CFD APPLICATIONS IN CHEMICAL PROCESSES

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Lecture 43: Modeling Multiphase Systems

Hello everyone, welcome back to another lecture on CFD applications in chemical processes. We are discussing the modeling of multiphase systems, and particularly since the last lecture, we have been discussing the implementation of the Euler-Euler methodology. Taking a case study where we considered a packed bed and specifically it is named as the trickle bed that operates in a specific gas liquid flow condition of the flow regime because based on the gas and liquid flow rate

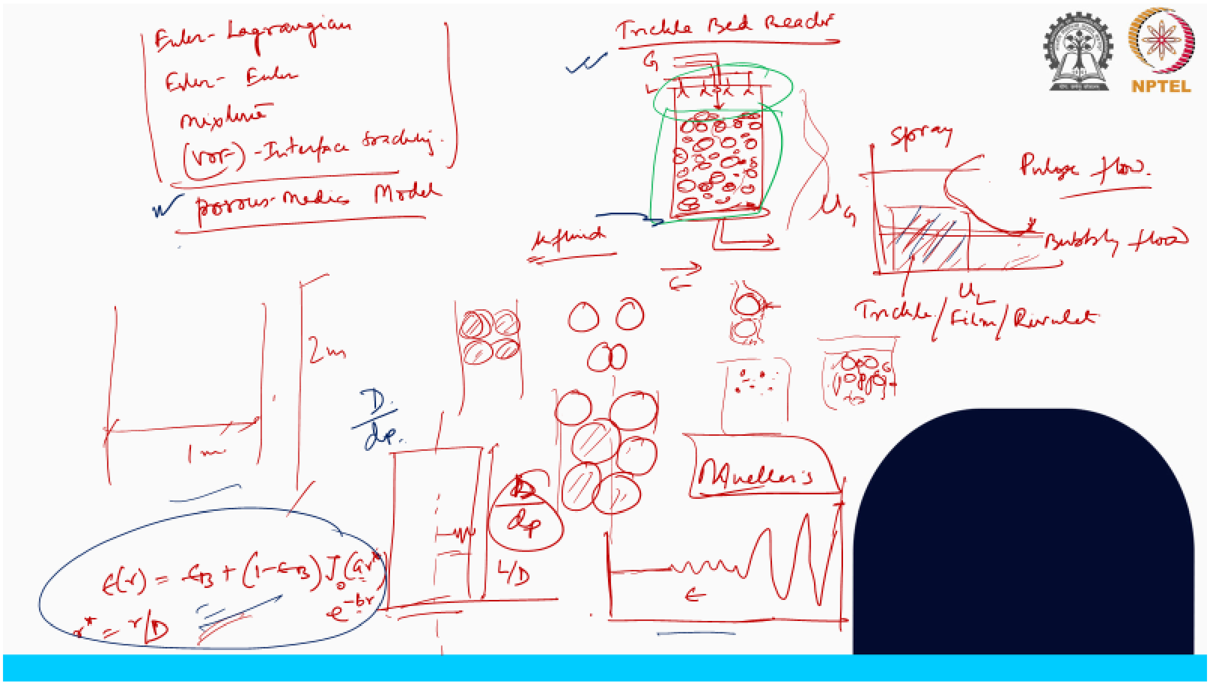
we can see that there exist different flow regimes or flow patterns, flow maps, and the trickle flow regime operates in the low gas and liquid velocity regime. And there, it helps in developing the closure models, which is why the information of this flow regime or the flow texture in a multiphase system is essential. So, we realize that there can be two broad classifications or ways of implementing this Euler methodology. One is considering individual catalyst beds. Draw that in the domain; the computational domain itself exists with their packing style or packing orientation, and through the voidage, the gas and liquid flow would happen.

