CFD APPLICATIONS IN CHEMICAL PROCESSES
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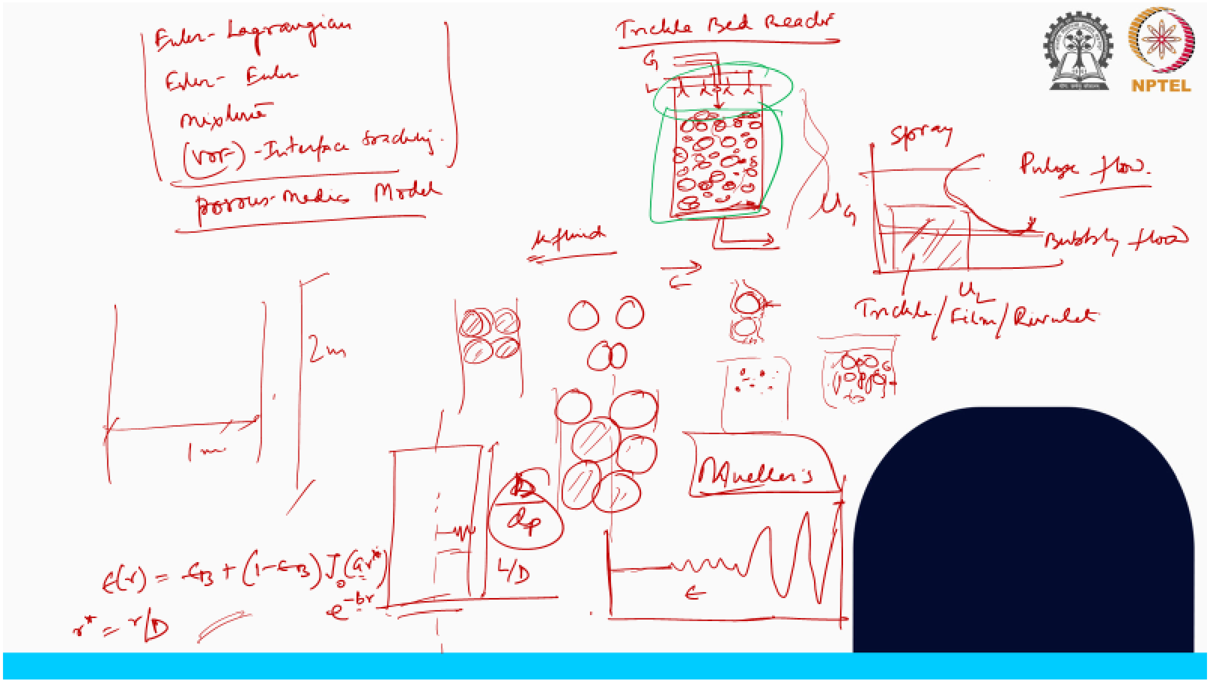
Week-09
Lecture 42: Modeling Multiphase Systems

Hello everyone, welcome back once again to another lecture on modeling multiphase systems in CFD applications for chemical processes. So, we are again discussing different modeling strategies for multiphase systems, specifically where multiphase flows exist. So, how we encounter multiphase flows and how we tackle those systems, we are discussing those with an overview that we had already seen, starting with the Euler-Lagrangian. Euler model, mixture model, and VOF, which is one of the front-tracking or interface-tracking methods. So, and there we also have to discuss, as mentioned earlier, the porous media model.

Now, we will do this with the help of a case study, which is the modeling of a packed bed reactor, or specifically, a trickle bed reactor. Trickle means when the gas and liquid velocity. So, in a conventional packed bed reactor, what happens? You have thousands or millions of particles, or the catalyst bed consists of thousands and millions of particles. You have a distributor where you distribute from the top the liquid phase, along with that comes a gas phase.

