CFD APPLICATIONS IN CHEMICAL PROCESSES
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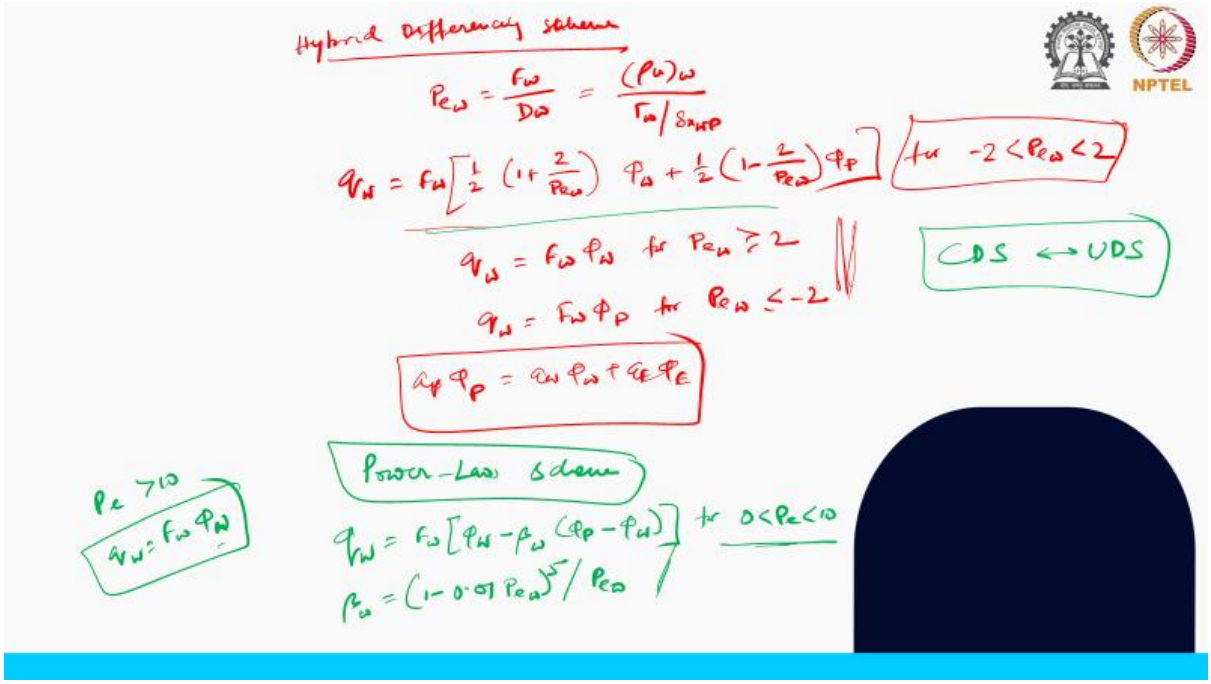
Week-06
Lecture 26: Finite Volume Method

Hello everyone, welcome back with another lecture on CFD applications in chemical processes. We are discussing finite volume method and its intricacies. So we are in the understanding of various differencing schemes and how it works. In the last lecture, we discussed about the upwind differencing scheme and how it improves on the central differencing scheme on certain category. That means when we have a flow that is convection dominant with the coarser mesh, we can improve the solution accuracy with the limited number of grids or the meshes.

Now, similarly, there has been a continuous development and we have other differencing schemes named the hybrid schemes. where everything now is basically, if you look at the genesis of it, it's basically try to overcome the limitation faced by the central differencing schemes for the convection, convection dominated problem. So that is why the focus is on the calculation of the cell Peclet number. And accordingly, the cell Peclet number is calculated. So the Peclet number, for example, on the west face is essentially is delta XWP.



