

CFD APPLICATIONS IN CHEMICAL PROCESSES

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Lecture 39: Modeling Multiphase Systems

Hello everyone, welcome back with another lecture on CFD applications in chemical processes. We are discussing different strategies for multiphase system modeling. So, specifically CFD modeling of multiphase systems that we are discussing. And we now have been introduced to the different categorization as well as the characterization of the multiphase system. And specifically we have discussed about the dispersed multiphase system and its characterization or say the categorization when it is dense, when it is dilute,

or even say what are the phase-phase interactions that can happen or what are the couplings between phases, how that happens and what are the modes that we can take into account those couplings, namely one-way coupling, two-way coupling and four-way coupling that we discussed. And we have also seen a generic expression that the kind of forces that may act on a single particle in a dispersed multiphase system. And again, the point is all the forces that are mentioned here need not be expressed taken into account in your modeling problem because some of the forces may not be that dominant or can be negligible or even absent.

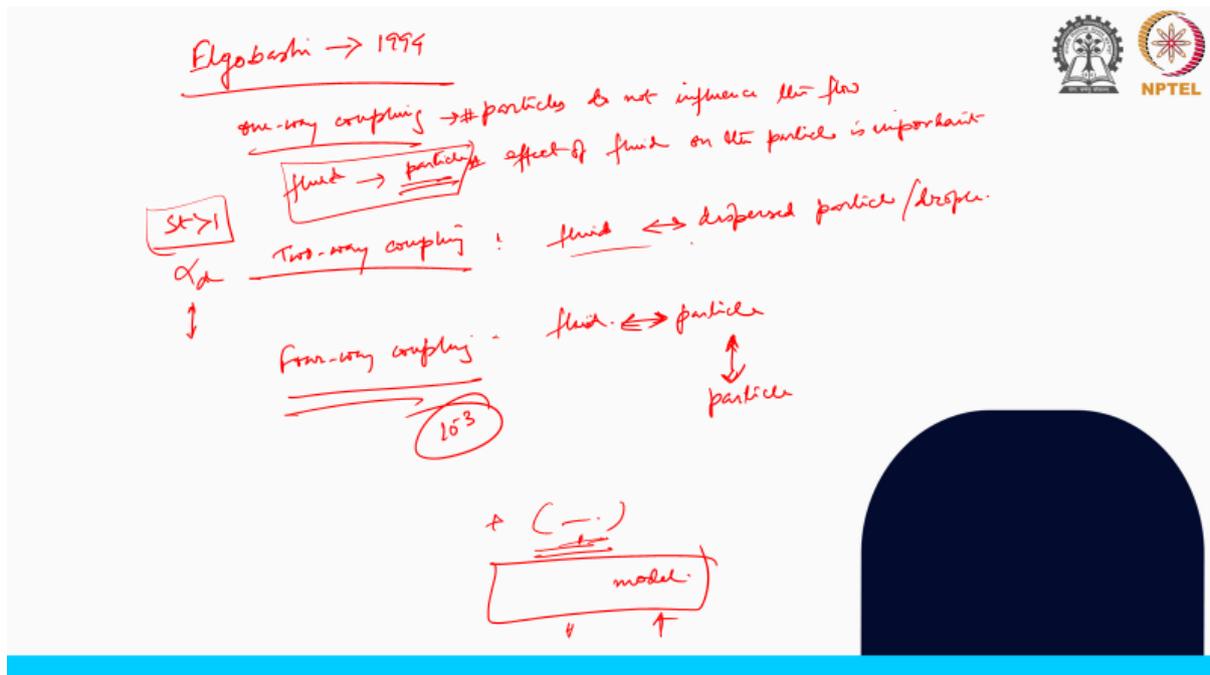
So, the point is based on these understandings I started with this modeling strategies that when we try to include one way coupling, two way coupling or even four way coupling. what should be my multiphase modeling strategy. Now, broadly depending on the reference frame on which we view the problem or the problem statements are developed the governing equations, there can be either the Eulerian framework or the Lagrangian framework. So multiphase systems are broadly classified into two major categories.

One is either it is Euler-Euler framework or the Euler-Lagrangian framework. So the point is that we are saying that it is either Euler-Euler system or Euler-Lagrangian system. Now, what does this mean? The name suggests that whatever the phases are, they are in the multiphase system. Again, we consider one phase as the continuous, the other one is the dispersed.

