CFD APPLICATIONS IN CHEMICAL PROCESSES

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Week-09
Lecture 41: Modeling Multiphase Systems

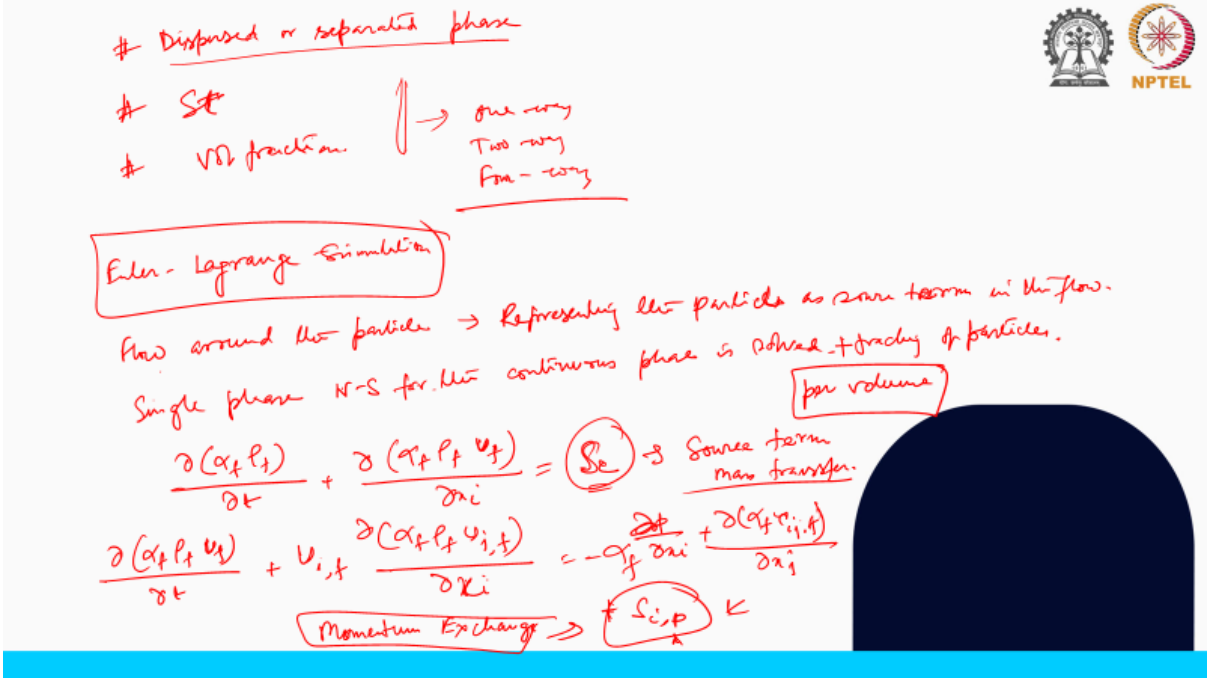
Hello everyone, welcome back to another lecture on modeling multiphase systems. In the course CFD Applications in Chemical Processes. What we were discussing is a brief outline of various modeling strategies in multiphase systems. We started with the Euler-Lagrange method, where we saw how the flow around the particle is resolved. And the individual particle—when we have to resolve an individual particle or droplet—from the Lagrangian framework, while the continuous phase was modeled per the Eulerian framework.

So, how that coupling happens between the particle and the continuous phase, and then we move to a broader objective or modeling strategy, which was the Euler-Euler model. Now, there we mentioned it as two fluid model or it can also be considered as the k fluid model where k is the number of phases that are involved and we are trying to simulate it from the Euler Euler standpoint or the Euler Euler framework. Now, there the important parameter we mentioned was the volume fraction by which the other phases were defined and the difference between the

grid cell and the control volume while developing the governing equations. Now we landed or we ended the last lecture at this point that those governing equations for the Euler Euler simulations can typically be written in this form where all the properties that are mentioned here are in the averaged value or the average term. Now, one subset—we will come back to the Euler-Euler model with an example later—but first, let us have an overview of the other models. So, we now move to the mixture model, which can

