CFD APPLICATIONS IN CHEMICAL PROCESSES

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Lecture 44: Modeling Multiphase Systems

Hello everyone, welcome back with another lecture on CFD applications in chemical processes. We are discussing modeling of multiphase systems and specifically Euler methodology. In the last lecture, I told you that we will discuss in this class the solution of or the modeling of a packed bed or the trickle bed reactor with two-phase Eulerian simulation. So I have a bed. Now this is packed bed. The catalyst particles are filled in this portion.

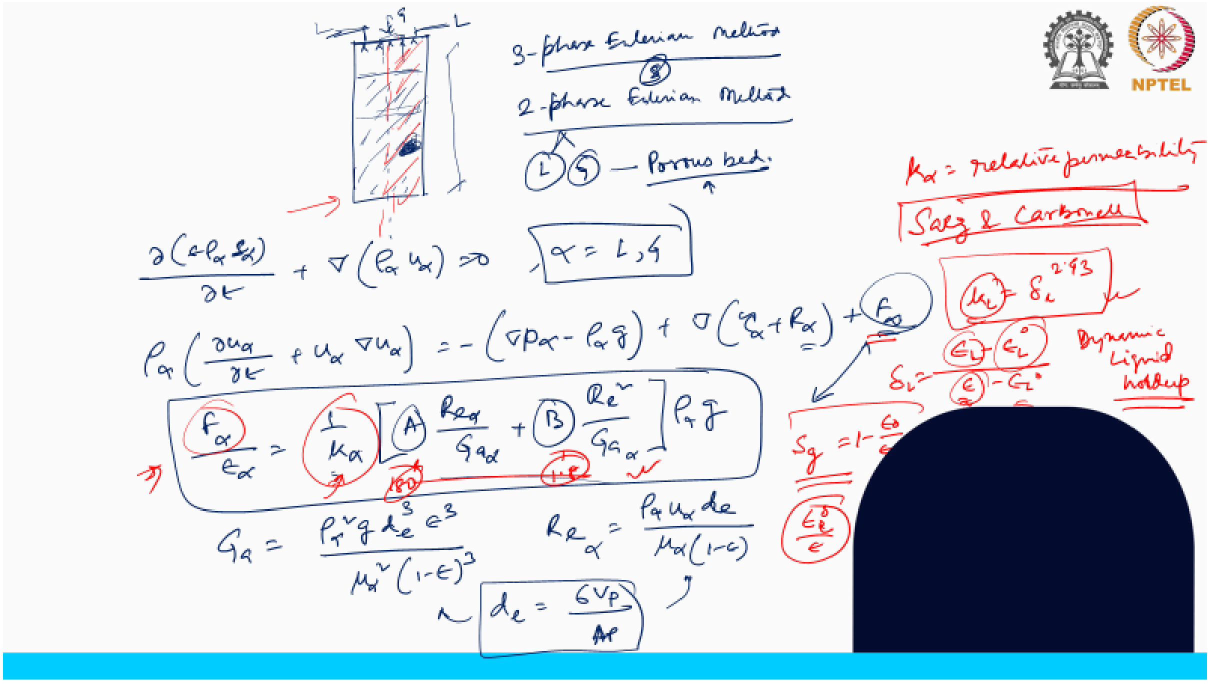
So, we have a distributor at the top. So, this distributor these are the liquid inlets and say I have inlet for the gas phase as well. So, these are the liquid inlets and we have the gas phase. We have seen the classical 3 phase Eulerian simulation where this packed bed was presented or represented in a manner that we although we had the solid particles, but we are not considering them individually.

Instead we are we represented those solid phase as the voidage profile as a known voidage profile. And then with the set boundary condition we solve the problem with few additional details that whether the bed is weighted already pre-weighted or it is dry that adds the complicacy to the problem the startup condition. And those three phase Eulerian simulations for this problem gives us even at the particle scale phenomena or it allows us to consider whether there is partial weighting of the catalyst bed or it is fully weighted condition.

But the point is, if we say industrial-scale reactor and we are not bothered about this particle scale understanding that whether it is partially weighted or fully weighted, rather we are focused on the overall pressure drop, the quality of liquid distribution because maldistribution would result eventually in hotspot formation where at some portion the catalyst would not be weighted due to this liquid maldistribution, and that would result in some hotspot formation, which is not desirable. So, if those are of our primary importance, that means how the liquid

or the gas—both their distribution profiles—are and whether such hotspot formations are happening along any axial location or even in radial locations. Then, we can think of an alternate strategy, which is implementation-wise, a 2D Eulerian simulation or 2D Eulerian method. And that means, by two phase two phase Eulerian simulation that means, only liquid and gas we will consider and the solid phase which was explicitly considered here in the three phase simulation would not be considered here rather the solid phase would be represented as a porous bed or a medium in which the flow resistances are represented by the voidage profile because we can understand that the voidage dictates the resistances: where the voidage is higher, the flow resistance is lower.