So, these are, say, the liquid inlet; you have a distribution system, which is the liquid inlet, and we have a gaseous system or the gaseous distribution system. So, the flow of gas and liquid will be from top to bottom because we are considering here a co-current downward flow, where at the bottom you have the collector. And the product goes; you are collecting the product. Now, in this case if you remember in one of the lectures I mentioned that gas and liquid this interaction when it flows over the catalyst bed is important because that dictates that how the phase phase interaction is happening. How closely it is interacting and accordingly it is resulting or yielding some product.

Now, for that or related to that, if you may also remember, I mentioned something about this—say, the liquid velocity, the gas velocity, and a flow regime map. That means you usually have such a kind of map or demarcation line. Where you have a velocity in which, or here in this portion, you have a certain flow regime. That means, when the gas and liquid velocities are on the lower side, what happens is that each and every particle, or those particles, tend to be completely wet by the liquid phase and the catalyst particles are completely wet depending on also the bed pre wetting condition catalyst bed was previously wetted before starting the experiments. So, there are a few criteria that exist, but the point is when the gas and liquid velocities are low or on the lower side, then this liquid actually trickles down the catalyst surfaces. And that is why the trickle-bed reactor name comes when it operates particularly in the lower gas and liquid velocity region. Keeping the fixed gas velocity, if you increase the liquid velocity to a substantially higher velocity, then what can happen is that you may achieve the bubbly flow, OK?



So, in bubbly flow, what will happen is there is a continuous liquid phase—it is completely filled with the liquid phase, and there are certain bubbles that are floating around or passing through. If you keep the velocity on the lower side and then increase the gaseous velocity, what will happen? You may find a spray rising. That means you have a suspended

Liquid particles or the liquids inside this bed voidage, and you are having a continuous gaseous phase, just the inversion of this bubbly regime or the bubbly flow. So, you have either spray at one extreme or bubbly flow on the other extreme. If you operate at a low velocity in both cases, then you have the trickle flow regime. Or you can also say the film flow, because there is a film or rivulet, as it is also called. So, in rivulet flow, you can expect that each and every particle or catalyst around which you have a film of a continuous phase.

And if the velocity of this gas and liquid phase is both higher. amount or high in very high flow rate, then what you get is the pulse flow, ok, where this whole bed is kind of in flooding condition. There is a high amount of throughput of gas and liquid that is passing through, those are having a lesser contact time between the phases and shorter residence time of the phases or the reactants. Now, depending on the reaction that you have chosen. to do in a packed bed reactor, there are also certain criteria; we will not go into how we choose a packed bed.