generally be classified as the subset of Euler Euler model when further simplification one stage further simplification because in Euler Euler we have already simplified we have taken the average either the ensemble average or the time average property and it is not at the particle resolved scale or the particle scale where we can resolve the particle level phenomena. So, considering the drawback, but its advantage is that we can apply it for very complex processes to have an initial assessment and to have the macro scale phenomena or macro scale parameters easily predicted or simulated. Now, one step further in simplification is assuming the coupling between phases is extremely strong and the relative velocity between phases is in equilibrium or local equilibrium. So, the important simplification in addition to what we have done in the Euler case is that we consider the interaction between phases to be extremely strong and the relative velocity

between the phases is in local equilibrium, which means this means that when one phase accelerates, the other phase also accelerates and grows together. So, that implicitly means that the phases accelerate together So, the point is that means we consider here only one set of governing equations: continuity and momentum, and that too considering the mixture properties of all the phases. So, one set of equations we solve here.



When we try to simulate by the mixture model, the unknown properties the unknown properties are of the mixtures, but not for the individual phases. So, the flow property and once we simulate it, what is done is the individual phase flow property of the individual phases are reconstructed with the help of an algebraic model, and this algebraic model is for relative velocity, and that is why it is often called the algebraic slip model.

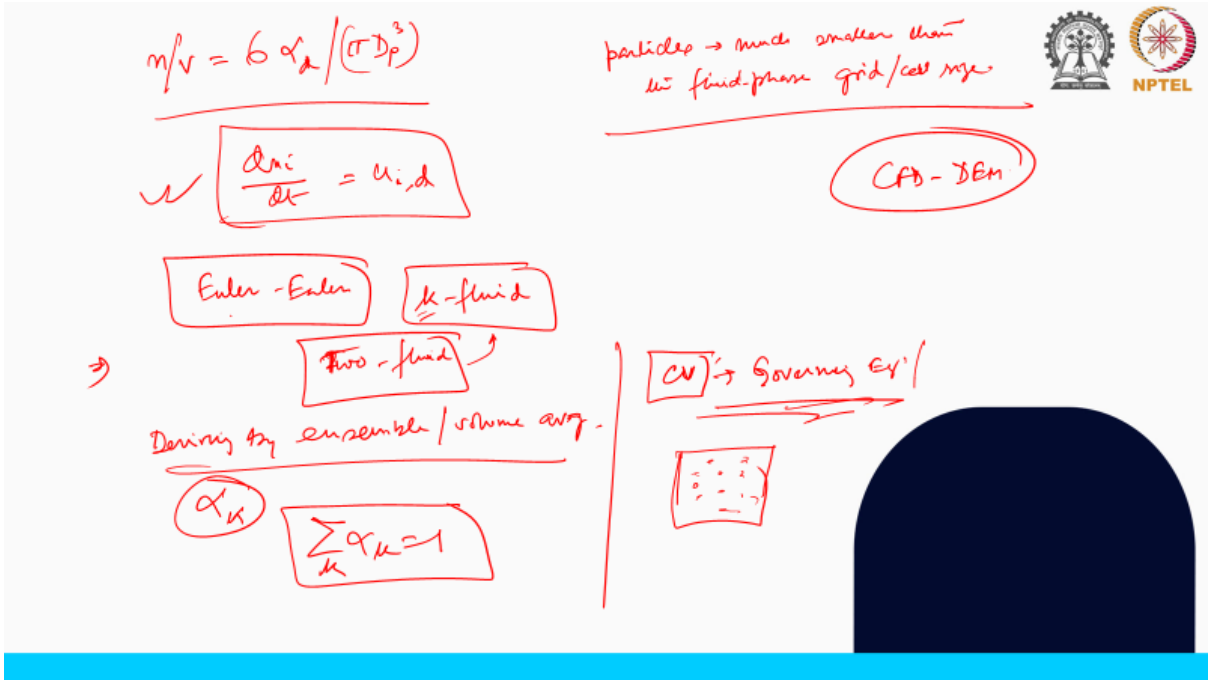
OK, so this difference or the individual phase velocity and its relative magnitude to the mean velocity is called the drift velocity, which, say, if I write in this form for phase k, OK. And the velocity relative to the continuous phase is known as the slip. So, it is an additional simplification to the Euler-Euler model where we consider the mixture property in the governing equation.

