CFD APPLICATIONS IN CHEMICAL PROCESSES
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Week-08
Lecture 36: Modeling Multiphase Systems

Hello everyone, welcome back with another topic and lecture on CFD applications in chemical processes. Today, we will discuss something about multiphase systems. Now, the point is, before we discuss multiphase systems or their modeling, we have to understand how we define multiphase in computational fluid dynamics. Because whatever we have discussed till now was based on single-phase phenomena. In fact, the derivations that we have done in finite volume method the details of it we have seen based on the single phase case and, but the point is that remains the pillar for foundation or understanding of multiphase system.

It is just that we are now having different phases in the system. So, the multiphase system is extremely important, the reason is that whatever application or the most popular applications or whenever we try to solve any real problem are involved with these multiple phases. So, the examples that we can think of: Starting with our day-to-day activities, materials, for example, we use sprays for several purposes, be it for deodorant, be it for insecticides, etc. The sprays, now those sprays, you know that they essentially involve liquid droplet flow or the gas and the liquid that are present.

So, there are liquid droplets suspended in a gaseous medium, and we eventually spray them over our desired places. So that means it involves two phases: one is the gas, and the other one is the liquid. So, the point I try to mention here is the multiphase flow or, in generic terms, the system. Flow means there has to be some continuous motion, and system means that it contains multiple phases. So, we will discuss this in a generic sense: that we have multiple systems.

Now that means, with the example of this spray you understand that there is between this gas and the liquid what we have So, sprays that we consider we have the gas and the liquid. Now, are those in equal volume that are there in a container when you spray it is essentially not. That means, what you have in that say compressed container where you have this spray be it say as I mentioned for insecticides or the body spray, you have the compressed gas in which the liquids are there in a limited volume.

So, which means we have two phases gas and liquid not in exactly equal volume, the one a higher volume generally we consider that as say primary phase for the modeling purposes and the other one is the secondary phase this is the general convention it need not be always true. At the same time there is we have a continuous phase and the other one we can say the dispersed

So, what happens here we have a continuous medium which is the gas in which the liquid droplets are suspended. and that gets stick to the surfaces with perfumes with antiseptic and all the other properties.

So, these are the things that happens the different liquid properties are attached to it for our different purposes applications. So, here the gas is our continuous phase and the liquid is the dispersed phase. So, based on this broad idea that we have a continuous say for example, again that we see a bubble column reactor. We have a pool of liquid and from bottom you have a gas purger where the gas bubbles are rising through the liquid pool or inside the liquid media. So, in this case in a generic sense or in a broader way that we have defined is that we have a continuous pool of liquid.

So, the continuous phase here is the liquid phase and the dispersed phase is the gas just opposite to this case. So, now based on this idea ok, although we will refine it later. So based on this, what we can think of that we have a continuous medium, so continuous phase and we have a dispersed phase in such system. So if that happens, say for example, gas we have continuous phase and dispersed phase is the liquid. We have seen this example that we have say spray dye applications.

Say spray painting. In all these cases, we have a continuous gaseous medium in which we have suspended liquid which is sprayed over it. If the liquid phase is changed to solid that we have a continuous gaseous medium and there are dispersed a few numbers of solid the applications that you see the classical fluidized or say pneumatic conveying, where the solids are transported with the help of a continuous gaseous medium. Say cyclone separator, okay.

So, these are the places what I am trying to show here that these are the places application areas where we find this kind of multiphase system. If in place of gas I have liquid. So, if I have liquid solid continuous phase as the liquid and dispersed phase is the solid The thing that you see in the start tank reactor or the start flow, start vessel or say hydraulic conveying. If we have liquid and gas combination that we had here gas and liquid which means the gas is the continuous phase liquid is the dispersed phase but

we reverse it that liquid is now the continuous phase and gas is the dispersed phase then we had the example of bubble column or flotation shells. aeration in mineral industries these are frequently used ok. Now, the point here is that it is not the conventional thermodynamic state that we consider as only phases in computational fluid dynamics. So, the point is not about thermodynamic phases like gas, liquid, and solid, but in CFD modeling, this is not in the true sense that we consider as multiphase only. Definitely, we will consider different thermodynamic phases at different stages, but it is not necessarily true.