But the drawback is that for a larger system for a commercial scale reactor of this size in the order of meters, such practice or such methodology would not be helpful for us because of the computational resources or the computational power demand by that methodology. And also, it is extremely difficult—nearly impossible—to draw such packing orientations if it is a random or structured packing of millions of particles. So, the alternate strategy is to consider the voidage profile that results from this packing or from the catalyst dumped inside the bed, and for that, there exist several porosity variations or voidage variation profiles inside the packed bed.

either some of those or one of those or we can develop our own from our laboratory experiments or the pilot skill experiments or some other techniques by which we can determine what is the voidage profile of our considered packed bed. So, one such well-established and frequently used profile in packed bed modeling is the Moeller's correlations. That correlation looks like something in here that I have shown here, which is the radial variation of the porosity. It equals the bulk, which is the average bed porosity, plus the variations that relate to the zeroth-order Bessel function and the r/d ratio, meaning the radial distance and the bed ratio.

A few things in a packed bed. Now, this is very specific to a packed bed since we are considering this case study for the packed bed. The thing is that this porosity variation depends on D/dp, which means the capital D by small dp, the bed diameter by the particle diameter ratio. For large-scale reactors, this D/dp ratio is very large because dp is in the order of millimeter-sized particles, and the diameter is in the range of meters. So, beyond a particular range, say around 15 or 20.

it is usually considered that this bed voidage or the bed porosity its variation from the center line for such large value of d by dp when it is much greater than 20 or so that the porosity variations is nearly uniform and it jumps to a certain value or it goes to 1 near the wall or at the wall. Such variations can also be taken into account while modeling. Now, this is problem specific, it is up to you and depending on this d by dp ratio whether you measured it or you are taking some correlations from the literature for the operating range for which that correlation is developed.

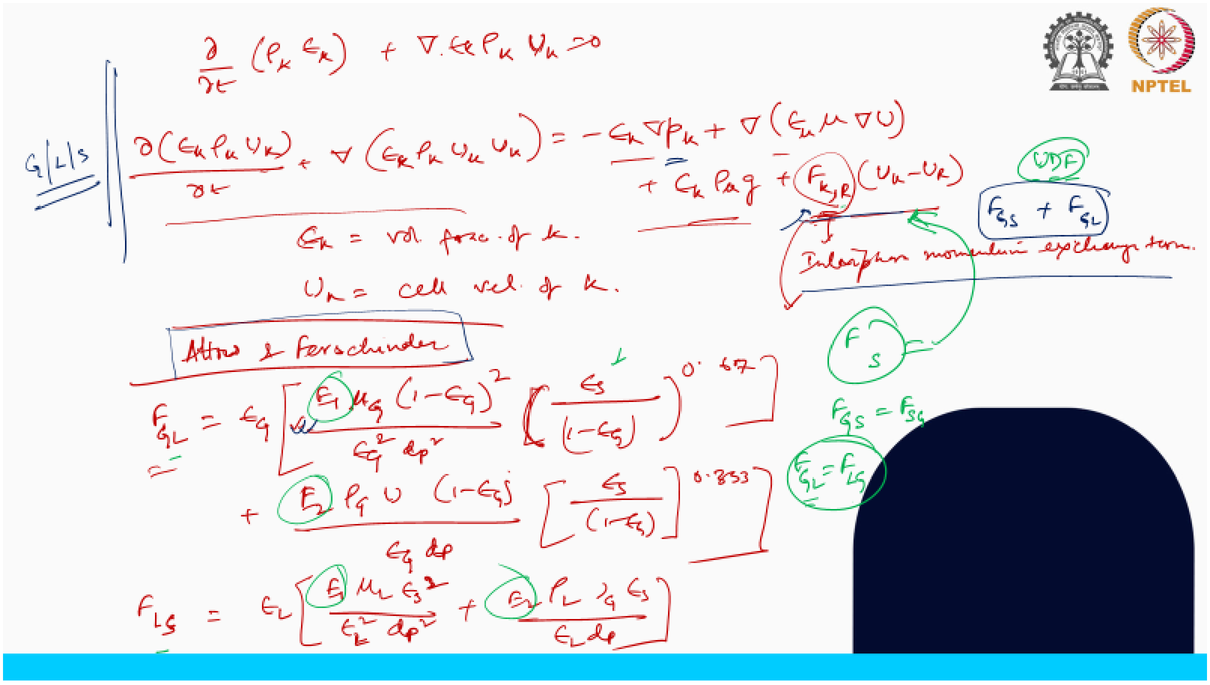


So, once we have taken this, the usual process is that we then consider the domain, the computational Now, here, since we are considering for the sake of simplicity that we have spherical particles packed or stacked inside this packed bed, those are having this known porosity profile. So, what is generally done? It is considered as a 2D axis-symmetric domain. So, this 2D axis symmetry domain is considered for the simulation instead of the full packed

because now we are not considering the individual particle and its orientation or packing style, but we are incorporating the resulting voidage their profile is passed or we implement that in the domain. So, once we do that then the job is to define the boundary condition since this is the axis This is the inlet, this is the outlet and this is the solid wall. At the inlet you have to then define the gas and the liquid velocities or their flow rate and this outlet is usually open to pressure open to atmosphere.