So, we solve for only one set of phases, which means combined phases considering the mixture properties, and whatever we calculate is for the mixture of the phases. And then, the individual phases' flow properties are reconstructed with the help of an algebraic model, the algebraic slip model. Now, the set of governing equations looks like something, where M stands for the mixture. is equal to 0, and the other case is the momentum, this is for the i and j. j of the term summation of k alpha k volume fraction rho k u i drift k.

u j drift k, this whole parameter where we have the subscript m stands for the mixture. And as I mentioned earlier, k u r i j k is the drift velocity for phase k. Which is nothing but if I consider the kth phase velocity, it is that ui drift k plus ui mean. This last term, this term, arises from the nonlinear inertia term in the Navier-Stokes equation, which can be written as alpha k rho k u i dr k u j drift velocity of the k divided by x j.

So, once one phase property or the mean phase properties are calculated, then it is reconstructed for the individual phase movement or individual phase properties. And these mixture values or the mixture density, say for example, mu m, is usually written in the form alpha k u k mu k. Where this mu k is for the dispersed flow, the viscosity for the dispersed flows, and this again has various techniques to estimate for the dispersed cases, be it granular flow or other kinds of flow. Which we consider what we do for the standard Euler-Euler process. So, the utility of this mixture model is that when we further require simplification in the computation because here we are reducing

the number of considered governing equations by the number of phases multiplied by 2. One continuity equation and one momentum equation for each phase that is being considered here, but here everything is considered for the single phase. So, let us take the example. say if you have say oil sand and water flowing together where there is a very dispersed or trace amount of oil and sand which is being flown with water or that case, by standard Euler-Euler simulation, you should have considered three phases: water, oil, and sand.But if the oil and sand are in very small amounts or do not necessarily need to be modeled or their influence properly understood, then what happens is that solving that whole system with the mixture model can reduce a great amount of computational effort for predicting the macro-scale properties.



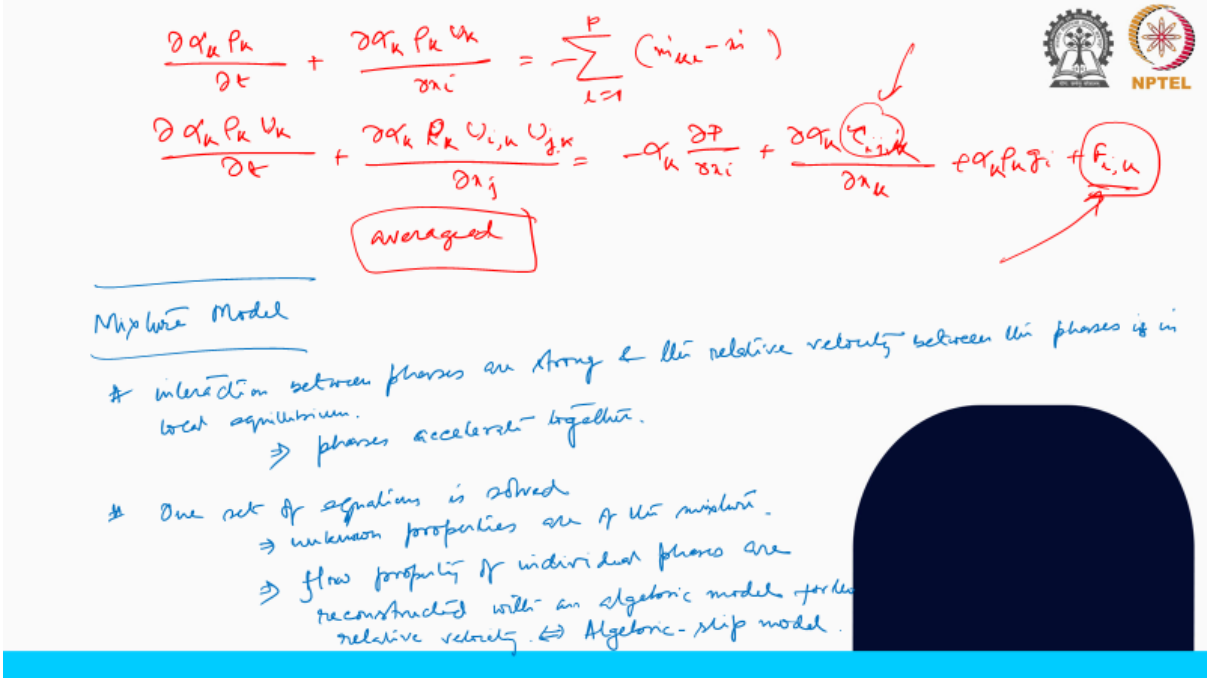
Because remember, this Euler-Euler model, from which this mixture model is derived, does not consider the particle-level interaction. So, in such cases, when direct numerical simulations or even a Lagrangian framework is not necessary for individual particle simulation, and if it is conducive to consider the mixture properties,