So, this voidage and the flow resistance—or the voidage or the flow resistance—that is incorporated in this porous bed Usually, if we consider uniform porosity of the bed, we give one single value and assume that an equal amount of liquid would pass through every location. But since we know that does not happen in this real packed bed scenario, that means there is a higher voidage near the wall, that means higher chances of flow going through the near the wall or the flow resistances are lower near the wall. Considering that fact, this 2D Eulerian simulation can work.



So, in this case also, the governing equation remains the same—that means we solve the continuity and the momentum equation, like the previous case. That means, if we explicitly write here, So, say this S is the—here you can consider as the volume fraction of it—and alpha is the corresponding Now, these are the stress terms that may arise. It is written in a generic form that may arise at the volume average, the viscous stress tensor, and the turbulent stress tensor.

But this turbulence does not occur in the trickle bit. So, we neglect that. And this F alpha is basically again the interface coupling term. It is written in a different form than the previous case, but again, it can be written in the instead of alpha if we replace that by k, it would eventually look like the previous case. So here, this is the volume-averaged interface drag term which is

The reason K is not written here is that we have introduced K here, which is different from the conventional Kth phase here, and that I am coming to this. So here, interestingly, this is alpha either for liquid or gas—no solid phase is considered—and this is the closure model, one of the ways of incorporating this interface coupling term. So, that is written here by the term k here; the rest you can find similarity with the single-phase flow argon equation, where GA is the Galileo number, which again, epsilon is the bed voidage, Reynolds number is for this case, DE is the equivalent diameter; if it is spherical, it is simply D or DP.

So, this equivalent diameter is nothing but the 6 VP by AP, which is the volume of the particle divided by the area of the particle. So, if it is irregular shaped particle the corresponding d e the equivalent diameter is calculated and by that we calculate the Reynolds number and the Galileo number and those are implemented here with the empirically fitted constant a and b. Now, the point is you look that these is except this part is similar to the single-phase Euler single-phase Ergun equation.

And indeed that is the case and that is modified for the multiple phase because if it is a single phase flow through the porous media this is the equation where this is our viscous part and this is our inertia part and again if it is the inertia part is neglected it boils down to the Darcy's So, the point is we find similarity except this part, which is to take into account the second phase or the different phases or the other phases than the single phase. Since we have two phases here, this K alpha is called the relative permeability. We understand permeation, the permeability, bed permeability—how easily it goes through around that place.

But here it is relative because we have two phases present. So, there is a competing mechanism in order to fill a void space when the gas and liquid are flowing, okay. So, this competing mechanism is represented by this relative permeability concept. So, this relative permeability concept was proposed by—again, all this comes from the research-centric understanding or from the detailed research on this particular topic. Since we are looking into its implementation, that is where we are going into a bit of detail on this.

So, these were developed by Saeg and Carbonell, two scientists, two researcher. And they proposed that this relative permeability is essentially dependent on the volumetric function—the volume fraction—which is represented in a different way here. So, usually, for the liquid phase, So, K L is related or was equated by an empirical relation: delta L to the power of 2.43, where this delta L is called the reduced liquid saturation, and that is defined as this epsilon l minus epsilon l 0 divided by epsilon minus epsilon l 0.

