CFD APPLICATIONS IN CHEMICAL PROCESSES

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Week-10

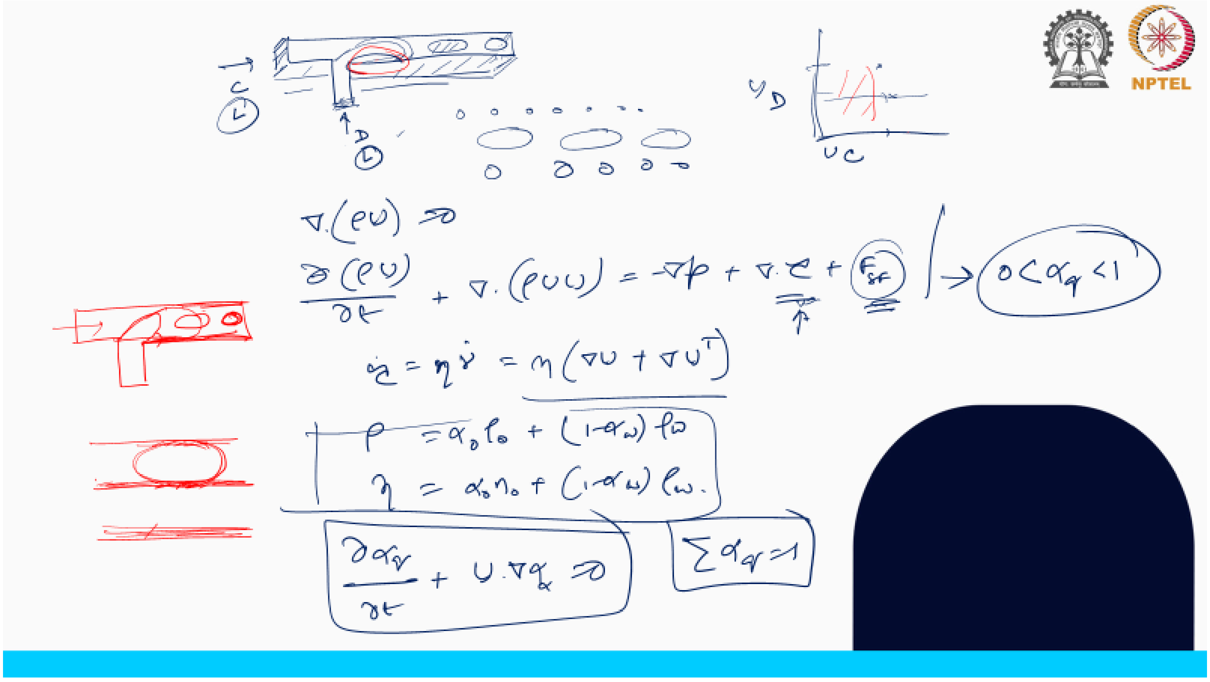
Lecture 46: Modeling Multiphase Systems

Hello everyone, welcome back to another lecture on modeling multiphase systems in CFD applications and chemical processes. We are discussing different multiphase modeling strategies, multiphase flow modeling strategies and one of the final segment that we are discussing is the implementation of volume of fluid method for which the theory we have discussed in the last lecture. Here, we will see how it is implemented, what the implementation strategies are, and what we should be careful about while implementing it. Taking an example of, say, droplet formation in a microchannel—consider a T-junction of certain known dimensions, a 3D T-junction—and the point is,

we have a dispersed phase that is flowing here we have a continuous phase and at a particular or at a given condition here the dispersed phase that generates depending on the contact angle and etcetera it detaches from this or from the system and it creates a droplet. Or multiple droplets, depending on the situation—whether it detaches or not. Such phenomena are understood using the volume of fluid method. It can also be done using other front-tracking methods, but usually, when done in a standard way, the volume of fluid method can also be applied. So, in this case, similar to that...

The previous understanding is that we have two different phases. Now, again, in CFD, as I told you earlier, two different phases do not necessarily mean two different thermodynamic phases. So, here, one liquid phase and another liquid phase. Two different liquid phases, but immiscible in nature, are flowing and generating a droplet of the dispersed phase. And for that the preamble is required velocity and everything are set because there again exist like the previous example in packed bed different flow regime or flow texture where the if we do not cross a threshold limit there may not be any chance of droplet development or droplet formation.

There is a possibility of the dispersed phase and the continuous phase flowing together in a stratified manner, for which we have seen the modeling strategy for stratified flow. There are chances that it detaches very quickly in those cases, we have multiple smaller droplets in certain cases. The development happens that it initially the droplet this dispersed phase develops the grows till and it blocks the flow of the continuous phase and then by shearing action it detaches and accordingly creates different shapes of the droplet not as the spherical droplet. So, all these things. taken care say as the primary understanding or the initial investigation that okay under this condition under a certain flow rate of the liquid and the gas or the dispersed phase and the primary phase here since both are liquid phases. So, I consider the continuous and the dispersed phase and their velocities.