It can happen that there are two liquids, say immiscible liquids, like water and oil. So, water and oil are flowing together. it would not mix there will be a separation we call that kind of flow as the stratified flow depending on the volume or the throughput with which this oil and water flow rates—because flow rate dictates how the flow pattern will be in a system. Not only flow rate, but also the corresponding phase volume fraction.
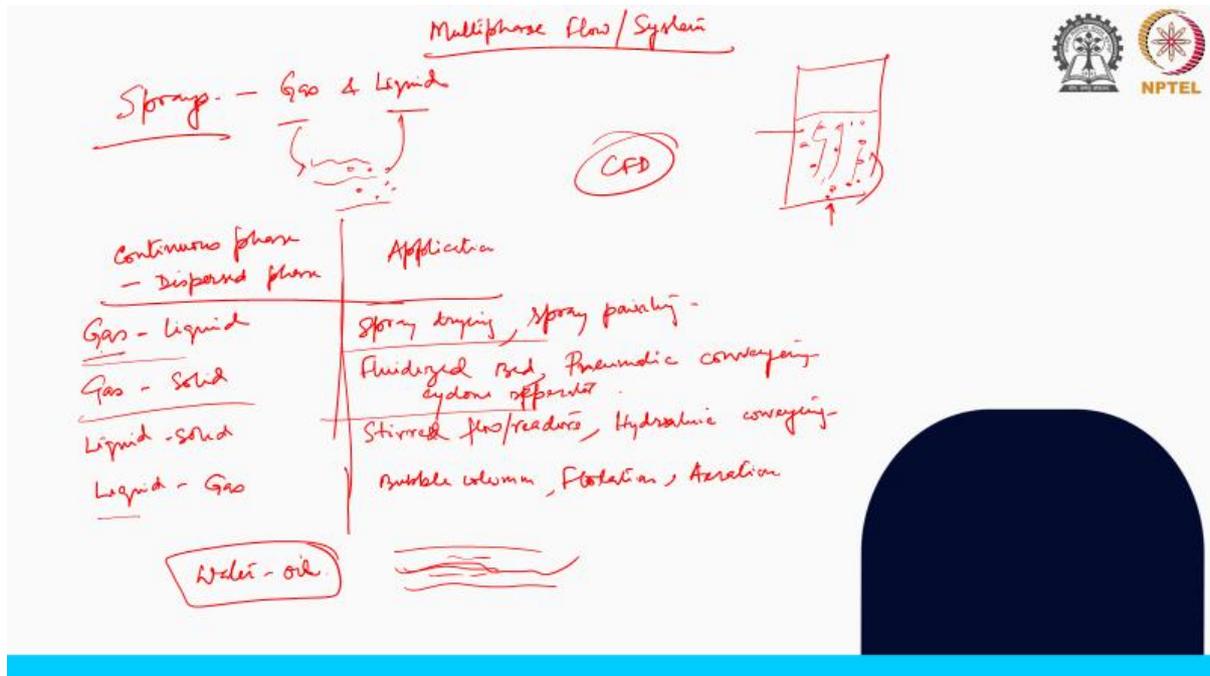
These things actually dictate how the flow pattern would be in the system. And accordingly, what will we have? We will have different modeling strategies in computational fluid dynamics. So, with the example of water and oil. Although here I have only one thermodynamic phase which is the liquid phase, our modeling strategy depending on what we are trying to predict or what

are trying to understand in the flow dynamics—we can consider water as one phase and oil as another phase in the CFD modeling strategy. So, that means oil and water flow can be modeled as a multiphase flow, depending on what we are trying to locate in that flow dynamics or in that flow. If we are trying to find out what would be, say, the interface of the oil and water while flowing—two phases are flowing—how this interface would behave. Then definitely I have to do multiphase modeling with the help of, considering water as one phase and oil as the other phase.

So, the point is now again depending on, say, how the flow is happening. If I have, say, this as the interface of one phase, and on top we have the other phase. So, if this is say phase 2 and if this is phase 1 depending on the velocity the flow pattern may be say like this what we are seeing here a continuous ah interface between the two phases or there can be are droplets of phase 2 or say dispersion of phase 2 in phase 1 depending on the volume fraction and the

velocity relative velocity between the phases. So, phase 2 may be suspended which means flow texture in multiphase this term is

important and you would hear it in different ah context what is the flow texture or the same thing also sometimes is called the flow regime what is the flow pattern ok so same fluids are flowing at different velocities with different volume fractions, which can result—or, in fact, would result—in different flow textures or flow regimes. OK. And multiphase modeling strategy would depend on this flow regime—in which regime you are modeling. So, from regime to regime, or for different flow textures, multiphase modeling strategy would be different.

