CFD APPLICATIONS IN CHEMICAL PROCESSES

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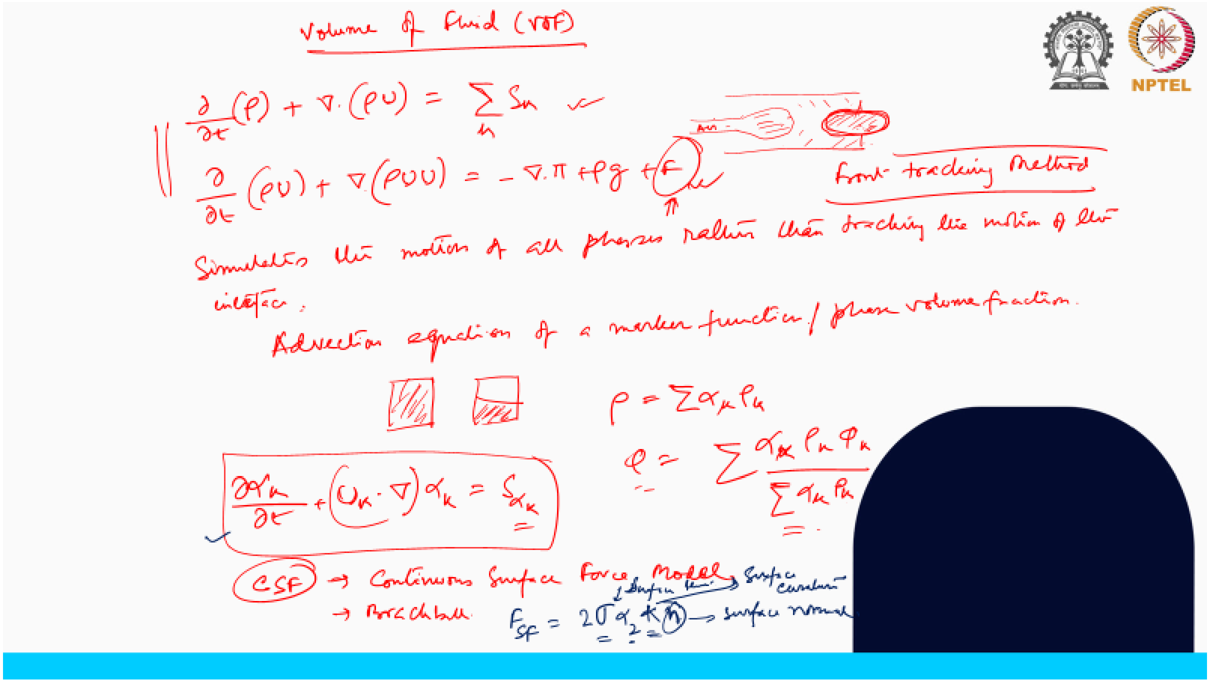
Lecture 45: Modeling Multiphase Systems

Welcome back, everyone, to another lecture on modeling multiphase systems in CFD applications for chemical processes. We are discussing different strategies of multiphase flow modeling systems, and so far, we have discussed Euler-Lagrangian development or the formulation, as well as the Euler-Euler formulation. In the Euler-Euler formulation, we further discussed the classical three-phase or the K-fluid simulation, or how to implement the porous bed formulation, taking an example of the packed bed reactor. Now, the point is, these methods are sometimes insufficient in certain applications where our objective is to track the interface.

Now, in such cases, strategies are available, and today we will discuss one such strategy, which is the volume of fluid approach, or the VOF. Volume of fluid approach. Now, using this VOF approach the flow processes around an individual droplet or particle or say in general dispersed phase are resolved not like exactly what we did in Euler Lagrange cases or even Euler cases although we do not actually resolve those particle scale phenomena. We take into account the interactions, the phase-phase interactions.

Now, in this VOF approach, all the participating fluids—I mean, the utility of this approach is that, for example, in a system, I have the generation of a droplet, okay. So, in a co-flow system where we have another phase, and that phase is growing and eventually detaches, creating a droplet. So, in such a scenario where we have to track the interface or identify the individual dispersed phase behavior—how it grows, how it collapses, how it breaks, etc. Such phenomena mean we need to understand the behavior at the interface of the fluid.