So, u c and u d. We set a certain point, we operate at a certain point where the detachment happens, and it creates some droplets. And we do not know what kind of or what shape the droplet would be, and our objective is to track that or to identify the shape of the droplet and its deformation, etc. So, the point is, we first generate this domain; we create the domain. in the preprocessor either by CAD geometry or by importing the CAD geometry to the CFD solver this T junction the 3D T junction

that we have of known dimensions that is depth, height, width etcetera all these lengths. So, these are all design parameters of this T-junction. So, those are drawn first. Then we give the boundary conditions: inlet, outlet—this is another inlet for the other. Where now, in these cases, the pure or single fluid is flowing through different inlets.

So, we need not bother about the discontinuity that may appear—that we checked we did for the packed bed condition—and where we made sure by dividing that with the volume fraction. So, the discontinuity does not appear because here the pure single liquid—a single type of liquid—is flowing in one inlet. So, we simply take the superficial velocity at this inlet, the velocity inlet, and the outlet in this case is open to the atmosphere. So, the pressure outlet boundary condition is taken. The solid surfaces are considered the impermeable wall. No-slip boundary conditions are set, and then we solve the governing equations, which are again nothing but equals to 0 and the surface force—the volumetric surface force.

Now, this stress term actually takes into account the fluid or the liquid types that we are handling. If we consider for the time being that we are taking here the Newtonian liquids—both are Newtonian liquids—then we use Newton's law of viscosity to calculate these stress terms. If it is not, then it takes into account the constitutive equations for different other types of non-Newtonian fluids, be it Bingham, shear-thinning, shear-thickening, etcetera. So, accordingly, the constitutive equations are solved for this term.

And this surface force we have seen earlier conventionally we use this Bragg-Wills continuous surface force model because that is mostly available in all the commercial CFD solvers and also easily we can develop the code if required for the open source software. Now again, if I write it separately, it essentially eta dot and in this case. Now, this is the generic form where the fluid can also be considered as a non-Newtonian fluid.

is essentially since considering here two different phases—say, if I consider here the continuous fluid that is going inside is the oil and water—these two phases. Then, considering the primary phase as, say, the oil and the water droplet inside as the dispersed phase, we accordingly write this O for the oil W for the water and eta which is the dynamic viscosity we are considering in this form and the equation for the volume fraction that we solve as the marker function So, again Q stands for either oil or the water phase whatever the phase that would be alpha Q is equals to 0. So, in each computational cell the volume fraction of all the phases

are conserved by this expression that alpha q is equals to 1. When alpha q is equals to That means that that particular cell is assumed to be completely filled with the other phase with its completely divide of the qth phase. That means whatever the other phase exists that completely has filled that reference cell and when alpha q is equals to 1 that means that particular reference cell is completely filled with the qth phase. And so this average quantities are then solved when these criteria are met or this criteria is set.

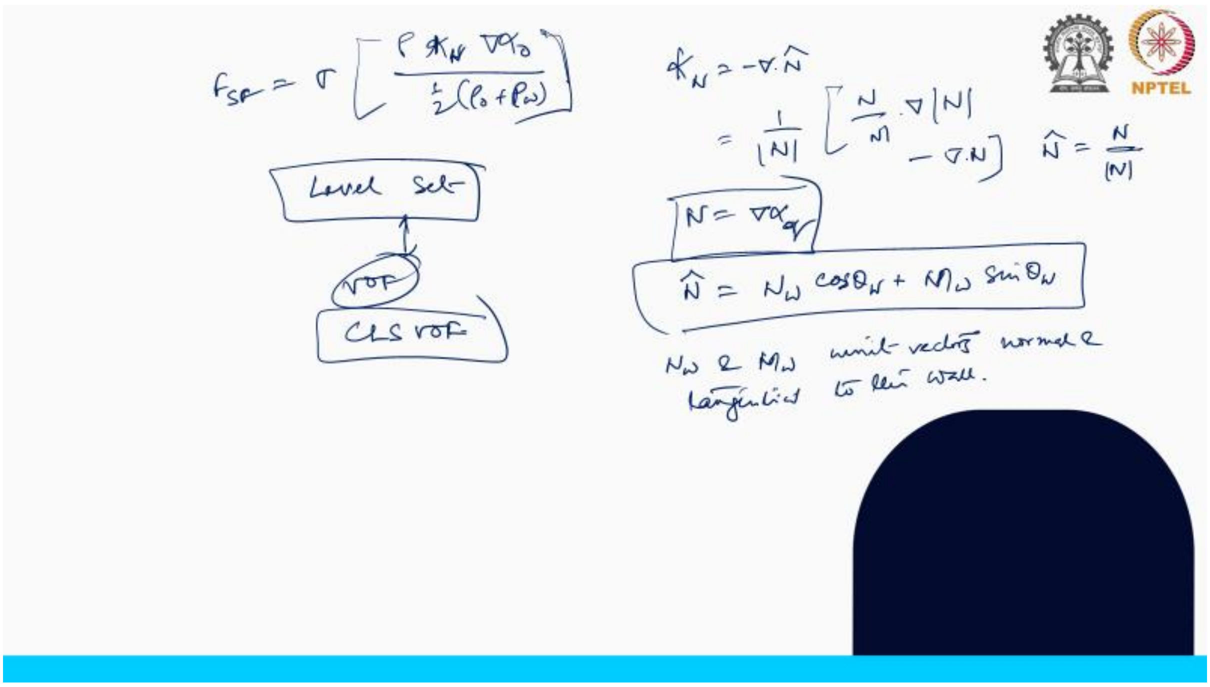
And this surface tension like in the previous case so this surface tension if I elaborate this force can be taken into account by this expression by the continuous surface model it is written in a bit different. So, this is the kappa again kappa normal half of rho 0 plus rho w considering here the phases are oil and water this is the n. So, this kappa n is essentially the surface normal that we have seen again, if I say this is the M hat. So, this is essentially 1 by N.