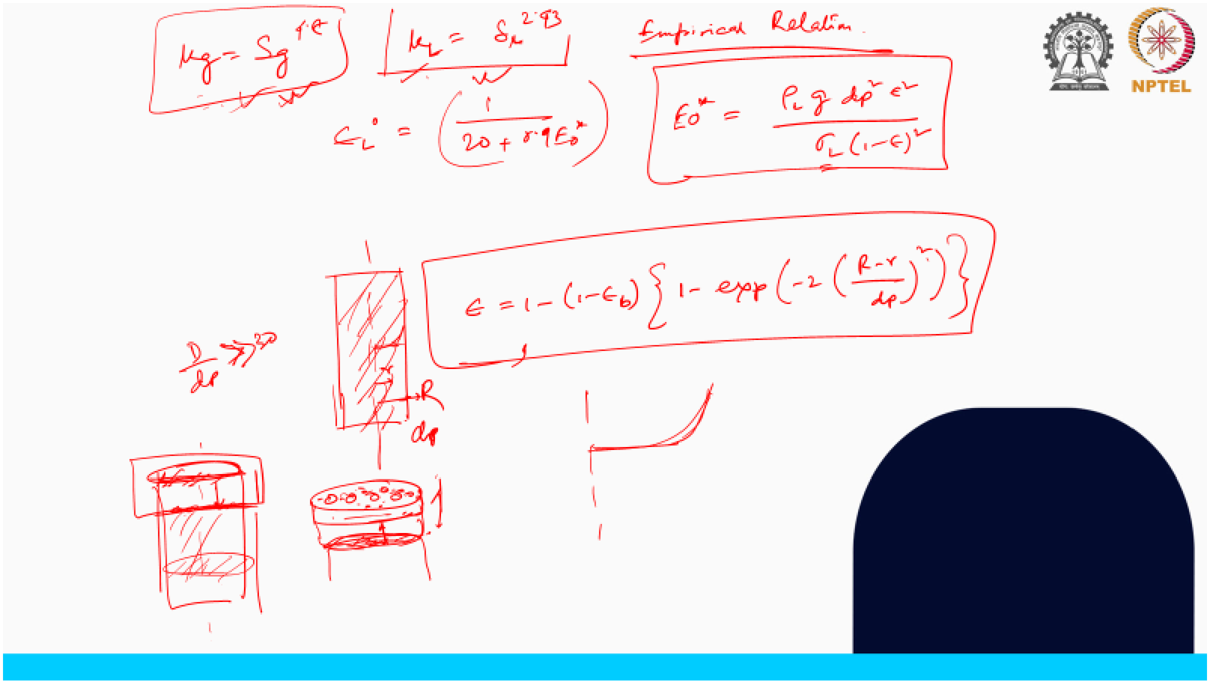
Now, what are these values? Epsilon l is the volume fraction of the liquid phase, epsilon l 0 is called the static hold So, this in other term we can consider as the dynamic liquid holdup. So, dynamic liquid holdup. standard terminology in packed bed reactor when we find out the liquid concentration or the gas concentration we call those as the gas hold up or the liquid hold up.

That means, how much volume fraction of the liquid exist per unit volume of the bed that is the liquid hold up or specifically here the dynamic hold up when that is in flowing condition or there is a continuous flow that is happening. But remember the start of operation that the bed is completely weighted ok. So, initially the bed is dry that means, your hold up liquid hold up is 0 in that bed. Then what you do you flood the liquid ok, you the bed is completely flooded with the liquid and all the interstices are filled by a single liquid phase.

So, somehow it is done experimentally and then we drain out that liquid and leave it for drying. So, initially it was dry then that bed with feel was filled with the pure liquid phase or the single phase and that single phase was drained out and after that we measure that bed liquid content. Whatever amount of the liquid would stick into the interstices or would be on the catalyst surfaces which is not would not drain out that is we called as the static liquid hold up that actually remains in the bed ok.

So, that is the static liquid hold up or this part. this epsilon is the complete bed voidage and again this is the static liquid holder. So, this is the reduced liquid saturation which is defined as this and the gas saturation which is if I say the SG is essentially 1 minus static portion divided by the bed voidage which is essentially is the for the liquid component and 1 minus of this liquid volume fraction is or the saturation. So, saturation is defined as this, this is the liquid saturation ok.

So, this is the L for the liquid saturation. divided by the bed voidage is the saturation corresponding saturation. So, this is similarly for the gas saturation. So, K L or this when alpha is L it is equated with this and when it is gaseous phase we have another empirical relation which is S g to the power 4.8. Now, this K L and K g 2.43 these are completely empirical relation which means with several experiments using different ah type of particle. using different type of particle, different size of particles, once these experiments are done, they found these relations are best fitted for those experiments or experimental points.



And these relations were developed or actually were provided by again different set of scientists or the researchers. So, now since these are again I am saying that these are research centric or specific to the your research if you are interested, but it is to show you that how implementations are done in the CFD model. You need not remember these expressions, you need not remember these empirical relations, but the point is where the value.

of the liquid hold up or the static liquid all these things are plugged in that you have to understand. So, you can make your model more accurate if required. So, that means once you give these relative permeability correlations and similarly these values, this static liquid holdup is also difficult to measure. So, but people have done it in the past for experimental conditions or lab conditions, okay. With lab experiments, they have come up with equations also. For example, one such expression is that the static liquid holdup can possibly be measured from this.

relation where this is the aod plus number and is expressed as this expression, okay. Such correlations for the static liquid holdup also exist. And here, interestingly, you would see that this liquid surface tension is incorporated while calculating the static liquid holdup condition. And these relations would go back here, which would help us evaluate the term F alpha in the momentum equation. So, this is where

These phase-phase interactions are incorporated with the help of F alpha, which is calculated based on K alpha, the relative permeability. Relative permeability is further estimated by different permeability correlations either developed experimentally or empirically considered or if you do your own experiment you can find out this correlation you can use it different values. Now again the point is as good as this the empirical relations would be that much accurate your phase-phase interaction would be and that would result in that kind of desired level accurate model predictions by the two-phase Eulerian model.