So, whatever the participating fluids exist in the system, okay. For those systems, for all the participating fluids, we solve a single set of conservation equations like we did for the mixture model, but with a difference here: the interface is tracked directly by several methods called the front-tracking method, but here with the reconstruction technique, we solve it. We do not directly track the interface by the volume of fluid method, but we indirectly reconstruct that by calculating the volume fractions or conserving volume fractions at a individual Euler Euler grid cell.



So, the governing equations actually are in this form. So, this is the continuity expression. This is the continuity expression; we need not explain it further, as we have seen it several times. We have written it in a very simple manner here. A single set of conservation equations, which are the continuity equation or the mass conservation and the momentum conservation. Now, in principle, what is done—or it is possible to solve this set throughout the domain—

even when there is a drastic change in the density and other properties across the interface. Because density, viscosity, etc., say, for example, if I take an example of this: say, an air bubble is forming in a liquid medium. So, we understand there is a huge—the order of magnitude—contrast in the density when this equation the single set equation is solved over the entire domain across this interface there is the air density and outside

we have a liquid density to account for and those are differed by order of magnitude. The chances of discontinuity or divergence in the simulations may appear, but suitable technique with the appropriate boundary condition and the time dependent behavior, we can track that we can solve those and those method directly called the front tracking method that directly captures this interface. But the issue is that these techniques are computationally extensive and demanding. It requires extremely fine resolution of the meshes as well as small or lower time step values, etc.

And also the consideration of the moving interface for capturing that. And the grid size that we take into account, the Eulerian grid size in the main domain. These two considerations are of paramount importance in the application of such methods. But we will not discuss those front-tracking methods here. We move on with the volume of fluid method, which is one of the most popular methods applied to track the movement of the interface indirectly, not directly.

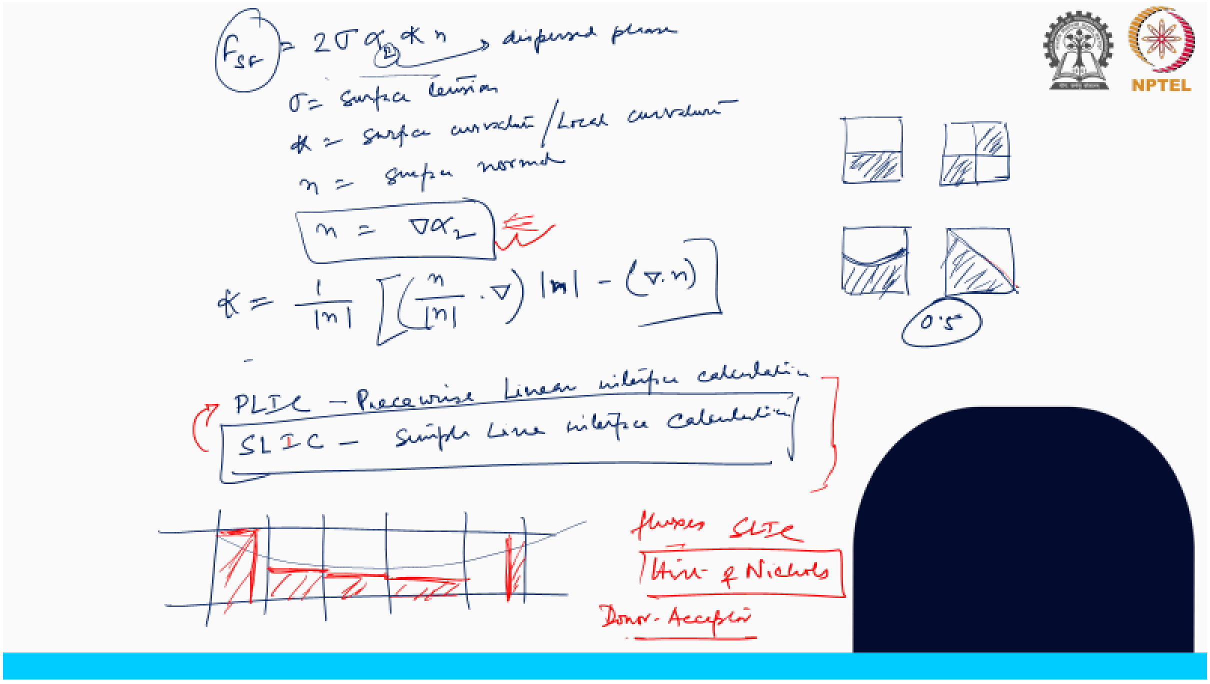
So, this VOF simulates the motion; it simulates the motion of all phases. Rather than tracking the motion of the interface, okay. So, the motion of this interface is actually indirectly calculated through this. Of the phases separated by the interface. So, this motion of different phases is eventually tracked by solving an advection equation of a marker function.