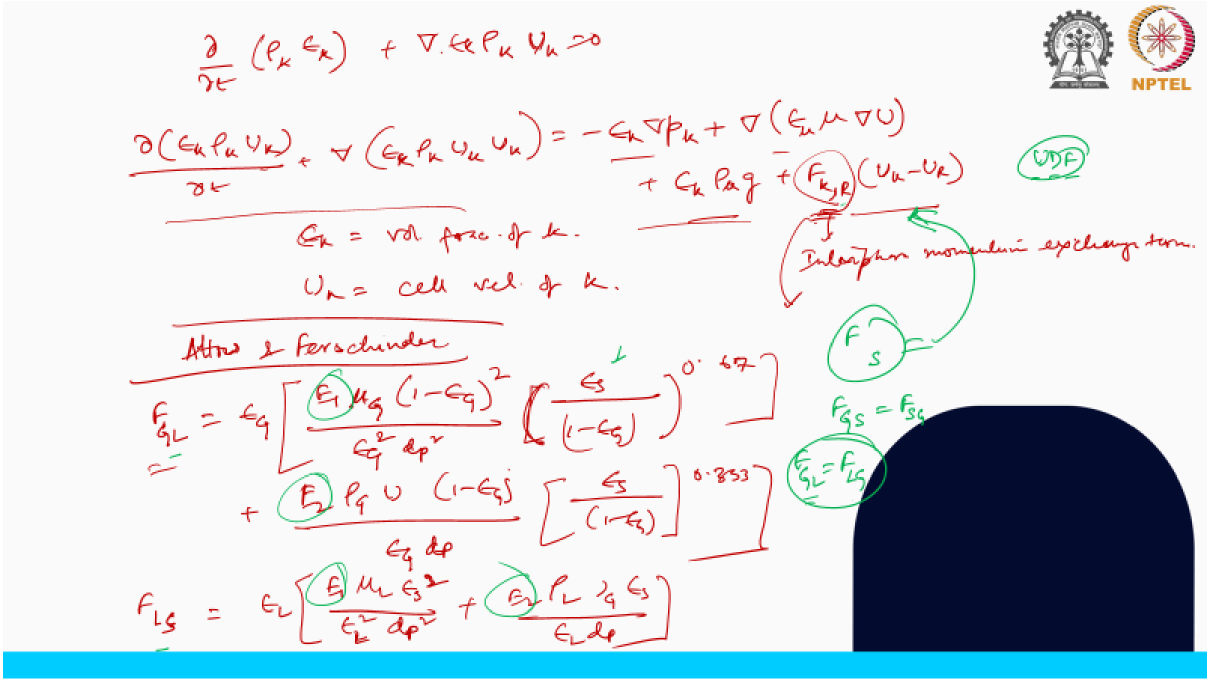
We consider that if you have chosen a packed bed and if you have to model this in the system by computational fluid dynamics, particularly by this Euler framework, then there are two different approaches that we will discuss here. So, conventionally now, you can think that there exist three phases: gas, liquid, and the solid phases. So, if we try to consider the Euler-Euler simulation in this case. So, then this process here is called the k-fluid simulation, or here the number of phases of k is 3. So, we consider there is a three-phase Eulerian simulation we have to do.

Now, there are a few things, a few intricate details. Since this is an example we have taken, we will quickly discuss how we will go to the simulation and, before that, what things we have to set in the simulation. Pre-processor, because we have discussed that for this simulation to happen, we have a pre-processor, then the processor, and the post-processing part. So, in the pre-processor, you have to design the computational domain or come up with the computational domain. You have to set the boundary conditions, the initial conditions, etc., and then you have to simulate in the processing part. And in the post-processing part, once you get the result, you analyze it for its desirable properties or the required properties that you are looking for. So, to set up this problem, one way is that you individually take into account these solid particles.

Now, remember, these solid particles in practice or in real conditions are touching each other. And also, those are touching the surfaces of the container or the vessel. Now, few researchers have considered the non contacting particles because of the meshing issue or the issues that are created by the discontinuity when we consider particles are contacted with each other and then the creation of the voidage is difficult. Although, when you consider this in three dimensions, there would definitely exist some voidage, but those would be different from the real-case scenario.

So, one way is to model these individual particles. Now, that approach is inherently difficult if you understand there are millions of them. Such simulations are considering those individual particles and considering their shapes individually and how those are touching the surfaces or how those are contacting with each other whether it is randomly packed or strategically packed. In reality, those are basically dumped.

So, you do not have a structured packing per se, but there are structured packings available to increase the efficiency of the reactor. So, depending on the scenario, whether it is structured packing or random packing, you have to take care of each individual particle or the catalyst. which is quite impossible for the real-case scenario when you have, say, a 1-meter diameter column with a 2-meter height. The real cases involve millions of particles. So, but in those cases also, considering that and considering two other phases, we have to write the governing equation and solve it with the appropriate boundary conditions.



The next strategy is that it remains a three-phase simulation, but we do not consider each and every particle separately. What do we do? We consider or take the voidage profile from the beds. And for that experiments have been done, several research have been done and it has been seen that the voidage inside this particle, inside this bed, this is the bed, and this is the center line—has an oscillatory profile. Specifically, the profile looks like this is the center line.