So that is why there is no generic or, say, the best CFD model for any multiphase problem. It is important that you set your wish list or what you are trying to find out for that problem. What is the objective of your problem? Say, for example, I have a packed bed reactor. I have packed bed reactor. And for single phase case what we have usually seen in the laboratory experiment for the UG classes that in liquid is flown and we have done the flooding experiment in several classes possibly you have seen the flooding experiment.

But at the same time if the gas flows, so gas and liquid So, co-currently flows downwards consider this situation. So, what I have that I have if I try to show you one plot which is say the velocity of liquid and velocity of gas. If I operate in the low velocity regime gas and liquid both are at low velocities. what will happen?

This liquid would eventually wrap this solid spherical object or say for the sake of simplicity consider these are the spherical packings or any kind of packings that would be. So, it would actually wraps this packing objects, it would be all over the packing objects and would try to wet all the packing surfaces, but also since the velocity is very low. So, what happens is that this liquid would try to find the lowest resistance path and would try to flow towards the wall of this bed because near this wall we have the maximum voidage. when it is packed with the spherical particle it has been seen that the voidage is maximum near the wall.
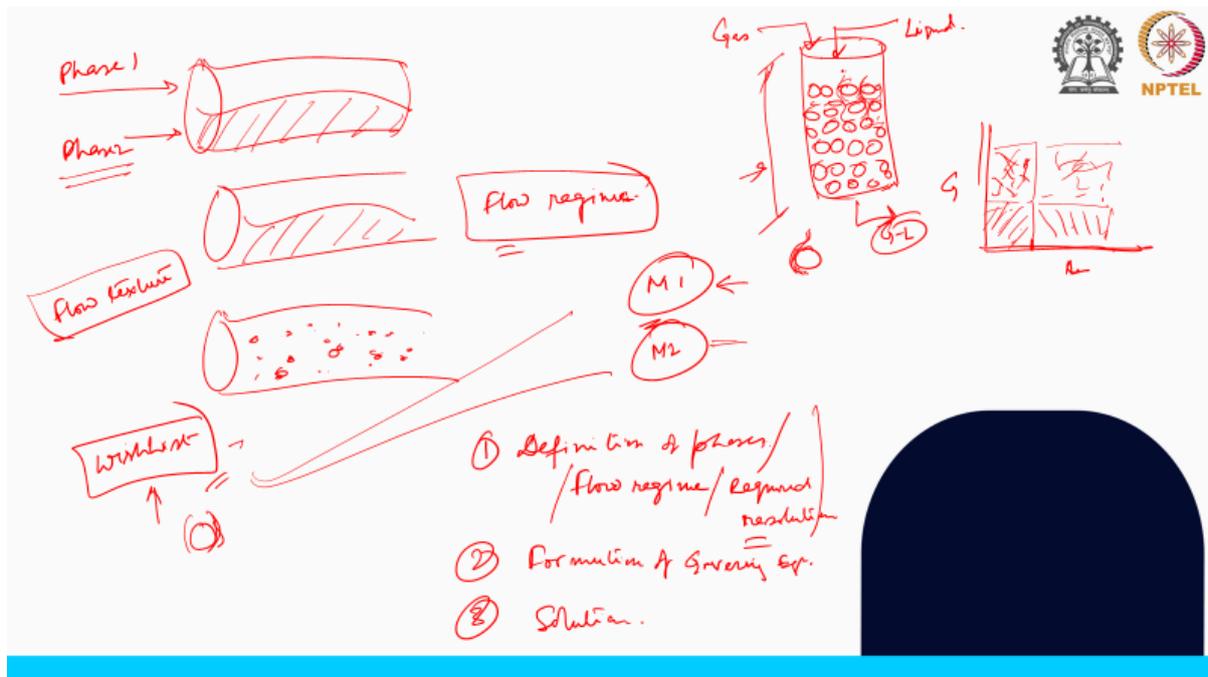
Since voidage is near the maximum is maximum near the wall the liquid would try to bypass those parts. So, we have a certain pattern we call that as the rivulet flow or the trickling of the liquid that if this is my spherical particle. So, basically so, this The liquid will partially or completely wet the particle and then will flow. It has its benefit from the application standpoint that all the catalyst particle because in the packed bed reactor these are essentially the catalyst,

These packings are the catalysts, and the reactions happen on the catalyst surfaces. So, if it gets wetted with the liquid, the liquid reactant and gas, Since both the velocities are low, it gets a much larger contact time. This interfacial area also increases due to the packed bed measure. So, the reaction happens if that is conducive.

