

CFD APPLICATIONS IN CHEMICAL PROCESSES

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Week-08

Lecture 37: Modeling Multiphase Systems

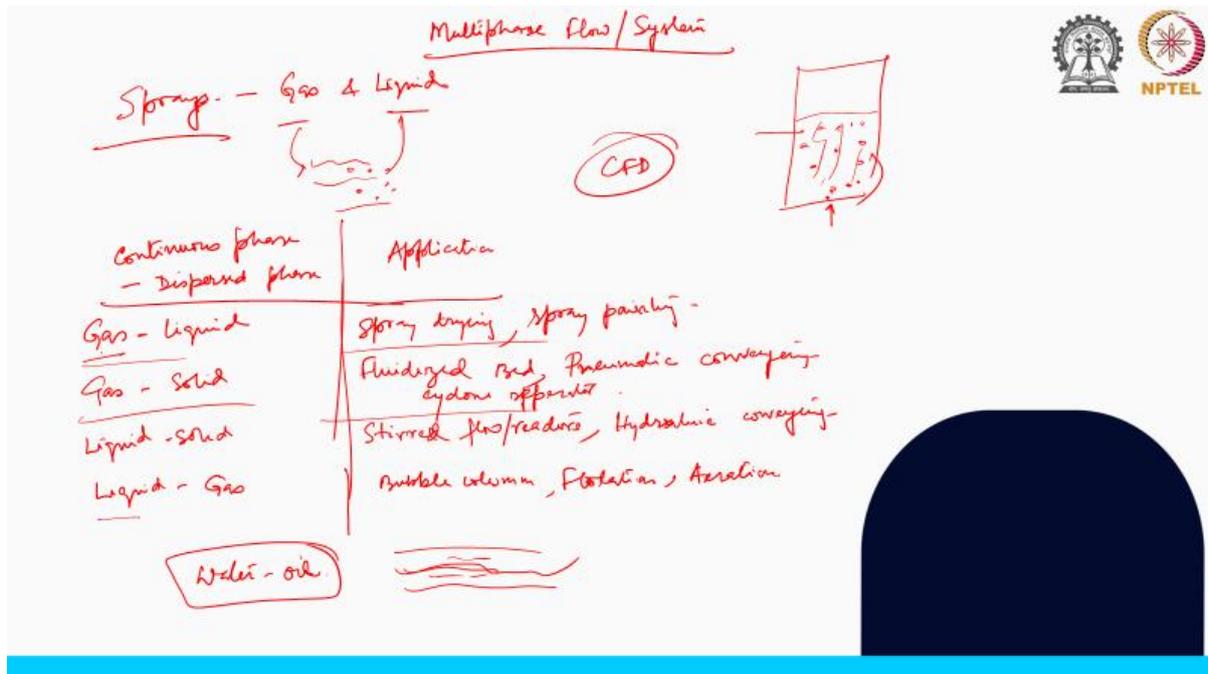
Hello everyone, welcome back to another lecture on CFD applications in chemical processes. In the last lecture, we started discussing multiphase modeling or the modeling of multiphase systems. We had some initial background on why multiphase modeling is essential. What are the types or what are the applications in the real world where we find such modeling useful? We also realized how the concept of multiphase is essentially different from the conventional thermodynamic state of phases.

So, here again, just to refresh your memory, multiphase here does not necessarily refer to thermodynamic phases. We can consider, or in fact we do consider, different thermodynamic phases as a single phase while doing multiphase modeling. In multiphase systems, we will see such examples. Also, it can happen that two different thermodynamic phase can be considered as the single phase and the other way round that a single thermodynamic phase say immiscible liquids, can also be considered as two different phases while doing multiphase modeling or when we do CFD modeling of multiphase systems. So, the example we had earlier was that a single thermodynamic phase can be considered as two phases.

The example I immediately gave was the flow of two immiscible liquids, say for example, oil and water. It is liquid thermodynamically, but in multiphase modeling and depending on the thing that we are trying to look into, that means the wish list or the objective of the problem, we may have to consider those two as two different phases. In fact, we do that when we simulate say the flow of emulsion, how the droplets deform while flowing through a constricted channel. So, during those kinds of modeling stages, although it is a single liquid phase flowing, that liquid phase can have several components, and those components are treated as separate phases. For the modeling of multiphase systems.