If we think in this way, then Euler-Euler suggests that the continuous as well as the dispersed, both phases are modeled from the Eulerian standpoint. if we say Euler Lagrangian standpoint or modeling strategy that means we are modeling dispersed phase by the Lagrangian framework and modeling or considering this continuous phase flow or the continuous system through the Eulerian framework. So, which means now you clearly understand this difference

between the framework. In Lagrangian framework, each particle trajectories are tracked or modeled or resolved.

But in Eulerian framework, we take the ensemble average or the volume average. The most say the easier to understand are these two averaging techniques, either the ensemble average or the volume averaging. So, the point is inside this Euler Euler technique or Euler Euler strategy, there exist several different or say specific strategies, specialized system that is applied for some specific problem. Say for example, this volume of fluid is essentially a subset of Euler Euler modeling. When this volume of fluid is essential, this volume of fluid is used in the problem where we try to identify the fluid-fluid interfaces clearly.



For example, say the droplet deformation in a flow, the droplet coalescence, the droplet splitting, etc. So, there we need to understand that how this fluid-fluid interface is clearly deforming. Similarly, this mixture model or the algebraic slip-slip model is also another subset of Euler-Euler model, where say for example, a suspension is modeled in a single Eulerian standpoint considering this phases two different phases considering a mixture property with the single equation there can exist and in fact there would exist another phases. So, that is why it would be the multiphase system.

So, if there are three phases or even the two phases we can use this mixture model in order to simplify the problem the solution strategy for the Euler Euler instead of explicitly considering the phases. And so these are basically the specific applied or specific application model and but in general this whole class you can consider as either Euler Euler modeling strategy or the Euler Lagrangian strategy. So, in Euler Lagrangian now since the basic is understandable for us or we realize that the difference between the Euler and Lagrangian framework.

So, Euler Lagrange model if we consider So, here fluid phase or the continuous phase is modelled as a continuum by solving the Navier Stokes equation. the disperse phase a large number of particles is modeled by Lagrangian framework. which means each particle the number of particle that we consider.

So, this large number of particles means a handful or a known number of particles we will resolve and in such cases each particle or say if there are droplet that we are considering as a dispersed phase their trajectories are computed that is the Lagrangian framework. That each and every particle that we have considered if a system consists of some million of particle each of the particles trajectory would be computed. And there if so now quite understandably

due to the computational resources, the limited computational resources and the time constraints. If it consists millions of particles, this has a limitation that it cannot solve for a very dense system or in fact a dense dispersed system or dense dispersed multiphase system. So, in such cases sometimes what is done that instead of each particle or trajectories to be computed, what it is done? A size range or a handful of particles say we consider the bundle of particles are assumed those say follow the similar trajectory. then those range or those size range if it happens for the same sizes or the similar sizes similar range of particle sizes say a micron

say 1 to 10 micron of particle is possibly behaving or would behave the similar way in a fluid than say 10 to 50 micron size particles. So, in those cases what is considered these size ranges. are a group of particle or a bundle of particle together instead of individual particle that is there in this case. So, if you have a size range before the study with from the flow characterizations that I have a size range where I know what kind of particle is there and or what is the size range of particle exist in the system and I club a certain known size range

that bundle of particles behave similarly if we assume that then this number of particles from millions it can be lower down to a reasonable number that can be solved by this Euler Lagrange model. So, it is not only based on the size, it can be based on the shape or different other characteristics that specific to that operation. I mean, when you expect those bundle of particles to behave similarly, be it on the size, be it on the shape or maybe other dependencies. So, in those cases, this Euler Lagrange models are used frequently. for comprehensive understanding that how each particle is flowing in the flow field or it is behaving whether the droplets are merging or whether the droplets are colliding etcetera.