So, pressure outlet boundary condition is provided here and this is the rigid or the impermeable wall that is defined. Once it is done, then we simulate or we run the simulations for the governing equation that I have already shown here. Now, since we have eliminated each other's cases of all the solid particles there, but still in the classical three phase simulation. the solids are considered here with their velocity 0 ok. The resulting voidage is imposed and two phase flow happens through the pattern.

While doing so, we have seen that there exist and one interphase momentum exchange term Now, this interface momentum exchange terms are nothing but the expression that we started understanding in the last lecture is that see FGL. FGS and FLS that means gas liquid interaction, gas solid interactions and liquid solid interaction. Here since we consider usually in the packed bed that the gas as the primary phase and then the liquid and the solids are the secondary phase in classical three phase Eulerian simulation. And these terms are actually replaced I mean are fitted in here instead of this FKR which is K for the one phase and the R for the other phase.



So, this FG, LFGS, FLS are actually fitted here depending on which phase you are solving this momentum equation for, either gas, liquid, or solid. So, if you are solving for the gas phase, then there would be two terms: one for FGS plus FGL. Now, these two terms have to be modeled. Now, as good as that model is, the predictions or the simulation of this case will be that accurate when we compare it with the experimental result.

So, now these are the closer models for multiphase flow or multiphase modeling. And the expression I stated, the one developed by Artaud and Freisneider, is that This is just to show you what parameters are incorporated in such modeled terms. This epsilon means the voidage, and when it is subscripted with g, that becomes the volume fraction of the gaseous phase in the system. We spoke about this E1, which is the empirically fitted constant.

0.667 plus E2. So, first, you can see—let me write it, and then I will explain. times 3. So, this expression consists your the voidage and this is basically the packing fraction okay and mu rho are the understandable properties the conventional properties and here now if you look at it the first term. is associated with the viscosity; the second term is associated with the density.

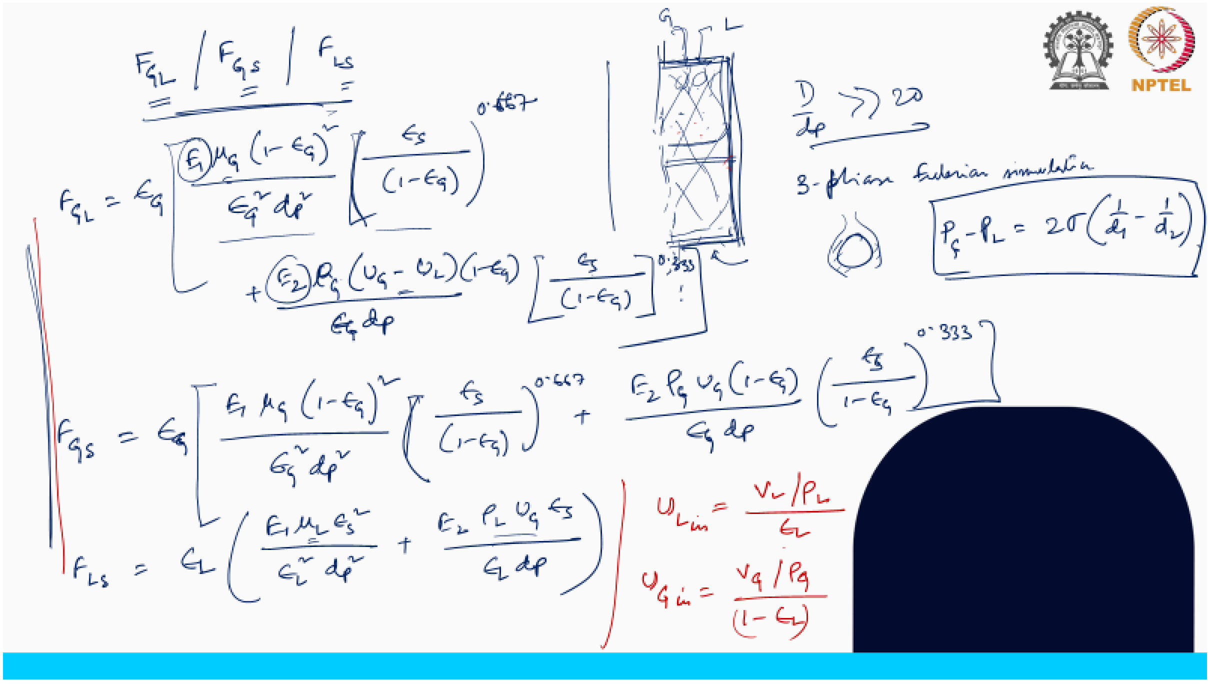
So, it is in a similar form to the Ergun equation, if you remember it, where we have the viscous part and the inertial part. So, contribution for the both the cases similar to the Ergun equations are here and these are the empirically fitted constants that depends on the catalyst particle or the particle size, shape and its characteristics accordingly these properties these values are fitted in here. Now, similarly, the FGS expression. Similarly, the FGS expression looks like this, similar to the previous one, but with certain differences: here we have the relative velocity, and here we have the UG component.