So this is one part, the other part that we had an example that two different thermodynamic phase, say for example, solid and liquid, these two are flowing together, say dilute suspension of some sand particles are flowing through a pipe. So, that water and sand particles that is a combined mix of this both phases are flowing, but if our objective is to consider or determine, say, the overall pressure drop through that pipe, then we can consider this solid and the liquid as a combined phase. Considering their mixture properties and so on, we can simulate that and have an understanding or an estimate of what the overall pressure

drop would be, and those are accurate enough in several cases. So, the point we stopped at in the last class was that the multi-phase modeling strategy would depend on the definition of phase. Essentially, the same problem can be solved in multiple ways by considering different phases, depending on the objective of the problem. For example, with the packed bed—the last illustration we had in the last lecture—we had a packed bed, and we considered that we had to estimate ΔP here. That is my macro-scale parameter estimation.

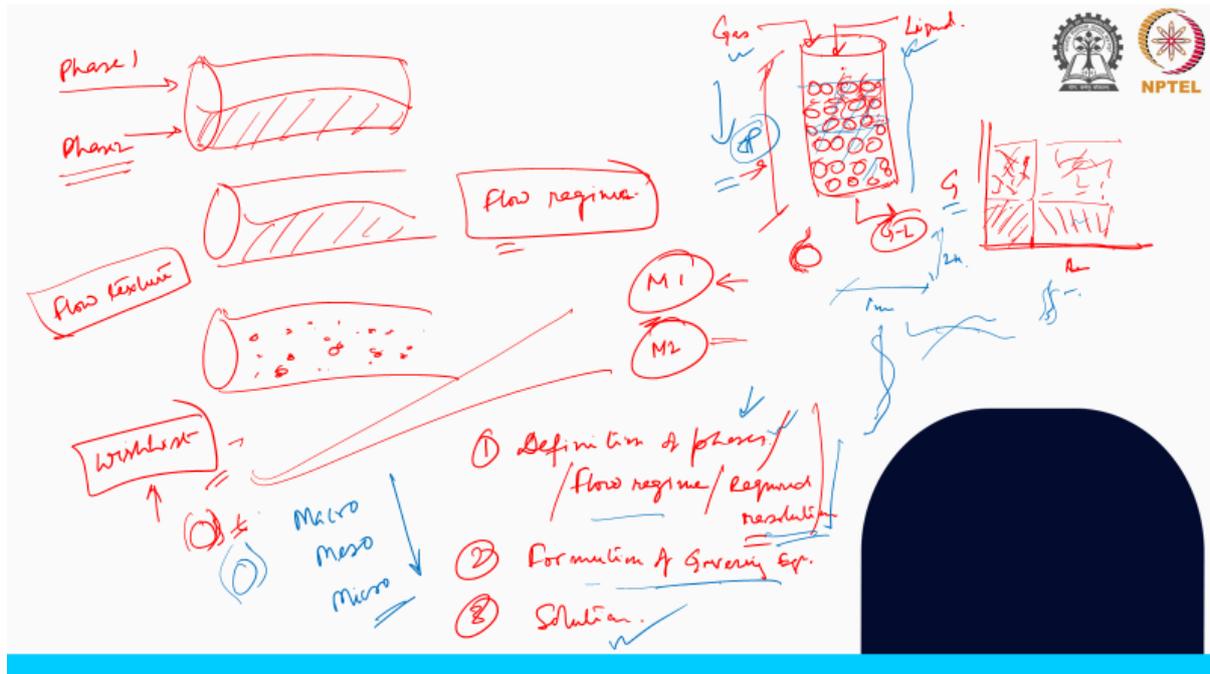


So, usually, these industrial-scale packed bed reactors are, say, 1 meter in diameter and 2 meters in height. So, you have millions of particles inside this packed bed. So, the point is, In that case, if your objective is to have particle resolved flow, that means whether the each and every catalyst or the bulk portion or certain section of the catalyst completely wet or not—such an objective, if you set it, then it becomes very cumbersome for the simulation and requires a special strategy, a different strategy,

than the estimation of simply this macro-scale property—that, okay, I need to know what the ΔP is, what my overall temperature profile is along the flow directions, etc. So, those are, I would say, the macro-scale properties that we are trying to simulate or estimate. So, in those cases, the problem domain or the problem Computational domain remains the same, but we have to use a different modeling strategy to quickly solve the problem. If we have to estimate this ΔP , now consider the point I was making about the definition of phase.