So what it does, it actually solves a polynomial which is, it has a bit complicated expression compared to the other. So I would not, plus half one minus two by number phi p. Again with it comes with a restriction that or the criteria for Peclet number of this range. we estimate the

flask at the waste face based on this expression when we have Peclet number in this range under this discretization or this differencing scheme. And phi, I mean Q, the flask that we are calculating W is essentially for

Peclet number greater than two phi P for Peclet number less than minus two. So you can see that based on this criteria, Peclet number, whether it is plus two or minus two, it actually adjusts or accounts for the flow directionality, which is very important. And the rest of the development remains the same. After replacing these expressions, we try to find out our form of phi in the AP phi P format, and then we solve the problem. It actually improves on the upwind differencing scheme because it takes into account the hybridness between the central differencing and the upwind differencing scheme.

So you can see from this part that when the flow is convection dominated, this whole thing essentially moves towards the upwind differencing scheme. So it automatically takes care if you write this generic expression of this hybrid and you put these restrictions of this Peclet number, then For the convection-dominated problem, it solves the upwind differencing scheme. And if it is not, then it goes back to the more accurate, because it is the second-order accurate central differencing scheme than the upwind differencing scheme. Because the upwind differencing scheme is a first-order accurate scheme.

So next comes the power law scheme. Power law scheme is again, better—supposedly it has been seen that it is better than the hybrid differencing schemes because it also solves the polynomial and typical expression for this power law scheme for the power law scheme. The waste phase plus calculation would look like something for cell Peclet number of this range, 10, where I have beta on the waste phase is essentially one minus 0.01 Peclet number. to the power five divided by Peclet number in the west face.

So for this range, it solves such polynomial and if it is Peclet number is greater than 10, then it is the upwind scheme. This is the capital W, this is the small w. So it further improves because here we had the CDS scheme, the central difference scheme for the Peclet number in between two plus minus. When it is greater than two, it moves towards the upwind scheme. So that is why it is the hybrid difference scheme.

That is it is CDS and UDS. It's combination of both. In the power law scheme, for the case of low Peclet number, it is solved by a polynomial, but for the higher Peclet number, it is solved according to the upwind differencing scheme. Again, all the differencing scheme discussion would not be feasible in this course of time. But there are also other differencing schemes that are recently developed. There are different order accuracy schemes.

For example, we have third order muscle schemes that are available in ANSYS Fluent, third order accurate because central differencing scheme is the second order accurate. So higher

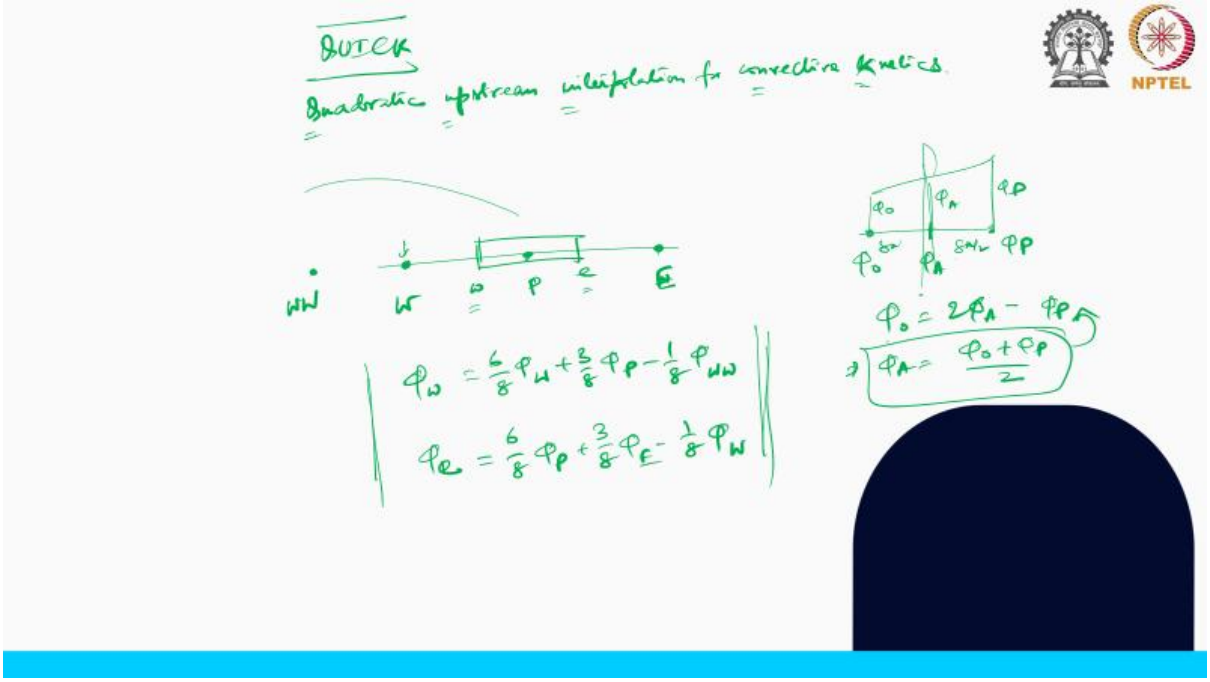
order differencing schemes are available. Based on your interest, you should explore those. But the point that we tried to mention here is that why such dropdown options are available in those codes that you must be aware of. That not only you should use its default first order differencing schemes, you should opt for higher order accuracy or