those who are not having drastically different objective that ok I require the overall pressure drop or overall flow properties for the mixture because we are simulating for a larger system extremely large system where Lagrangian simulation would not work because we do not require those much those many information for all the particles. So, in those cases, Euler-Euler is sufficient, but again, for extremely large cases when you have to transport, say, oil mixed with water including various sediments, through a pipeline that ranges for miles, covering miles of area or miles of distance, in those cases, also in a pipe having a diameter in the range of, say, a meter, In those cases, this mixture model can easily give you initial estimate or very rough estimate of what is happening in the fluid or what would be the

pressure drop that you require your pump to be set in order to make that amount of thirst to have the flow happening. So, in such applications, mixture models come in handy or, in fact, in say, riverbed flow. A real scenario. In those cases, these mixture models are extremely handy because they reduce a substantial number of phases, as we are considering the mixture properties. So, the governing equations become applicable for only one phase, considering all mixture properties.

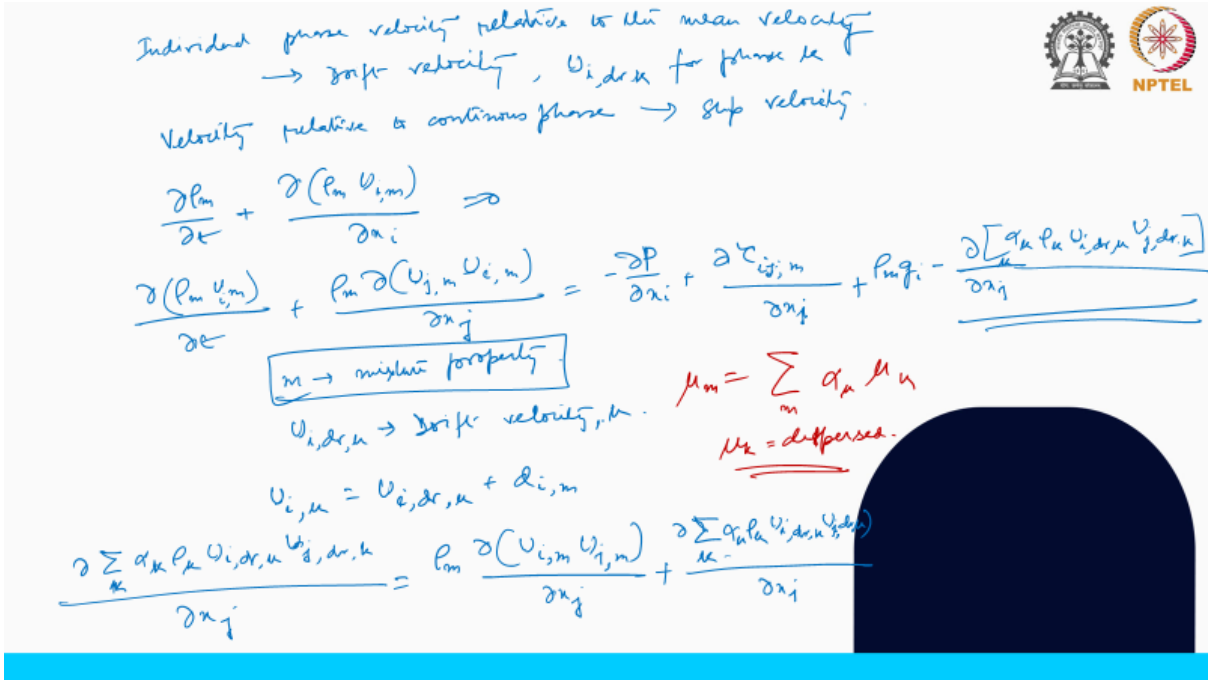
So, this is the mixture model, and the other important model is for stratified flow or when the interface is truly important to demarcate or to understand. That means, here, like in Euler-Euler cases or in Euler-Lagrange cases, we are not concerned about how the interface between the