Here, essentially, three phases exist: the gas, the liquid, and the solid catalyst or the packings. So the packings consists, actually creates the voidage, the bed voidage, it has interstices pores through which the gas and liquid flows. Now the point is, if your objective is to calculate ΔP , okay, what you can consider for this problem to easily solve is that, say for example, you

have a porous medium as boundary condition, in which the flow is happening without considering individual catalyst particle and their packing orientation. What you can consider instead of that that ok, I have analyzed what can be the voidage characteristics, what is the voidage profile inside the bed in radial directions or in the axial directions.



And then based on that, I define my boundary condition considering this as the porous medium or a porous jump condition. There what you are doing, you are essentially defining a domain with some boundary condition that takes care of the bed voidage and the flow resistance and you are solving only the two phase flow that is the gas and liquid phases. because what we will see later in the later part of this lecture or maybe the next lecture different modeling strategies and here since the number of phases increases the number of equations that we will solve for each phase or maybe considering two phases combined is complex than the simple single phase flow. So, as you increase the number of phase

in the computational you have to solve more number of equations. And we have seen how difficult that would be when we discretize those set of equations because essentially those governing equations are set for each phase and those governing equations are discretized and then we solve for it either iteratively or in a more implicit manner. But iterations are there because we have to reach the convergence. So, if our objective is to find out the delta P, the macro scale property, then we have an approach where I can only solve for two phases here.

The flow of two phases through a porous medium. that considers the orientation of packing and its flow resistance etc in all three directions so that means this is a two-phase simulation the other strategy can be which is more exhaustive and more comprehensive is that I consider each and every catalyst particles and their interstitial spaces Those voids, remember, where the

flow is happening, that is our computational domain. So once I understand what are the interstitial pores, if I draw those in intricate details, considering the particles orientation and say their pores and etc.,

That becomes a comprehensive three-phase simulation that involving solid particles. There, although solid particles do not have any movement and we set the velocity of the solid particles as zero, we will see that in certain modeling strategy, we still consider the solid particles, this set of solid particles as a one fluid stage or one fluid media that is having zero velocities. and that is more comprehensive or exhaustive than the previous strategy of two phase simulation. So, that means, we can have three phase simulation, we can do two phase simulation.

which one would be more faster definitely the two-phase simulation but with some approximation or some simplification of the domain but if that simplification does not affect much on the accuracy of this macro scale property predictions we can accept that strategy with proper validation with the experimental data so that is why in order to simplify your simulation because So, those who do these CFD simulations one thing they remember and they follow is that we do not over complicate or over I mean we do not make it more complex than what can be done in a simplified manner. And of course, the simplified strategy would require model validation. with the literature data or experimental data or analytical solution for the benchmark problem.

But the point is that in the commercial CFD solvers, there are several buttons exist that you would be tempted to make the model more and more complex. The switching all the possible buttons on and you think that all the physics have been incorporated and my predictions are accurate. that would not be the case in most of the cases. So we try to keep it simple based on the objective we choose the appropriate modeling strategy for an efficient solution. So that is why definition of phase based on your objective is very important and that dictates the modeling strategy for the multiphase flow or the multiphase system.

Similarly, we discussed about the flow regime or the flow texture by citing this example in this pack bed for the gas and liquid velocities and we understood that there can be different flow texture inside the system and accordingly our modeling strategy we will see that also varies because at different flow texture we have different interaction between the phases And in that case, our objective also varies. Okay. Accordingly, if the objective varies, our modeling strategy also changes according to that. And definitely the required resolution that whether it is a macro scale property that we are trying to observe, predict or simulate

Or what is the mesoscale which is in between macro and microscale. Macroscale in the sense of say meter scale, microscale literally in true sense at the micron scale and in between we have the milliscale or the mesoscale interaction. So, this actually depends when we talk about this

length scale this actually depends on the problem statement. One problem statement, if we consider it has macro scale properties, we can have micro scale details of it and their intermediate scales, we say the meso scale. So, macro, meso and micro scale.