higher order accurate differencing scheme because those are more accurate. in the calculation. But at the same time, you have seen that with increasing order of accuracy, the computational demand naturally increases, but at the same time, these differential schemes are developed based on certain philosophy or the operating range. For example, the cell Peclet number was a criteria for using central differential scheme. So we must not be trusting just by default values in the CFD code or the CFD solver that are available and we mostly use.

We should be looking into their help files, their theory guide, their manuals to understand that how that differencing schemes have been derived or what is the expression of that and whether it fits my problem statement or it tracks my problem statement. Accordingly you should use the higher order differencing schemes for example there is also a popular scheme that is available I will quickly mention this is the quick scheme which is the full form is that quadratic upstream interpolation for

Quick scheme, you take the all first letters of this and the acronym is the QUICK, Quadratic Upstream Interpolation for Convective Kinetics. What it essentially does, we will not go into its derivations or details of it. The point is what it does that now when say, for example, if I illustrate this small thing, you would understand that if I have my point P, we always try to estimate the values at the cell faces or the control volume faces because those are the points that are unknown and this is my capital E and this is my capital W, west point, east point and this is the point P.

So till now what we have done or we have seen the all the schemes are using either the two points or one point considering the upstream location. But here in the quadratic upstream interpolation convective kinetics, the quick scheme, it takes the two upstream points. So, say for example, estimating the phi waste phase, we will require two bracketing nodes, which means definitely the phi w and phi p and one further upstream point, which is phi ww. That means one further west point. So what it does, it actually takes a quadratic function.



Okay. And that form is solved here. Its approximation is solved, but definitely putting into continuity at the junction between the considered quadratic functions. For example, when the point P shifts to the other points. So essentially, say for calculation of phi, again east point, I will have two bracketing nodes, which is covered by P and E. And I will require another upstream point, which is in this case, west. And we then take its weighted average value. And that is six by eight plus three by eight minus one by eight.