Bussel-Brownian or D'Arcy RRD $Re_p \ll 1$

$$m_p \frac{d\mathbf{v}_i}{dt} = \mathbf{F}_{i,drag} + \mathbf{F}_{i,pres} + \mathbf{F}_{i,wind} + \mathbf{F}_{i,magn} + \mathbf{F}_{i,elec} + \mathbf{F}_{i,Lift} + \mathbf{F}_{i,therm} + \mathbf{F}_{i,turb} + \mathbf{F}_{i,grav}$$

\mathbf{v}_i = linear velocity of the particle
 m_p = mass of the particle

→ Euler-Lagrange Model
 → Euler-Euler
 → Mixture Model or Algebraic-Slip Model
 → Volume-of-Fluid Model (VOF)
 → Porous-bed Model

C → Euler-Euler
 D → Euler-Lagrangian



So, all those things can be modeled, but the limitation is that the drawback is that it can be used for only low volume fraction of dispersed phase system. Because of this obvious limitation, if you have to solve millions of particles with this Lagrangian framework, it would not be computationally feasible. Now, the point is, that means here you have this two-way coupling. So, that means the dispersed phase is sensing both the phases—dispersed and continuous—both phases are sensing their presence together. So, this is the two-way coupling.

Now, the Euler-Lagrange model with four-way coupling means whether the particles are colliding or whether those collisions are happening, whether that results in particle breakage, etcetera—those are still very difficult and specialized processes. It is not easily feasible; it is not easily done in modeling or through research. Details of the four-way coupling by the Euler-Lagrange model are usually done in a very problem-specific way. There are different strategies—for example, the hard-sphere approach, Monte Carlo approach, etc.

that can be augmented with this strategy of the Euler-Lagrange model, where you can sense this four-way coupling. But it is not easily done through the Euler-Lagrange model. It requires further different modeling strategy for example the discrete element modeling and etcetera that is there for this four way coupling meaning the particle-particle interactions of the dispersed phase. The other strategy

the broad classification from that is the Euler-Euler model. Now, in the Euler-Euler model, what happens is that different phases are all treated as continuous. And momentum, as well as the continuity equations, are solved for each phase. So, all the phases that exist in the multiphase systems through the Euler model are solved using the Navier-Stokes equation and the continuity equation, irrespective of their thermodynamic state. So, that is why in one of the

examples earlier, I told you that for a packed bed, or even for a fluidized bed, if somebody goes for Euler modeling strategy, they had to consider that the particles, the solid particles or the solid catalyst in case of packed bed packed bed—are also a continuous phase with velocity zero for the case of a packed bed, but for the fluidized bed, having a different velocity, and then it is solved. as a flowing fluid. So, the point is, this Euler model takes into consideration averaging.

Euler-Lagrange Model

- # Fluid phase is modeled as a continuum by solving N-S; the dispersed phase → a large number of particles is modeled by Lagrangian framework.
- # Each particle or droplet trajectories are computed.

low vol frac. of dispersed phase

Euler-Euler Model

- # Different phases are all treated as continuous phase and momentum & continuity equations are solved for each phase.
- # Interpenetrating quasi-fluid

Best! Empirical model

phase vol. fractions are defined over a CV

The image contains two logos: the Indian Institute of Technology (IIT) logo on the left and the NPTEL logo on the right. There are also some diagrams: a simple sketch of a particle or droplet, a grid representing a control volume (CV), and a large dark blue semi-circular shape on the right side.

So, say, for example, if you have several dispersed particles here, the phase volume fractions—each phase volume fraction—is defined over a control volume. And then, some averaging techniques are used to derive either time- or volume-averaged equations for all phases. So, averaging techniques—there are various averaging techniques to derive the governing equations. We will not go into those details, but the point—the essence—is that the phase volume fraction is the key or one of the major components in this Euler-Euler model. And when we talk about this specific, in the true sense, Euler-Euler model, What does it do? These phases are also considered as interpenetrating medium or interpenetrating quasi-fluid, we can say. What does it mean? The interpenetrating quasi-fluid; all phases are considered as interpenetrating quasi-fluids. Which means that usually, when we have a void space, the consideration can be that at a time, one fluid can stay there.

If that happens, then if another fluid tries to come into that void space or the interstices, you can track the interface to see how it is getting displaced. And that is specifically what the volume of fluid method does. It clearly tracks the interface. There are several other interface tracking methods. One of those we are discussing here is the volume of fluid method.

So, we will discuss it here. So, the point is, if you can consider interpenetrating quasi-fluid or interpenetrating media, that means at the same time, multiple fluids can coexist at a certain location. That is the assumption of interpenetrating fluid medium. And due to this assumption, we cannot resolve the particle-scale phenomena or the microscale phenomena with the help of the Euler-Euler method, and also due to this averaging technique. That it takes average.