Handwritten notes on a whiteboard:

- $\alpha_d = \frac{\sum_{i=1}^n v_i}{V}$ where $v_i = \frac{4}{3}\pi r_i^3$
- $N_d = \text{Total no. of particles in volume } V$
- $D_{d,i} = \frac{6(V_i)^{1/3}}{\pi}$
- $L = D_{d,i} \left(\frac{\pi}{2\alpha_d}\right)^{1/3}$ = Distance between the particles (assuming particles are homogeneously distributed)
- $\alpha_f = 1 - \alpha_d$
- $\alpha_f + \alpha_d = 1$
- $m = \frac{\alpha_d \rho_d u_d}{(1 - \alpha_d) \rho_f u_f}$
- $St_T = \frac{\rho_f u_f L}{\mu}$
- Stokes no. = $\frac{\rho_f u_f L}{\mu}$
- $\rho_d = \text{timescale of the dispersed phase}$
- $\rho_f = \text{of turbulence}$
- bulk density $\rightarrow \alpha_d \rho_d$
- $St_T \ll 1$ → flow dilute
- $St_T \gg 1$ → flow dense

We go into more details, the particle level details in the micro scale phenomena. So once we set this, we choose the modeling strategy. There are different modeling strategies we will see. Then accordingly, the formulation of governing equation happens. We do formulate the governing equations and once the governing equations are set, those partial differential equations

essentially are discretized by one of the methods that we have seen either the finite volume, finite difference or finite element and then those are solved the solution part. So, until now or before the last class, we have seen how to discretize the governing We will not go into the formulation of the governing equation in the future lectures, be it about multiphase or some other systems that we will discuss. What we will understand is how different systems are categorized for the sake of modeling or CFD modeling. Now, what we have also understood in the last class is that there are continuous and dispersed phases or

In other words, broadly classified in multiphase systems, there are primary phases and there are secondary phases. So, if we go back to the continuous and dispersed phase understanding, we understood one of the characterizations of such flow that depends on the volume fraction. So, if I consider the volume fraction, of the dispersed phase, that is the superscript or subscript that we have written as D. So, alpha is the volume fraction, and the way it is estimated is essentially per unit volume. The dispersed phase volume fraction is basically the volume occupied

by the particles in a unit volume of the system, which is say V , if I consider the individual particle volume v_i . So, for i equals 1 to n , the number of dispersed particles that are there in the system, and if we have a total volume. So, the volume fraction of the dispersed phase or the volume. So, this is the dispersed phase volume fraction; this is how we usually estimate it. where this v_i is the volume occupied by a particle or a droplet. Now, this total n is the number of droplets or the number of particles in the dispersed phase or the others in the system, the total number of particles.

that are present in volume total V . So, this dispersed phase these are some of the fundamentals we will quickly go through is that this dispersed phase if it is spherical calculate this individual particle or droplet volume fraction, and that would be say capital D if I consider its diameter, the droplet diameter or the particle diameter for the individual cases that is essentially 1 by third. This assumes that the volume occupied by the individual particle having a spherical shape. but in most cases it is not the spherical shape it can be of different shape then the concept of sphericity comes into play.

that we know what is the sphericity. Sphericity we define for of the same volume of the sphere and then we determine the diameter of the sphere and we determine what is the equivalent diameter of that particle and if sphericity 1 that means it is the spherical particle. And the typical distance between the particle in the system assuming these are homogeneous homogeneously arranged ok. So, that would be $6 \alpha d$ to the power one-third.

This is where L is the typical distance between the particles. considering or assuming particles are homogeneously distributed. the volume fraction of the continuous phase is essentially. So, if this is α we consider for the fluid that is the continuous phase then it is essentially $1 - \alpha$ that we calculate from here. So, essentially what happens is α plus αd is 1 this has to consult.

