CFD APPLICATIONS IN CHEMICAL PROCESSES
Prof. Arnab Atta
Department of Chemical Engineering
Indian Institute of Technology Kharagpur
Week-08
Lecture 38: Modeling Multiphase Systems

Hello everyone, welcome back to another lecture on multi-phase system modeling in the CFD applications of chemical process course. We discussed in the last class that phase-phase interaction, or even for the dispersed phase, depending on their volume fraction, whether it is a dense or dilute suspension, accordingly, the phase-phase interaction changes. So, a broad classification was proposed by Helgo Bassey in 1994, which gives us an idea a very generic idea of what kind of interaction can happen in such dispersed flow processes or flow systems when we have dispersed phases.

So, if the dispersed phases are flowing with the continuous phase and the continuous phase is unaffected by the presence of the dispersed phase, then whatever the characteristics of the single phase as it is flowing, the continuous phase, that kind of modeling strategy we may use. And that is called one-way coupling. So, one-way coupling means the particles or the droplets do not influence, OK, do not influence the bulk flow, OK.

So, that means the effect of the fluid on the particle is what is important. So, the effect of the continuous phase fluid on the particle is important or dominant. OK, ah. So, how the particles interact with each other we do not bother about in such a scenario, and that is called one-way coupling. If these particles have a Stokes number, OK, that is larger than 1, then what happens? The volume fraction of this dispersed phase that means is sufficiently large that we cannot just discard the presence of the particles in the fluid.

The fluid senses that there are something it is not the pure fluid is flowing. So, the presence of the dispersed phase is failed by the fluid phase or the continuous phase while flowing. So, in such case that means we the both the phases essentially senses their presence and we call such scenario as the two way coupling. So, the effect on the flow is no longer independent of the particles that are present. the flow senses, feels the presence of the other phase or the dispersed phase that are present.

Now, here still it is not dense enough, the volume fraction is not that sufficiently large that two particles also feels their neighbors presence of the droplets. And that is why we call this as the two way coupling that the fluid understands that there is something with the dispersed particle or the droplets that are there. Both senses each other while flowing. So that means the dispersed phase imparts its characteristics on the flow also. But when this alpha D is further increased or say Stokes number goes very high, then the presence of the particle, a single particle is also failed by the other particle.

So that means particle-particle interaction, now particle-particle may hit each other. Say again, go back to the thinking of the sand is being flown in a pipeline. If you increase the sand volume, what will happen? The sand, the particles also will collide with each other and that may result in breakage of certain bigger particle. So that means particle-particle interaction is also there.

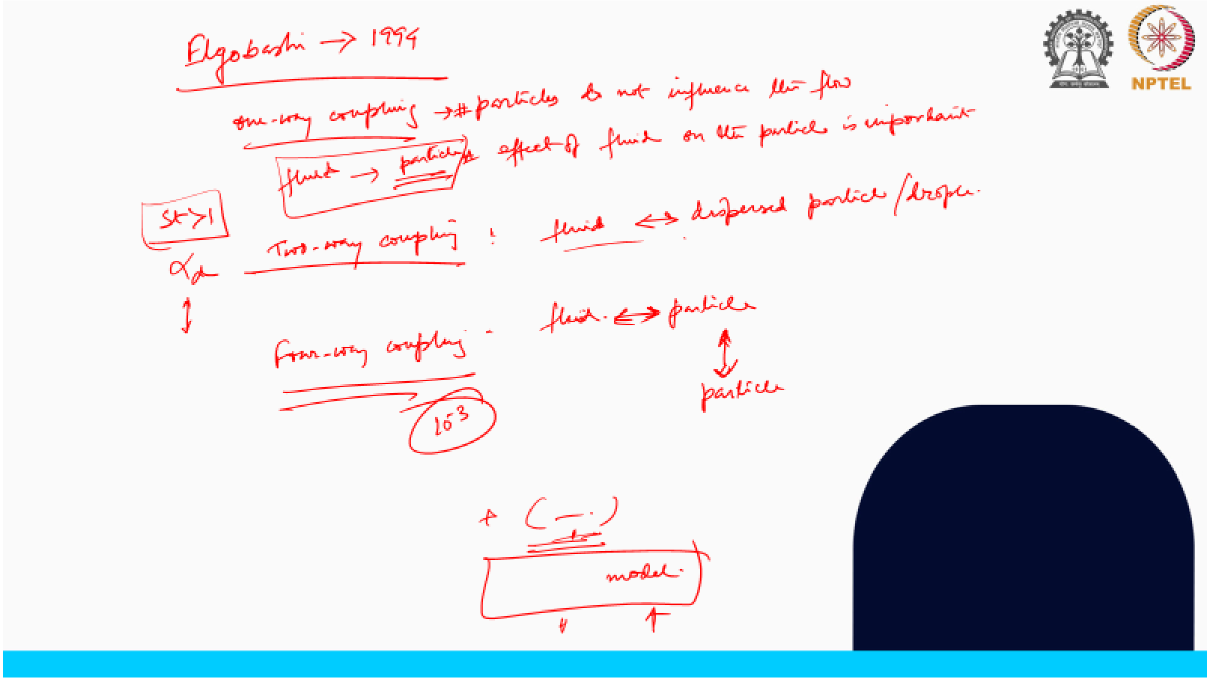
And we cannot neglect for that such scenario because that frontier, that agglomeration, if it is not breaking, then maybe they are sticking to each other. And depending on the other examples, the particles may have agglomeration nature. So they may agglomerate, they may grow in size when they collide with each other. So in such cases, the flow characteristics, the flow pattern changes effectively. So, we cannot neglect this particle-particle interactions further.