two phases evolves. if that is of particular interest in some problem or for your problem then there we require a different category of model and that is we called the front tracking such as one of them, the Volume of Fluid (VOF). This is one of the front-tracking methods.



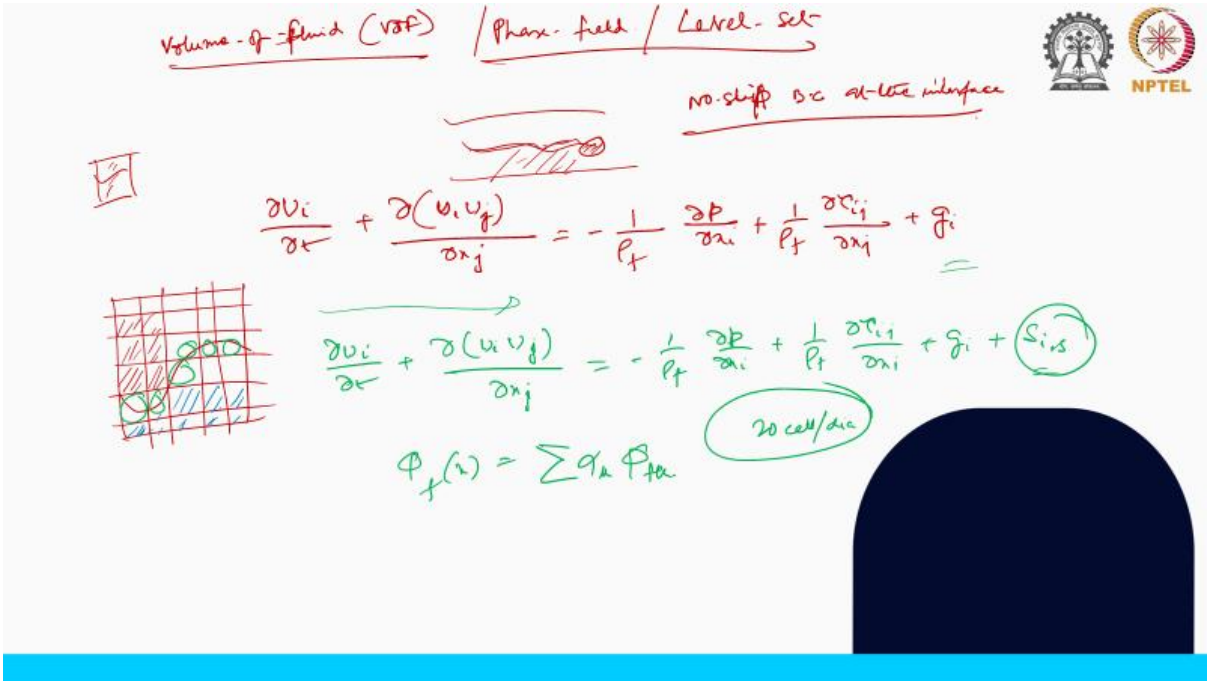
There exist other methods to track this front or the interfaces, to name a few: the phase-field method or the level-set method. So, these are similar kinds of methods where this phase phase interface, say for the bubble or the droplet or whatever other phases are present in the medium, are clearly identified. So, in those cases, one particular assumption is inherent: the no-slip condition at the fluid-fluid interface. So, we consider a no-slip boundary condition at the interface.