where I have this n hat is equals to n in the vector form. So, since it is written in all the cases in simple manner. So, this surface normal n is essentially the gradient of the volume fraction. For the qth phase, this surface normal in any reference cell is essentially given by this expression. Here, Nw and Mw are the unit vectors normal and tangential to the wall.

Now, several assumptions are usually done while implementing this VOF strategy for this droplet development understanding is that we can consider a static contact angle which is independent of the moving contact line or the velocity. Because the surface normal cell when it is away from the wall along with the contact angle it governs the local curvature of the surface and that is utilized to calculate this surface force and that in terms also is applied in the momentum equation. Now, the contact angle can vary dynamically between an advancing and receding contact angle.

If the contact angle remains within the range of advancing and receding contact angles, then the contact line essentially does not move. So, typically, the use of a static contact angle has been proven adequate for analyzing flow behavior. This applies to microchannels and is used for microchannel cases. So, this dynamic contact angle can definitely be applied here as well, further complicating the whole development. For better accuracy, this can also be resolved by defining the level set function, which can further be coupled.

So, there exist again another set of this front tracking method or the interface tracking method is the level set function that further can be clubbed with this VOF model calling this as the CLS VOF model. Now, the point is C stands for the combined level set and VOF model which is more accurate than the single set of either level set or the VOF model because the inherent drawback of this VOF model that is that the limitations in considering this static or the dynamic contact angle But the level set tracks that very beautifully and more accurately.



But level set suffers from the conservation of the traditional level set method suffers from the lack of mass conservations and when these are to combine the level set and the VOF method it actually conserves the mass through the VOF as well as it tracks the interface more accurately by the level set method. But anyhow, the point is So, once these are implemented and also if you have a multiphase the non-Newtonian liquid further this tau or this expression will require constitutive equations for the expressions or in order to find out the apparent viscosity.

Once those are incorporated into this momentum equation, because now we have resolved this surface force to the continuous surface force model proposed by Braqueville. And the other terms are solved again for the mixture properties when this is the criteria. Or when this criteria is met, then all the properties are calculated through the mixture properties, or these governing equations are solved for the mixture properties. We solve this problem the iteration actually goes on through the discretization that we have seen earlier by the finite volume method in the finite volume setup or any other discretization technique. It can be solved, and then what it results in is the phase volume fractions with time steps, as well as the flow field and the pressure field.

Whatever the desired thing we have, we need, we require, we collect that information and then look for model validation. But the thing that is essential in order to implement this, as we have seen earlier, is that the VUF model requires a very fine grid. And the choice of contact angle dictates here in this initial part, and it eventually dictates the shape of the droplet if it touches the surface for that operating condition. So, if the situation is that for your flow condition, the dispersed phase grows and before it grows further, it immediately detaches and creates suspended droplets, then the influence of this contact angle is not dominant than when it actually blocks the whole surface or whole flow path of the continuous phase, and then it elongates and after a desired level—after a threshold—it actually detaches and creates the larger droplets.

So, in such cases, since there is a significant portion of the contact angle or the contact line exists, but if that again has to be taken into account, if the contact line the advancing and receding contact line contact angle does not I mean it appears to be within the range within the certain range then this contact line does not move essentially such cases, the choice of static contact angle may suffice your requirement and may predict the desired level of accuracy or the result with desired levels of accuracy. But the point is, when this flows inside the channel, practically what has been seen or what can we understand is that there would exist a three-phase contact angle.