So, and that case we call as the four-way coupling. That means the fluid and the particle interactions are there and now the particle-particle interactions also exist so here we had two way coupling here also we have another two way coupling between the particle and that is why we call that as the four way coupling and here we had just one way coupling that this fluid is completely unaffected by the presence of particle so fluid actually dictates the complete flow irrespective of the presence of the particle or what kind of particle that is there.

So, the typical range of this dispersed phase we say is very dense or typically when it is above the value of 10 to the power minus 3. then this four-way coupling comes into usually play. So, the point that we have here in one-way coupling, the dispersed phase senses continuous phase, but the continuous phase remains unaffected by the presence of the dispersed phase. So, in such case, we can simply model that system as say a single phase flow because we are not bothered about this influence of the particles.

And those tracking of the dispersed phase may be done in some post-processing unit. But when we have two-way coupling, then dispersed phase senses the continuous phase and the continuous phase senses the presence of dispersed phase. So, the presence of dispersed phase then should be reflected in the governing equations actually that would happen in the momentum equation. Because in all these cases

the flow is happening if the flow is happening then we have to solve for the set of continuity equation and the momentum equation the Navier Stokes equation. So, then in the momentum equation there have to be momentum exchange between this continuous and the dispersed phase. So on the right hand side of the Navier-Stokes equation, the terms would start appearing when we have the multi-phase modeling stress. In single simple phase or simple single phase cases that we have seen earlier, the momentum equations, we had the pressure term, the shear stress term, and if there is any source term. Now, here this source term actually would account for this momentum exchange when it comes for this multiphase modeling cases along with if there is any other source term.



So, now this phase-phase interaction would appear on this right hand side of this Navier-Stokes equation. In the four-way coupling, further this is augmented, further this is complicated. So dispersed particles are also now interacting with each other. There is wear and tear can happen, agglomeration can happen. So the model for particle-particle interaction would further appear when we resolve that dispersed phase.

And suitable modeling strategies have to be adopted. okay so the details of these terms that would now appear on the right hand side of the momentum equation for the phases that we will solve because we have multiple phase we will solve it for a multiple phases so now the point is how do we resolve those terms how do we encounter how do we estimate those terms say for example momentum exchange between the two phases, okay. So, we call it in a multiphase flow system, particularly multiphase flow modeling, the interphase drag term, okay.

So, these interphase drag coefficients or drag terms would have to be estimated; otherwise, that particular term on the right-hand side of the Navier-Stokes equation cannot be solved. Or the whole equation remains then complex. So, those terms we have to solve or resolve first. Now, here comes different opinions or different philosophies or different genesis on how we resolve those phase-coupling terms. And that, I mean, since this term I am introducing here in this course particularly, you may be aware of it, but related to multi-phase flow modeling,