So, it is nearly uniform up to a certain particle diameter, then it oscillates, and then it reaches a maximum near the wall. So, this is, say, if I say the voidage is epsilon. So, this voidage profile is something like that, from the center line towards the wall, where near the wall, we have the maximum voidage profile. And incidentally and in fact, fortunately the researchers have modeled this voidage profile for which we have an equation and

equation for the packed-bed case, which we call Müller's equations. By Moeller's equation that has the say profile something like this that in the radial direction this voidage is essentially the bulk voidage which is the uniform till certain value or till certain particle diameter. Now, again for the packed bed, there are certain important things: one is definitely the L by D ratio, which is the length of the bed and the diameter of the bed. for a certain L by D this is this profile is important and this mainly is dictated by the bed diameter to the particle diameter D by D p.

So, for a certain D by D p range the profile looks like this is the Bessel function. Now, this A— So, this is the say r by r star if I for the time being if I write r star multiplied by e to the power minus b r. This a and b are the empirically fitted constant, r by d, and j 0 is the zeroth-order Bessel function. So, the overall point here is that we usually have this voidage profile known. People do experiment for example, MRI and all to understand this voidage profile and they have reported more complex or complicated function recently as different profiles. But in most cases, this standard Euler's equation fits well with the numerical simulation. So, the point is, such voidage profiles can be implemented in the domain and also— So, this goes for the radial variation of epsilon, which is the velocity voidage profile, and also there we can have a Gaussian distribution along the axial length. That means, for a particular radial position, we can also have the Gaussian distribution of the voidage profile. Those can also be imposed or integrated into the domain instead of individual particle consideration.

So, instead of individual particle consideration, we can consider various voidage profiles because that gives us the flow path. And, in computational flow dynamics, what is important is to create grids or meshes or to solve the governing equations in those grids where the flow is happening. So, that is essential part you must remember that we try to find or we try to make meshes or grids on those parts only where the flow is happening, because there the for that part the flow governing equations are being developed. And the rest we either set as the boundary condition or some other conditions that are fit for the problem.

So, the point is, once we define this domain with the help of this, what we solve is the mass balance—the continuity equations. So, if I write that for the kth phase, it is essentially rho k epsilon k plus u k equals 0. This is the continuity equation or the mass conservation equation and the momentum equation for each such phase. where this pressure is shared by all the phases. So, where this is the volume fraction of the kth phase or each phase rho is the density and corresponding k is for the kth phase,

uk is the cell velocity of the kth phase in that cell, p is the mean pressure. by all phases that are present in the system. FKR, this term is the interphase momentum exchange term. So, the point is this term eventually represents the rate of change of momentum of the this whole part rate of change of momentum of the kth phase and this right hand side presents pressure force, gravitational force or the gravitational acceleration, average shear stress and the interface momentum. term that are present in the system.

Now, in this case, the gas-solid usually what happens is in this case the liquid and solid, these two phases are considered as the secondary phases, and gas is considered as the primary phase. So, solids, although stationary, are considered as another phase or the third phase here. setting its velocity as 0 in those cases. Now, this FKR is the interphase coupling term, and I told you earlier that this term we have to now model or we have to consider how this phase-phase coupling is happening. And for that now you consider that for this particular trickle bed, now these equations what we have written are applicable

for any of these fluorescence be it spray, be it trickle, be it bubbly or the pulse fluorescence. This is the generic set of equations, but what matters is the closure of this FKR. that is the interface momentum exchange term, those are then varying from regime to regime or flow texture to flow texture. Because in this condition, you have this film or revolute kind of flow at very low velocities, but as you change it, it gets bubbly or becomes a spray-type condition. Now, when you try to understand this gas liquid interaction with the solid for this film flow, it is certainly different from when it is suspended

gas bubbles are suspended or the liquid droplets are suspended in the continuous medium. Now, from this fundamental of the film flow or the revolute flow, these coupling terms are developed. And that is why, when those are fundamentally or analytically developed, it becomes—when we close this—a particular flow texture or resin-specific, okay? So, in this case, again, fortunately, research has been done, and researchers have proposed these interactions or the force coupling terms. Through empirical or analytical relations.