Or it is essentially the phase volume fraction that demarcates different phases. So, when a control volume is not completely filled by one single phase, in that case. If an interface exists, then in that computational cell, the mixture properties are used to solve this set of governing equations. And once we consider these mixture properties, then there are minimal chances of divergence due to this abrupt change in density or the other properties because it takes into account the average properties, and it calculates in that cell. This governing equation solves for those.

So, the point is the density in that case is considered by this expression, where k is the kth phase and any other property that is considered here is something like this kth phase. So, this is basically alpha k rho k. So, the average of any other variable than the density is calculated like this. Those are replaced when a cell is not filled with a single fluid.

And the volume fraction alpha k for each fluid is calculated by tracking the interface between the different phases throughout the solution domain. So, that kth phase volume fraction or the advection equation that is solved is S alpha k. This is that particular phase's source term if there is any. So, this marker function is solved that identifies this interface in a particular cell. And then the mixture adapts whether the mixture properties should be taken in that particular cell in order to solve these governing equations or not.

Now, since here the curvature or the contact between two immiscible phases is there, that is why it becomes important to model the surface tension effects also in this particular system. And specifically, since multiple phases exist, we do not call that surface tension, but it is the interfacial tension or interfacial phenomena that is necessary to model. Now, there exist several models by which this F term, the interfacial drag term, is modeled. The surface force is taken into account by this term here in the momentum expression.



One of the popular methods is the continuous surface force (CSF) model, which is the continuous surface force model proposed by Brackbill. He developed this CSF model to describe this interfacial surface tension. Now, how is it modeled for two-phase flow? Say, with a dispersed phase or the secondary phase, if I denote that interaction as, say, if the surface force is 2 sigma alpha 2 kappa and heat.

So, this 2 represents the dispersed phase or the secondary phase. This is the surface tension. So, the surface force is modeled like this, where this normal term is the surface normal that acts on the interface, and kappa here is the local curvature. That is denoted with the expression that I will show you. So, this is the surface curvature, this term, and this is the surface tension.

So, if I write it again clearly, then you would understand that Fsf is 2 sigma alpha 2 kappa n, where sigma is surface tension, the 2 subscript stands for the This is the surface curvature or the local curvature. n is the surface normal, which is the surface normal for the secondary phase volume fraction alpha 2, denoted by this expression. The local surface curvature is defined by this expression.

So, here the volumetric source term volumetric force that acts as a source in the momentum equation has been resolved by one of such method that is the continuous surface phase model and that has the other expressions detailed here. So, the point is that with the surface tension model, adhesion and other phenomena can also be modeled by this strategy. So, that means since surface tension is involved, adhesion can be resolved—meaning the contact of the fluid with the surfaces and the fluid interactions are also dictated by the contact angle that develops due to the surface curvature caused by surface tension.

So, to ensure accurate implementation of surface tension and wall adhesion phenomena, the solution method we use must maintain a compact and sharp interface that we can identify. So, to accurately predict the evolution of different shapes of droplets or bubbles that we are trying to identify, accurate implementation of these surface force phenomena, including the contact angle and related properties, is extremely essential. The point is

For small-scale phenomena and deformable gas bubbles, we must ensure accurate estimation of local mass and heat transfer rates near dispersed phase particles. But one of the disadvantages—or the biggest disadvantage, we can say—is that VOF is also computationally very demanding in terms of grid refinement. So, if we have a large number of dispersed phases to identify, then applying the VOF method is also very demanding in such cases. I mean, it is difficult to implement because of this individual capture, as we have seen the drawbacks in the Euler-Lagrange method as well. Now, the point is, how do we understand this curvature?