And FLS, the liquid-solid interaction, is represented. So, similar to this G L or G S and F S, here also you can see that there is a viscous term, and this is the rho u term, which is the inertial term that exists in these expressions. Now, these models or this closure is developed considering this fundamental force balance when there is a thin film of liquid that is wrapped around the spherical catalyst particle. And accordingly, their interactions were measured, or their analytical development happened based on such experiments. So, these expressions are represented by these equations.

So, these expressions or these closure models—again, this is specifically one closure model—similar to there being further developments. New models—I mean, this was developed long back when the fundamentals of CFD modeling for the packed bed were developed. And then, gradually, such models were further refined, and several other closure models were also developed. But this kind of model suitably or appropriately predicts or simulates the packed bed reactor, even for a larger scale. So, the point is, there are also a few intricacies that exist in this packed bed modeling.

One of them is that the considering the capillary pressure inside the bed because when there are immiscible fluid that is gas and liquid—there would exist a curvature of the bed. phases and that results in the capillary phase which capillary pressure which usually can be written in this form due to the pressure difference between the two phases. Now, this P here in the governing equation I mentioned that this P actually the pressure is shared by all the phases. But this difference in the gas and the liquid that results in the capillary pressure, this pressure difference

actually also sometimes are incorporated in the model. That also depends on the bed pre-wetting condition. If there can be two different scenario, one is that the bed was soaked in the liquid phase overnight or prior to its startup operation. And then slowly the liquid the gas phase was flown over the catalyst bed. That is one condition and also parallelly the liquid phase was fed in.



The other startup condition is that the bed was completely empty, the dry condition and the gas and liquid started to fill in. So, now you understand that based on this startup condition of the reactors, there will be two different dynamics that would happen for the flow or the internal reaction systems and its yield. So, depending on the startup condition of the reactor we also have to consider few more details in the modeling, but we will not go into the very specific detail of those because those are again quite research centric discussion and also those are specific to the particular reactor. But, in general the generic statement may be done such that the startup condition also dictates the simulation behavior or the model details that we have to adapt in a particular methodology.

and then these are with the boundary conditions that I told you is solved. Again one of the tricky part is that usually when there are two different fluids are coming to the Now, usually the flat velocity profiles are implemented for both the cases that is at the inlet, but there are sometimes a chances that discontinuity at the inlet when you just define the superficial velocity that is not accounted by the bed voids. The point is once it enters this superficial velocity when it enters in the bed it flows through the interstices or the

I mean that by this three phase classical Eulerian simulation that we consider that through the voidage our set profile. Through the set voidage profile, that liquid flows or the gas flows, and when it happens, It is, although the interpenetrating media, we are considering that in one place both fluids can coexist. So, based on that understanding, when it is flowing through the interstices, the main consideration or the calculation becomes based on the interstitial velocity or the interstitial velocity, and how that interstitial velocity and superficial velocity are related is—

Interstitial velocity is the superficial velocity divided by the bed voidage. So, usually, when we define that inlet for a particular phase to avoid any discontinuity in the simulation, what is done is that— this liquid inlet velocity, the velocity that is given here is the volumetric liquid flow rate divided by rho divided by the epsilon l. is the mass flux divided by the corresponding density, and this is the— Corresponding liquid fractions that we consider. We start the simulation that way.