Now this front tracking method can also include say the direct numerical simulation where each and every phases or the particles are clearly resolved, details are unnecessary, instead of DNS, we can use the Volume of Fluid, phase-field, or level-set method. So, because in all those cases, we require a no-slip boundary condition at the interface, and we also have to resolve to the Kolmogorov length scale when it comes to direct numerical simulation. Now, these methods actually solve a combined single-phase Navier-Stokes equation that has the type of where this local fluid properties for example, density, viscosity or these scalar quantities are given by the presence of their phase volume fraction.



So, here what we do? Only one phase is present in the properties if the that phase is present in a particular grid or a cell, but when it comes to say one cell is occupied by two different fluid, then it comes that cell we solve it by the volume averaged or volume weighted average properties are used that are shared between two or multiple phases. So, volume fraction essentially is modeled by the continuity equation that we have seen earlier for the Euler case.

And this single set of momentum equation is solved for this stratified kind of flow where we have to understand the interfaces. Now, this front tracking method phase field method, level set methods these are all similar in nature, but there are several distinct advantages or disadvantages or the pros and cons of this methods which we will not discuss at this moment. But what we do here is that we will focus particularly on the volume of fluid method that one of such examples that is also implemented or can easily be implemented by the finite volume method and it is accessible in most of the standard CFD solvers that uses this finite volume method as the discretization scheme.



So, this volume of fluid method it uses the value of the volume fraction on a particular grid or the cell basis that describes the position of the interface. So, for example, if you have this grids and your interface is something like this that is evolving in nature. So, here what we have to track or here there will be several cells that are filled with simply one phase and the other phases are filled completely with the different phases. So, in these cases

Where this is the case. So, only the fields that are shared—say, for example, these are the cells which are shared by both phases—there we use, we tried, we—this method uses volume fraction or the volume-weighted average properties in order to find a smooth tracking or the smooth interface it tries to track. But in the other cells where it is filled with only one phase, in those cases, it is the single phase, just like this stratified kind of thing, it is solved. So, basically, this interface, when it is not straight, then

immediately what happens there is the influence of surface tension that we have to take into account. So, when there is a finite curvature, the surface tension force comes into play, and this surface tension force in this stratified equation is included as an additional source term. So, the thing that it looks like is that u ij xj and, say, for example, so in this case, even if I plus there is a source term that we include here and this source term actually takes into account of this surface tension forces and that eventually helps us to understand this influence of surface tension and the interface curvature.

So, now it is only for the cells where the cell is shared by the phases—in those cases, the momentum equation is different from those for the single-phase cases. And the volume-averaged properties—that is, we have seen earlier—which means the volume-averaged properties of any scalar that we write is essentially alpha k and for the number of phases that

we have for that particular phase. So, in these cases, one of the major drawbacks—we will again come to this volume of fluid in detail, taking a case study. So, here, one of the drawbacks is that the accuracy of this model

Despite it conserves mass compared to, say, the level set method and is better, it still has first-order accuracy, and very fine meshing is essential. So, the range, as a rule of thumb, is that if you try to capture a dispersed phase with a diameter d, you have to consider, say, around 20 cells per diameter size to capture the interface of that particular dispersed phase. So, we can understand that it requires very fine meshing because we are capturing particle-scale phenomena. And this source term we have to resolve for the surface tension by surface tension models those are also available given models if the problem is solved it is fine

have to write your own user-defined function to solve those interface surface modifications of the surface interface evolution pattern. So, with this brief overview, I stop here today, because we have just seen Euler-Lagrange, Euler-Euler, mixture model, and volume of fluid—a brief overview of them. We will go into some details of a couple of these in my next lecture, and we will also cover the porous media model or the porous bed model—how it is implemented with the example of a case study. So, thank you for your attention today. We will be back with the next lecture.