One of such relation that is very popular is suggested or proposed by Attow and Ferschinder is that FGL that means, the gas liquid interaction The expression looks something like this—again, E1 is the empirical constant, and that comes from the Ergun equation. Because here, if you consider or if you remove one phase, usually this pressure drop— And the other parameter, specifically the pressure drop, can be predicted by the full-phase Ergun equations. So, these empirical constants are similar to the—

But, again since these are the empirical relations or empirical constant this number or the value of E 1 and the other values can vary and that has to be adjusted as per the particle those also depends on the particle shape sizes or nature. So, these are the fitting constants, and that is why, when we use these Euler equations or the Euler model— It already comes with simplification and then several of these closure models, which further— The empirical relations or empirical fit make it less accurate than the DNS model, of course, or the Euler-Lagrange models. But as you can clearly see, for the industrial-scale problem, these are the best possible or the most efficient ones that we can use.

So, just to show you the pattern or the parameters that are involved, because these are important, or again, these are merely for reference. One need not memorize this expression, but to show you what the parameters it involves are and what the things that are necessary to know to model this are. So, what you see is that the proposed phase, particularly the gas and liquid interaction term. Similarly, they have also proposed the term for the liquid-solid interaction, and where all these epsilon g l are the volume fractions of the corresponding phase, l stands for the liquid, g for the gas.

These E1 and E2 are essentially empirically fitted constants, and they have certain values for certain types of catalyst particles that you use or that fit your objective. So, the nature, you can see, is quite complex, and the terms that are involved in this problem. So, here, these E1, E2, as I was saying, are empirically fitted constants; these are the volume fractions of the corresponding phase, S stands for the solid, G stands for the gas, and L stands for the liquid. So, similarly, what happens is that you have F_GL, which is gas-liquid, F_LS, and you also have F_GS expression, OK.

So, the point is while writing for each and every phase say for example, now you replace K with the liquid phase and the corresponding R here comes twice because one is with the liquid-solid and one with the liquid and gas, and accordingly, these expressions are solved with this equation, OK. And in this case, yes. So, similar this gas liquid and gas solid these terms are then solved here corresponding to here also one has to understand that f l s g is

essentially the g s and f g l is essentially f l g. So, when you write for the liquid phase of the gaseous phase if you Come across LG or GS; it is essentially a similar term, but you know, with a different sign, it would involve because those forces have to be balanced. So, the point is The gas liquid momentum exchange term and the gas solid momentum exchange term all these there are certain models are available see in conventional or commercial CFD models.

You will have several interphase coupling terms, and there are options to choose from those. So, if you choose from those, it is the default model that you are solving, and if it does not satisfy your problem or if you are not with those interface coupling terms, you have to write your own forces that you deem fit for your problem as the user-defined function or user-defined code in the problem or during the solution. In conventional terms, or say, the most commercially used is ANSYS Fluent, where those are mentioned as the UDF, which is the user-defined function. So, and then with the appropriate boundary conditions—that is, the velocity inlet and the velocity outlet or the pressure outlet

and with the other designs of the internals, this problem is further solved. So, I will stop here today and again in the next lecture I will be back with this content, but with the addition of few other features because here what we have seen is simply a solution that happens in this part. But, what about if someone wants to further also try to design the distributor part, how a single model or how multiple models can fit into a same problem or a single problem to solve our overall objective. So, we will take it to the next lecture; we will continue from here in the next lecture, and until then, I want you to grasp this idea that how it is happening you can further look into the reference books that i already mentioned for the details and if you are definitely interested in particularly packed bed.

So on this note i stop here today and thank you for your attention.