So, the point is again, we consider a 2D axisymmetric domain. That is shown here. For this 2D axisymmetric case, we consider this half of this part. We impose the similar voidage profile because that voidage profile you can see that this voidage profiles are there it is necessary for the calculation of K L and K G. That means the relative permeability is essentially dependent on this voidage profile.

So if it is varying in all the direction, similarly the relative permeability values would vary in different direction, which means the bed is of not uniform resistance. Accordingly the flow would happen in different direction. So now the another part that comes, so once we do that we can solve this part. ok like we have done earlier. Again this void is profiled that I told you

If you take a longer larger bed where d by dp ratio is much greater than 20 or 30 then certainly what you can do you can consider the uniform bed voidage and a profile say that goes uniformly and suddenly goes valid to goes back to 1 at near the wall. So, such profiles also exist and for such profiles let me write one expressions because that is also available in the literature. ah that is that kind of profile has been proposed already. So, such profile if you plot

For different values of R, which means if this is my center, this is the R, this is the DP is the particle diameter and this is the complete radius, which is capital R. You would see such kind of profile exists that it goes to value 1 near the wall at the sharp point from the display. see which is relatively easier to implement because these equations have to be fed into your default CFD model that are usually not available in the commercial CFD solvers. So, you have to incorporate the porosity profile in the model by this user defined function in ANSYS fluent or in other way in open form. So, with this you can solve this part again as I told you there exist several empirically fitted constant that has to be considered carefully because remember empirically

fitted constant means those are derived for a certain range of particle size particle shape or a particle or a say operating condition. if your objected problem, if you what you are solving the problem, if that problem is outside that boundary, then you have to tune in or you have to tune this empirically repeated constant values that are there in your model. then those default values or whatever values it is considered for the one particular research papers they have given you this relation saying that okay now my A and V values are 180 and 1.8. So, this is 180 and 1.7, 1.8 such kind of value, but they did their experiment with spherical particle of different sizes etc. You have cylindrical particle or cylindrical catalyst in the bed.

So, these values will have been to be adjusted accordingly so that you get more accurate result. So, the other point that I was trying to discuss is that once you do this part there can be another opportunity to improve the model. I told you say if my objective is to find out the liquid distribution profile in the bed, which means I also have to model my distributor which is at the top. So, how do we do that in Euler Euler because Euler takes an approximated or say weighted average quantities. So, if I have to have an understanding of precise velocity or the volume fraction distribution at a distributor where I have a clear distinct path or the entrance of two different phases.

ok, then we can decouple this whole problem into two different or by the two different modeling strategy. What we can consider is that this distributor part we solve it by tracking their interfaces or how good is the distribution after a certain millimeter or centimeter from the distributor section because usually the bed starts after a certain distance from the distributor. There are some supports so that it does not really destroy the catalyst with such high velocities. So, there are certain gaps from the inlet of the distributor to the packing portion.

So, we can consider that surface and we can understand that how the velocity or the phase distribution at this surface from where the packed bed starts. So, we are decoupling this that till this portion I will use one strategy or the modeling strategy to understand my phase distribution and taking the inlet of the packed bed as the outlet of the previous one and solving the rest of the part. And then, we can also find out at different cross-sections in the post-processing what the phase distribution is. So, this means that if you are not confident or not convinced by the solution of the Euler simulation for the distributor,

you can use different font tracking method or the interface tracking method such as the VOF method, which we will discuss in the next lecture, that we apply VOF method for the distributor design and taking the outlet or the result of the VOF as an inlet to my Euler-Euler simulation. That starts with a simple packed bed or porous bed. So, we have to be improvising with the strategies for a given problem in order to simplify it, but not that simplification where it would not result or give me a realistic result of the accurate solution. So, on this note, I will stop here today because this is the part where we have extensively discussed Euler-Euler simulation.

In the next lecture, we will move to the other specific method, which is the volume of fluid method. It is also quite interesting to see. We will also discuss one example with the volume of fluid method, and then we will move on to the other topic. So, on this note, I thank you for your attention.