And this choice of static contact angle is important in such a scenario when you have this three-phase contact angle. But when it is not contacting the solid surface, this is the first phase; then, that contact angle, whatever the choice would be, does not influence this whole formulation.

So, this has to be kept in mind: whether this wall is hydrophilic or hydrophobic. Now, hydrophilic or hydrophobic—this nature is actually incorporated through this contact angle value in this formulation.

Now, we will not go into the details of what the contact angle value should be when it is hydrophilic or hydrophobic. That choice or that study is separate. You can look into what hydrophobic nature is, what hydrophilic nature is, and how we define that. But mathematically speaking, that nature is incorporated in the CFD model through the choice of an appropriate contact angle. And that is a very important part while solving such a problem.

And the other practical problem that those who do research in this area face is the capture of a thin film of the continuous phase near the surface. If it is not captured, that means, in that case, the droplet eventually touches the surface. And then, definitely, the static contact angle would not help or would not be sufficient to capture the actual physics of the flow. But if there is a sufficiently thin layer of continuous fluid that means it is there is no three phase contact angle for such cases is not relevant for such a problem, or the static contact angle would definitely be sufficient for that problem.

Now, in order to capture this thin film near the surface, the grid has to be resolved; the grid has to be finer. to a very greater extent and then it would require too much of computational resources or huge computational resources in order to resolve those continuous film of the continuous film of the continuous phase or the film of the continuous phase. So, these things have to be kept in mind, but the point is these are extremely research-specific or problem-specific. If you are doing research in this area, then this information would be helpful.

But the intention of this part of the lecture is to explain how the implementation happened, okay? Or how we apply the VUF model to a certain case. Taking here the example of droplet development or the droplet formulation or the droplet. In a microchannel, in a T-junction microchannel, where I have two different liquid phases—immiscible liquid phases: oil and water. So, the water droplet is forming inside the oil or the other situation may also happen that depending on again then this flow texture or the flow regime would change the velocity and all this thing would have to be set in such a manner

There can be the inverse emulsion stage, where you can have the oil droplets in a water medium as well. Now, these are the say specimen liquids that I have mentioned here the water and oil this can be a different combination different set of fluids and that is how the emulsions are formed or the emulsion studies are done in the detailed research you will find out the formation of the emulsion the stability and all this criteria depending on the properties of the characteristics of this liquids. So, the point is if we now if I now try to summarize this whole thing that what would be the choice of multiphase model once again the summary is that the choice would depend on the wish list or the objective that you have that what you are trying to look into. What is the computational capacity that you have? The resources you must have—you have— You must do a trade-off between the desired level of accuracy and your set objective. While doing so, you have to choose the appropriate modeling strategy. You can always do a direct numerical simulation for all the parts, tracking each and every particle for the dispersed phase simulation, which would be, I mean, the best strategy in terms of accuracy.

But with limited computational resources, if that is the constraint or the time, so considering all these constraints, the choice of other models, for example, Euler-Euler model, Euler-Lagrange model, and in the Euler-Euler model, two specific models we have seen, the algebraic slip model or the VOF model or even the porous bed model. So this choice depends on how large the volume fraction you are tracking okay and also what are the coupling that you are trying to capture what detailed level of phase phase coupling you are trying to capture is it a one way coupling is it a two way coupling is it a four way coupling are you looking into droplet droplet interaction if it is so then

that that kind of appropriate model for example here the VIF model is more appropriate or even the CFD-DEM approach that I very briefly spoke about although we have not discussed the DEM which is of the scope of this work, but the combination of the DEM and CFD can work in such cases. So, what is the best CFD model for multiphase flow? There is no fixed answer to it. It is problem-specific, research-centric, and based on the wish list or the objective for your problem. The desired level of accuracy, the time constraint, the computer resource constraint—whatever you have—and based on that, you find the best strategy.

A single problem, a given problem, can be solved by different multiphase models, and there will be different levels of information. Level of information means: Is it a particle-level or particle-scale level, or is it a macro-scale level or meso-scale level—that is, the cluster of particles or the cluster of dispersed phase? This kind of level, which is the meso-scale, depends And that also directly influences the choice of your model for the multiphase flow. So, on this note, I will stop this discussion here on multiphase flow.

In the next lecture, we will move on to the other topic and introduce turbulence, which is another vital aspect of CFD modeling. But again, remember that whatever we are discussing here This is a brief overview of each and every topic to give you a flavor of how all these things are modeled by the CFD modeling approaches. Each subsection itself can be studied in greater detail and can constitute a full course on its own—the multiphase, the turbulence, the reactive flows, etcetera. So on this note, I will stop here today and thank you for your attention.