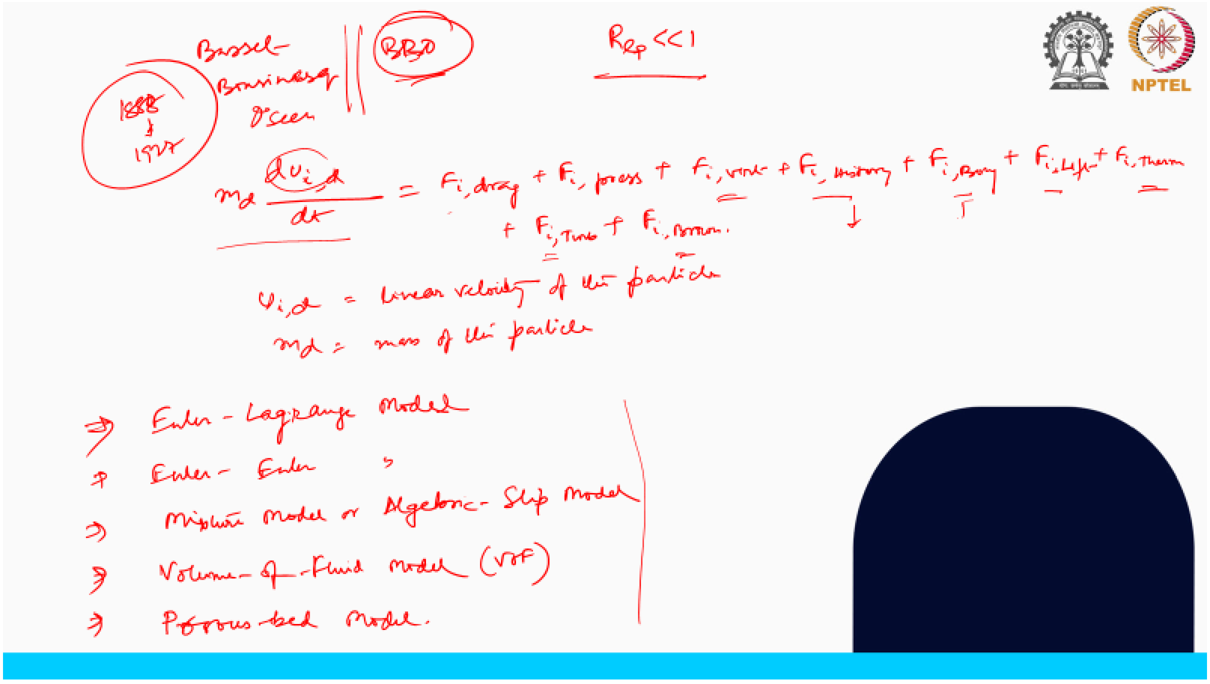
the meaning of this closure model is that we try to close or resolve this term, phase-phase coupling term, by a specific philosophy or by a specific understanding because again as I told you the problem that you may be solving can be unique that has not been done earlier but the same class of problem possibly has done by someone else earlier and during that time he or she may have proposed That if you do or if you resolve this coupling term like this with say any empirical result, empirical correlations or maybe some analytical derivations considering that particular phenomenon, phase-phase interactions, how they resolve.

So, to resolve that term, we can have several strategies or several models again. We call those as the closure model in a multiphase system. Now conventionally in several disciplines when we say the closure model for flow problem people also understand that this is the turbulent closure model because turbulence, also when we discuss this, we will see turbulence also requires several strategies to resolve different length scales.

The interactions of the eddies at different length scales requires different model. So that is why we say in those cases also the turbulent closure model. Similarly analogous to that here also we had confusion Those fortunately are gone away with the development of different strategies. For the multiphase cases, there has been established models that addresses this particle-particle interactions, particle-fluid interactions depending on the flow regime or the flow texture.

And we call those as the closure model. So, those closure models are usually user-defined. because as I told you your particular problem may be unique, but if it falls into a generic class you can possibly use the default closure models that are provided in the commercial CFD solvers. We will name those couple of them while going for a specific strategy. So I hope this is very much clear to you that there exists closure model and modeling these closure models or understanding these closure models are in fact the essence of the multiphase modeling.

Because in multiphase flow modeling, we essentially would solve the Navier-Stokes equation and the continuity equation. how the phase phase interactions you are handling is the key step in the multiphase flow modeling along with the definition of your phases that we discussed exhaustively earlier. So, now if we look into this say what are the forces usually acts on the dispersed phase. So, that Newton's second law actually is the foundation for that, that what are the forces that acts on a dispersed phase, typical dispersed phase. Now, along with that, when a flow is happening, in that flow, what are the forces that acts?



So this was original, I mean, at the very beginning was resolved by Bassett, which is usually called the BBO equation. That describes that few small particles in a uniform flow with particle Reynolds number much less than 1. There in such scenario this BBO equation tells us that what are the forces acts on a dispersed space.

