. So, that is why this Euler-Euler method comes with several closure models that you have to resolve or take into account. Now, several closure models are well-established and can be readily used, but there are several places where you may have to develop your own closure model. that fits your specific problem. And how do we develop the closure model?

It comes from the fundamental understanding from the particle scale or from the mesoscale information. So, due to this simplification, it is easy to use or easy to apply. The easy-to-apply nature of this model makes Euler-Euler extremely popular in multi-phase modeling. So the point is a small volume, which is much smaller than the large-scale flow texture or the structure, but it is much larger than the individual particle size. That is essentially the control volume.

On which the governing equations are developed. So, here, remember the difference between the control volume for deriving governing equations and the conventional grid size. So, on one hand, this is a very important thing that you must remember: the control volume for deriving the governing equation. Because you need to estimate elemental analysis. You have to do the elemental analysis, or you have to consider a small control volume over which you will do this averaging or develop the governing equation.

But this is not your grid size. Do not get confused with the grid size. Grid size is when you have your governing equation and then you are discretizing it. So, the size of the control volume in the case of this Euler equation, it has to be say smaller than the large scale flow structure that exists in the system, much larger than the individual particle or the dispersed space that is there in the control volume. So, volume fraction in this case is defined based on this distribution of phase and the size of the computational domain or the computational volume that we have here.

So the point is, in a two-fluid modeling equation or say this k-fluid modeling part, each phase will have its own. Momentum equation and the continuity equation. But it will be conserved by this equation that the summation of the volume fractions of the kth phases or the number of phases is essentially 1. So, the equation would look like for all the phases, considering that conservation happens. rho k for the continuity equations.

So, this is the part in the continuity equation that appears due to mass transfer. This L stands for the number of phases from 1 to p. So, p number of phases can exist, and this equation is for the kth phase. So, to be clear, there can exist a number of phases, say 3 or 4, in the multiphase

system, and this equation is particularly for the kth phase only—one phase—and k can be 1 to 3 again, but the total number of phases here is 1 to p, p number of phases existing in that system.

And so, this m k l and l k essentially are the mass transfer rate, the amount of mass transfer happening from phase k to l. And, this is the continuity equation, and I can write this for the momentum equation as well. So, considering So, here this term, Fik in the momentum equation, is the interaction force with the phases or within the phases. So the point here is that this is where you would require several closure models in order to account for this phase-phase interaction.

So, these equations are not trivial to solve. Quite evidently you can see that analytically it is not possible to solve. And that is why the CFD different strategy is there. One of them is the finite volume method by which we can discretize and solve it and that we are looking into it here. But the solution part again we will not go into the details because we know the algorithm by which it can be discretized and can be solved.

The point here we are looking that where this phase-phase interaction comes in for the multiphase case. and this is the point where the different phases actually interact with each other because this equation is for a particular phase that is the kth phase. So, similarly such equations has to be written for all the phases that exist in the multiphase system for the Euler Euler case. So, here you would require another closure for this tau. We will see in future

If it is a simple Newtonian case and the simplest possible case, then it is easier. We have the standard relation. But if it is not, if it is due to turbulence and other dominant factors are involved, then we require some other closure for that term as well. Okay, so again here, All the terms that appears in this governing equation or these equations are the average variables per unit volume.

So these are the average variables instead of the point variable. Those are not the point or the instantaneous variables; these are the average variables that are here. And that is why we will see that some specific turbulence models that do not resolve or do not operate on the averaging basis—say, for example, the RANS or the LES—those are difficult to combine with this Euler-Euler model and usually are not combined for resolving turbulence in the case of multiphase flow. So, with this, on this note, I will stop here.

We will, in the next class—in the next lectures—see the other models, that is, the mixture and also more of the Euler-Euler model. And then we will be done with this multiphase modeling strategy. Thank you for your attention.