There are other techniques by which we can actually solve this reconstruction of the interface because, say, I have four different cells and I have the information. That half of it is filled by the liquid or, say, the different phases. There can be several such combinations of possible surface or interface configurations for the same value of volume fraction in a control volume, which here is 0.5. So, in all four cases, in this control volume, we have the consideration of, say, 50% dispersed phase that exists in one cell.

What would be my actual interface or the accurate interface in such a scenario, or how does it reconstruct from this information that it is 50 percent full? So, my interface looks like this way, or which one is the more accurate one? So, the point is, as we have understood now, that if we have an interface value, say, a transport marker function—for example, here we have seen this volume fraction. Then, there exist different methods by which this surface interface is reconstructed, and two of those such methods are PLIC and SLIC. One is called the piecewise

linear interface calculation, and SLIC is essentially simple line interface calculation. So, initially, this SLIC which is simple to implement, was used, and that considers, say, if I have this kind of grids and if I have, say, actual reconstruction or actual interface like this, then what it considers that I have a full value of it in this case. So, what it considers is that flask that we calculate

This flask that is parallel to the reconstructed interface is estimated in this case for this PLIC and is different than this SLIC scheme. So, the point is when we calculate, it depends. So, it is an approximation of this SLIC was essentially initially developed by Hart and Nichols. They developed this SLIC technique that uses an approximation, so approximations are these that these are my interface which is quite abrupt in the case of coarse meshing. But the point is it uses an approximate interface reconstruction where the forces at the interface align with one of the coordinate axes. And that is why, depending on the volume fraction, that is developed or that kind of structure is developed here, that it may look like some parallel interface lines that are aligned with the one that is aligned with one of the grid lines.

And that depends, that the alignment actually depends on one of the coordinate axes and on the prevailing direction of the interface normal that is calculated from this expression. And when we compute the flux in the direction To this reconstructed surface, the upwind flasks are used, which means that they conserve the directionality of the flow. And flasks that are in a direction perpendicular to the reconstructed interface are estimated using the donor-acceptor method. So in donor acceptor method, one computational cell is considered to be a donor when some fluid is withdrawn from it or flows from that cell to the other cell and in which it is coming, we identify those as the acceptor cell.

So this happens between the two neighbor cells that the one becomes the donor cell, one is the acceptor cell. So the flask again, the flask that we calculate when in the direction that we have parallel to the reconstructed interface, that time we use the upwind scheme and when it is perpendicular to the reconstructed surface, that time we use the donor and acceptor method. And in PLIC which is more accurate than the SLIC scheme which is piecewise linear interface calculation. What that is done is that in that case interface that is calculated within the computational cell is approximated by a straight line segment that cuts a cell like this.

The cuts a cell with a slope that is determined from the interface normal. And this interface normal is calculated from the gradient of volume fraction. okay. And the line segment that cuts a computational cell in such a way that the volume is equal to the value of the marker function of that cell. And then based on this, so if I draw a couple of cells that would be more clear.

So, again if I draw a couple of So, there what happens it cuts the surfaces like this where it is more accurate to the actual interface curvature. And these line segments actually preserves the information of the volume fraction these are aligned with the volume fraction value. The marker function essentially takes into account the volume fraction and accordingly cuts the cell.

So, SLIC and PLIC both exist, but the point is it is better to use the PLIC scheme when possible if we have the options available because It is more accurate than the SLIC scheme, and it creates or gives us a more accurate interface than the SLIC scheme, which is the simple linear interface calculation. So PLIC is preferred or more accurate than SLIC in any given situation. So with this basically this gives us an overall idea that how it is implemented or how what are the governing equations of the volume of fluid method and how it operates and in the next lecture we will see a brief overview before we move on to the new chapter or the other topic which is on turbulence that how

this volume of fluid can be applied to capture one example, particularly for the droplet. And in terms of execution, what are the considerations that typically should be made when we take into account or try to apply this VOF method. So on this note, I will stop here today, and in the next lecture, before introducing turbulence, we will have a short overview of this implementation of the VOF method for the practical case. Until then, thank you for your attention.