Now, consider keeping the gas velocity constant and increasing the liquid velocity to a higher value. This flow texture would then break. And all the pores or interstices would be quickly filled, and the liquid phase residence time would be much lesser. And what would happen? The chances of bed flooding can start.

So, which means the gas and liquid would interact in a different way than what it was interacting when there was a lesser amount or the velocity of the liquid was lower or the flow rate of the liquid was lower. Similarly, if you keep the liquid velocity low, you get a different flow texture or flow pattern on that side and the higher liquid side with a constant low velocity. Keeping the velocity of the liquid lower or the flow rate lower means I am talking about the superficial velocity, which in fact dictates the flow rate. So, keeping that low if you increase the gas velocity what would happen this gas would take this liquid with it very fast and eventually this while be there will be the liquid droplets

that would be forming and that would flow inside the bed. So, kind of again spray kind of phenomena would exist inside the packed bed. So, that regime is another different type where the gas and liquid interaction is happening in a different way. When you further say increase the liquid velocity with the higher gas velocity the bed quickly possibly would flood depending on the situation.

And you have a complete different flow texture or flow pattern inside the bed because there again you have changed the gas liquid interaction time period etcetera. And in all the 4 cases here If there are say only consider I have four cases. So from research people already demarcated this velocity ranges where this velocity for a particular set of fluid where this regimes would end where it starts or where is the transition. Like just for the single phase we have seen laminar transition and turbulent.

So, similarly for the multiphase cases there are several such transition or sub areas where the flow texture is different. And in those specific places you will have to use a different modeling strategy because your objective may be different in different cases. Say for example, here again with the packed bed. if I have to understand that what is the overall pressure drop ok. If my objective the wish list contains only say the velocity the pressure drop the calculation of a macro property what is the total pressure drop

happening for my case), this is the only thing I would like to know. I do not—I am not bothered about what is happening inside. If this is my objective or this is in my wish list, then possibly I can use the combination of, say, both phases as a single phase and grossly estimate what the velocity can be. Or I can still use a multiphase model—which we will discuss later—what kind of multiphase model, but we can use, say, multiphase model 1 to quickly predict that. But that multiphase model 1 can only predict such macro-scale properties—that is the limitation because it is easier and faster, possibly. But if you are looking, or if your wish list or the objective for that problem is to see whether my catalyst particles are completely wetted or partially wetted.

whether my catalyst are fully wet or partially wet because that dictates my reaction efficiency or the conversion part then I will not be using the model M1 shift to a different model or use a different model, say model 2, which means for the same domain, for the same setup. Based on your objective, you have to choose your best alternative of the modeling strategy in a multiphase case. There is no single-use model. Even in model 2, there can be a possibility of several other different types of models that can predict whether the catalyst particle is fully wet or partially wet. Again, there will be a different range of applicability for that particular modeling strategy.

So, the point is the choice of wish list or the choice of objective—what is the objective? Sometimes, the objective you cannot choose; you are given the objective of a problem. So, what is that objective? Based on that, you have to decide your modeling approach in a multiphase case. The first point is the definition of phases, okay. So, the definition of phase is very important. We will discuss this further because the same problem— The same objective— depending on the accuracy, we can decide how many phases we can consider for a particular problem.

So, again in multiphase CFD modeling phases are not truly in the sense of thermodynamic phases this you have to be very careful about, and you have to be completely aware of it—that I can consider two liquids as two different phases. I will also discuss later that ok again liquid and solid I can combine it and consider it as a single phase because it is convenient for me also acts—I mean, sometimes it gives us whatever result we were looking for. So, phases—the term is flow regime—this is equally important.

And the required resolution of the result. This is what I just spoke about that if my resolution is at the macro scale properties, I do not require this micro scale phenomena that completely wet or what the flow texture is, which I would say is meso-scale or micro-scale phenomena. That dictates the modeling approach. So, phase, flow regime, and required resolution dictate my modeling strategy—or our modeling strategy—in multiphase cases.

Accordingly, the formulation of governing equations happens. And third follows its solution. So, in the coming classes, what we will discuss mostly is this first part: the definition of phase, flow regime, required resolution, and accordingly how the governing equations can look like. We will not go into the formulation part. We will see what the governing equation is and how it accounts for different phase-phase interactions, which we will see in detail and have briefly discussed today.

We will not go into the solution part. So, with this understanding, I stop here, and in the coming classes, we will continue discussing the multiphase system. Thank you for your attention.