Mixture Model (Algebraic Slip Model)

- # flows of phases are assumed to interact strongly and it is not necessary to solve the momentum balances for different phases separately.
- # viscosity is estimated for the mixture.
- #

Volume-of-Fluid (VOF)

- # Interface between phases are tracked.
- # drawback -> large number of drops or bubbles.

Porous media Model

Either, as I told you, the couple of averaging techniques are the ensemble average, volume average, or maybe the time average. The phase, the governing equations are developed for all the phases. And that is principally based on the phase volume fraction and their velocities. So, the point is now in this case quite reasonably—I mean, quite understandably—then this Euler-Euler model can handle very complex flows. But it does not give you the best result. Again, the definition of 'best' is very different from person to person because it depends on the objective of the problem, but it requires—

This Euler-Euler model requires several empirical models or empirical sub-models for the closure of the phase-phase interactions and other cases. So, it requires several closure models. And as good as your closure models are, that good would be your Euler-Euler prediction or model result prediction. Okay. So, this is what we are showing—a very brief overview of the overall strategy.

Now, as I told you, one subset of the Euler-Euler method is the mixture model or the algebraic slip model. So, here what happens is the flows of phases are assumed to interact strongly, and it is not necessary—to solve momentum balances for different phases separately. So, not all the phases are solved or resolved by individual momentum balance equations. We consider in those cases those are not explicitly taken; the viscosity is estimated—

for the mixture property. The velocities of the different phases that are calculated from buoyancy, drag, and other forces actually yield the comparison of mean velocity of the mixture. So, the velocities of the different phases that are calculated from buoyancy, drag, and some other forces actually give the relative velocities. Instead of the mean velocity and that is why we have that concept as called the slip or the drift velocity which will go into the details when we specifically talk about this mixture model's governing equations.

So, it results in a relative velocity, and that is measured. What is my mixture velocity, the mean velocity of the mixture, and the individual phase's relative velocity? So, basically, what it does is solve the Euler-Euler model while considering a lesser number of phases in the system. And a lesser number of phases means you have fewer governing equations to solve. Here, the mixture properties are taken, and these mixture velocities or mixture properties are considered when we solve the momentum balance equation.

And the other specific model that we will look into is the Volume of Fluid, or the VOF model. This is again a subset of the Euler-Euler model, but here, specifically, the interface is tracked—the interface between. So, the interface between phases is tracked, and since it has to be resolved between the phases, it has a drawback: it cannot be used for systems where you have several such interfaces or several means.

A large number of drops or bubbles. One example is this. If you have millions of drops or millions of bubbles to resolve, then this Volume of Fluid method is difficult to implement. Because it goes into the resolution of this particle scale or I would say here for example it's a droplet scale or the bubble scale so each and every bubble is being tracked tracked means the air interfaces are tracked how it happens we will go into this the details later but this is just to give you an overview of

that the possible models of the multiphase system where we can use these different strategies for different purposes. And in the other case, the porous media model or the porous model, or the porous bed model, we have already discussed that when you have to understand the pressure drop across, say, a porous bed, and that bed may contain multiple particles. So, it is extremely difficult to resolve individual particles. Navier-Stokes equations for those individual particles as well by the Euler-Euler strategy.

So, again this is a subset of the Euler-Euler model where this instead say directly we calculate this pressure drop from an equation that looks like an Ergun equation case of multiphase flow with several empirical equations, one can say the relative permeability concept. So, the point is, there we need not model the catalyst particles inside the bed due to their complex nature and complex shape. Nature means the complex shape; those are static there, the velocities are there.

So, the point is, those particles may have different shapes, different porous structures, even say, the foam-like structure the catalyst can be.

So, those are difficult to resolve at the particle scale. And if your objective is to understand the pressure drop or the pressure drop profile, etc., at the macro scale, then you need not resolve those particle-scale phenomena. In that case, this subset of the Euler-Euler model comes handy because the bed void and their resistance to flow act as a boundary condition to the Euler's equation. So, the point is, we have an overview now of what the different modeling strategies are that comes from the Euler or the Lagrangian framework be it either it can be either Lagrange Euler Lagrange model or can be Euler Euler model and in Euler Euler model

I can have or we can have several subset of the or variations of the Euler Euler model. To name a few, we have seen the mixture volume of fluid or the porous bed model. So we will now go into the details of this, how the governing equations look like or what are the points where we need the closures, and we will start discussing this from the next lecture. So with this, I thank you for today. We will see you with the details of this in the next lecture.

Thank you.