But later I mean because this happened in the range of say 1880 and say 1882 in the order of 1927 in this era this was developed and slowly it was further made robust for a wide range of Reynolds number. And a more generic framework was proposed that on a single particle if I say that U of the dispersed phase of the individual particle. is essentially are the drag if I the pressure forces then I can have. So, it is not that all the forces can be acting on a particle.

It depends on the flow situations or the operations that you have in hand. Some of the forces may not exist for that particular scenario but it is a generic expression that what are the forces may be possible in any situation. Then you can have the history force also you will have the buoyancy force. this you have the lift force plus thermophoretic forces plus due to turbulence additional forces and also the Brownian motions the forces due to Brownian motion.

So, here this UID term is essentially the linear velocity of the particle, and md is the mass of the particle. Okay, F_I drag is the drag force. The second term on the right-hand side is the pressure force due to the pressure gradient. This is the virtual mass force that arises due to the acceleration of the surrounding fluid.

in certain situations if such situations appear that there is a certain acceleration of the surrounding fluid then the virtual mass is generated so the virtual force is there have the history or the Basset force. This Basset force can appear due to changes in the boundary layer. This is the buoyancy force due to gravity, and this is the lift force—the Saffman and Magnus lift force—that can occur due to the velocity gradient and particle rotation in the flow. Then you have the thermophoretic force, which can appear due to the temperature gradient. This is the thermophoretic force. This is due to turbulent fluctuations—any additional force that can be generated on a particle.

And the last one you can have is the Brownian force due to molecular collisions. So, all these forces, as I told you, may not appear in your particular problem. But your particular problem may involve some of these forces, and this is for the individual particle—remember. So, this has to be summed up for all particles. Now, depending on the situation that whether you have one-way coupling, two-way coupling and all, this is a generic framework where the forces are understood

with two-way coupling, four-way coupling, etc. So, the point is, depending on these forces, understanding of different forces that can arise at different time or different scenario, you have to have the expressions for each and every forces and that you can have analytically for a single particle and there exist different expressions or different equation for each and every forces. If you are interested in going to these details, what are those, how actually are those happens?

Say for example, I can tell you this virtual mass force may be dominant or may be one of the dominant factor in the bubble column reactor. So similarly, in microfluidics, I may have to omit this buoyancy force it is not necessary that the influence of gravity is not there in the microfluidic flows. So, we can drop this buoyancy force term while deriving this particle-particle interactions and all these terms that we have to consider. So, this the reason it is shown here.

is to have your understanding covered around this that there can exist different forces and your modeling strategy would be dependent on the understanding of these forces that are present or that you anticipate in your problem statement while solving it. So this leads to essentially the choice of different modeling strategy in multiphase flow. So, what are those strategies? Now, once I write those names you would realize that essentially depends on the framework, the reference framework from which you are looking at the problem or you would resolve the particles.

If you think of resolving each and every particle in the flow That means you have to solve for these individual particles, their interactions, their trajectories, etc. If you are not bothered about this individual particle movement, then you can model the only fluid phases that are present in the system. So the choice of these forces also depends on the understanding of your dispersed phase system that how dense it is, how dilute it is or how it is going to behave what I am anticipating.

So, the point is this actually leads to the choice of different multiphase modelling strategies. as the Euler Lagrange model or I can have Euler Euler model. I can also think of a variation of the Euler Euler model which is say the mixture model or we say also algebraic slip model. We will go into these details of this models one by one.

We can have volume of fluid model and also the example that I told you, we can also have the porous jump or the porous bed model or the porous media model. Okay, so we will go through this in details in the coming lectures one by one. The point here, each model can be used or are used for different purposes. Or even multiple models can be clubbed to solve a single problem in a multi-scale manner. That if I try to resolve

the particle scale it is essential that I have to use the Lagrangian model Euler Lagrange model and the deduction from there this particle fluid interaction can be clubbed to my broader objective or a macro scale objective where I can use Euler Euler model. The VOF model for example the here the volume of fluid or the VOF that takes care of the individual particle be it a droplet or other particle, how it deforms, how it agglomerates and all these intricate details can act as a closer model to the macro scale Euler Euler simulation. I will stop here today.

We will go into these models one by one in the coming classes so that we can understand how multiphase models are usually solved with the minimum mathematical expressions so that you don't get bored by all these mathematical expressions, derivations, etc. Based on your interest, you can refer to the reference book or research papers for the derivations and broader applications of those. What I will tell you is when to choose one and why it is so. So with this note, I thank you for your attention today.

We'll see you in the next class.