And G, for the gaseous case, is also similar to that, but this is 1 minus epsilon L because we have to understand if the voidage is epsilon—if the voidage is epsilon— That means one space can either be occupied by the gas or the liquid phase. So, that means the total volume fraction for both phases can be, at a certain point, if the maximum is 1 in that case. So, that is why, or that is how, we try to avoid the discontinuity in the simulation for such cases, for these packed bed cases. And no-slip boundary conditions are set for this impermeable wall.

Grid independency tests are essential for any simulation; we discussed this in detail earlier. So, here also, as the first iteration, we do the— Grid independency test with this set of equations. So, with the number of cells, usually, it is increased twice, 1.5 times, thrice, something like this, and then we reach a grid-independent result. This is the time dependent simulation, which means the unsteady state simulation and the unsteady state simulation requires

careful choice of the time step with which we are marching towards the solution. So, the time step has to be chosen wisely, but we generally start with a very low time step. And corresponding to the desired level of accuracy that we set as the tolerance limit for the solution, the results are obtained. So, the point here is that by this three-phase, classical three-phase Eulerian simulation, we can simulate a large-scale packed bed reactor where three phases are explicitly considered. And when these solid phases are considered here, they are considered with their voidage profile in the pale, that is, how these solids are packed, their orientation.

The interface coupling terms are modeled; this is one of the model descriptions. There can be several others; you have to look for them in the CFD solvers. theory guide or the theory descriptions when you choose a different closure model because this phase phase interaction one drop down or the options would come to you consider multiphase simulation. There, you have to choose an appropriate closure model or the interphase coupling term or the interphase drag terms. I mean, for which operating range, for which flow regime, that interphase drag is suitable, you have to be careful while using that because that has to be in line with your choice or chosen set of the operating condition if any because those solvers are generic in nature the CFD solvers so they would provide several options to choose

from the interphase coupling term, and those may be developed for different flow regimes, one from each of the flow regimes or may be a couple of them from all the flow regimes. The choice of flow regime, why it is important, we have discussed because it actually has different flow textures. So, if you are solving for the trickle bed, make sure that the interphase coupling terms are chosen for the trickle flow regime. If you solve for the bubbly flow, then consider the closure models that are developed for that particular flow condition. So, the point is in this case, and then these parameters in these empirical correlations.

So, the question may arise, so if we use this exactly this set for irregular shaped particles as the catalyst set. or say different shape of the particles than the spherical shape. Whether this model would not be applicable? It would be applicable, but then here comes these parameters which are the empirically fitted constant. This E 1, E 2 you may have to vary these values and see or if you can determine these values for your kind of particle shape or the sizes.

then this model would fit in better or would predict more accurate result for your operating condition or for your case. And so, you can convert this disadvantage of Euler methodology which comes from the several empirically fitted constant values to your advantage by tuning in this parameters as per your requirement. for more accurate result ok. So, this is one strategy in the next lecture I will tell you or I will show you that the same thing the same domain or say the same problem can also be solved by another method with the Euler Euler methodology, but with

two phase Eulerian simulation or say the porous bed formulation because we have seen this porous bed and I told you that I will give you an example that how this model is implemented for the multiphase case. takes into account of the solid phase explicitly, but with also the help of the voidage profile where this startup condition and the bed pre weighting whether it is partially weight etcetera can also be model or can also be those information can also be given as an input to the bed or to the computational model so that the results can be more accurate even at the particle scale.

But if those are of not my objective, if my objective is the macro scale property, then I can further simplify this model or further simplify this problem with two phase Eulerian simulation. So, in the next lecture I will describe that strategy. And with the same example or the same case study. So until then, thank you for your attention.