So, this inertia of these phases that are there in the multiphase modeling is sometimes expressed by the concept called the bulk density which is αD multiplied by the ρD . Because instead of simply considering ρD which is the intrinsic density. in multiphase modeling it is the bulk density that is used to understand the potential of inertia by the for this flow. Because now there is another point: the loading—how much of the dispersed phase is there, how dense that phase is, or whether it is a dilute phase. So, for that, the parameter that is also understood is called the mass loading.

or the mass flux and that is estimated by something like this. This is the flux that is coming. So, that is why the velocity appears. So, $1 - \alpha$ $\rho_f u_f$. So, it is now you see this is the bulk density multiplied by its velocity and here in the denominator you have the continuous

phase or the other phase which is essentially the continuous phase its volume fraction multiplied by the corresponding volume fraction and its velocity the superficial velocity.

So, that gives us the mass loading or the mass fraction of the dispersed phase in the system. Now, here in the multiphase system, time scale and length scale are important. Say, the time scale of interaction or the travel of the dispersed phase in the system, and the length scale that we discussed—is it the macro scale, micro scale, or the meso scale phenomena? Now, it is difficult to define a single scale for all the flow problems in multiphase, as I told you—it depends on the problem statement or depends on the objective that we are setting. So, usually, we specify the dispersed phase time scale and the continuous phase time scale as a ratio, and that number we call the Stokes number.

And the Stokes number is defined something like this—for say, the turbulent Stokes number—where this τ_d is the time scale of the dispersed phase. And τ_t is the relevant time scale—the same time scale of turbulence that will come later—what would be the turbulence? But turbulence we can understand as the formation of eddies and chaos in the flow system. So, say this eddies that we can immediately think of in turbulence is that the wake formation that happens. Now, say if I have this Stokes number that we defined here.

So, this Stokes number if I write it as turbulent Stokes number here. So, if this is much less than 1, then what happens that this turbulent eddy that is formed the particles or the dispersed phase also follow the same trajectory. If it is much less greater than 1, in case it is much greater than 1 or infinity kind of value, that means the behavior of the particle cannot be correlated with the flow characteristic. and if it is near about 1 that it is dependent these are related that means say if stokes turbulence number is near about 1 then 1 happens that particle trajectory

also influence the turbulent trajectory the turbulent eddies and correspondingly we have the interaction of both them. both of them in between. But for very low value, much lesser than 1, it completely follows the flow characteristic. There is no individual identity as such of the dispersed phase in the system because it follows the continuous phase trajectory. So, the point is similar to that

people discuss or derive or set various non-dimensional number including this say the collision Stokes number. Similar to this idea that if I define this Stokes number of collision then it is the turbulent. So, it is the time scale for the dispersed phase and τ_c say the collision time between the particle. So, inter particle interactions this measures. So, this τ_c represents the time scales for the inter-particle interaction, particle-particle interaction of the dispersed phase.

If this is much smaller than 1, then we consider the flow to be dilute. If it is greater than 1, then we consider the flow to be dense. The reason for such categorization is that we will have different levels of interaction between phases. If we have dilute particles, then you understand

that if the dilute particle I have to simulate, then I need not bother about say the particle-particle collision, particle-particle attractions and et cetera,

because all the particles has almost lost their identity and it is following the continuous flow as it is flowing. At the same time, when we have dense particles, then there can be chances of acclimatization, there can be chances of settling if those are not carried with the continuous flow effectively. So, in a pipeline with the sand and water example that we cited earlier, if we have dense flow, then the chances of sand particles settling on the pipe at the bottom of the pipe would be much higher so accordingly in such cases the modeling strategy has to be different than the dilute suspension where the

particles the sand particles are easily being carried away by the continuous water flow in the pipeline and there will be no deposition because dense particle will have the corrosion effect in such example in the bends and etc. But in dilute suspension, we may not need to model such phenomena. So, this leads to the understanding of phase-phase interaction, particularly in this dispersed phase or, say, this continuous and dispersed phase interaction, that at which level we have to consider becomes one of the vital parameters in the modeling strategy. So, we will stop here today.

In the next class, I will discuss that level of interaction—what interactions can happen and how, based on those interactions, the modeling strategy would differ. So, thank you for your attention. We will see you in the next lecture.