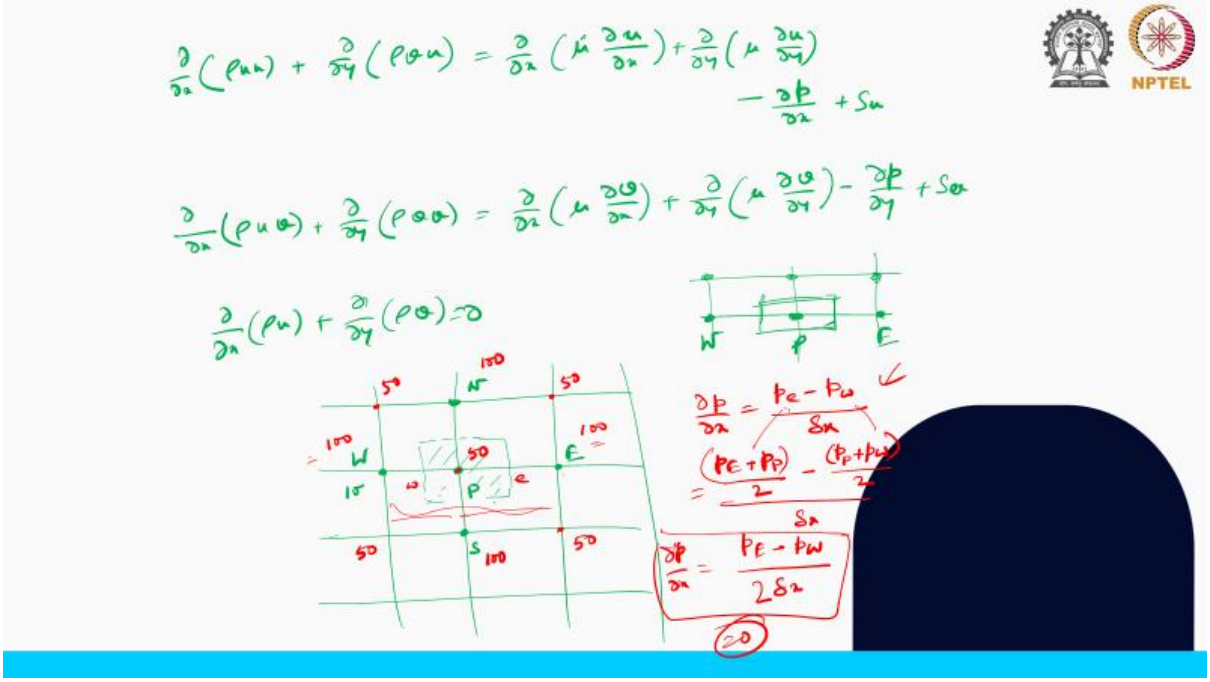
So this is six by eight plus three by eight minus one by eight. In the case of, so this would be fine for all the nodal points two, three, four, what are the intermediate nodal points? And we can do this formulation. But in the case where we do not say for the control volume one, if you consider, if you again imagine the control volume one and control volume five, in those cases, what will be my waste-waste point?

That means the WW point. OK, so in that case, we will have to consider an imaginary point outside the domain. And we have to estimate or say kind of we say imaginary or the mirror node. And then we take the weighted average again. Say, for example, if we do not have, say, this nodal point after this boundary.

So we consider there is a mirror node. Say we consider this is the phi A is the boundary and the phi P that we are calculating. So, essentially it is phi 0, phi A and phi P. So, this is the domain boundary that we have. So, what we assume here is that phi 0 is, so this is delta x by 2 and this is delta x by 2. because this is the control volume one as for our drawing that we did earlier.

So in this case, what we consider again, we approximate this value by this assumption that essentially it is the Phi A, it comes from the thing that the Phi A is Phi zero plus Phi P divided by two. Since we know phi A, we consider phi zero as for this expression. So this is one way of doing it. The point is that if we use quick scheme, we have to do such estimation and we have to do such implementation. So again, I am pretty sure that if you are further interested in this upwind scheme, you have to look into the details of the problem

of these given differencing schemes that are available to you, provided by the CFD solvers, usually commercial CFD solvers and all. And then, accordingly, you have to choose your appropriate one. Alternatively, the other way can be like the thing that you have done for the grid independency test, where you have taken five numbers of grids: 10, 15, 20. And then you have possibly narrowed down to a number that takes care of the time and the accuracy that you require. That means the trade-off between the time and accuracy, which is your mesh-independent, the grid-independent solution.



Similarly, there is also the possibility of a differencing scheme-independent solution. You must try different discretizations of these differencing schemes. For the same problem and the same number of grids, you may see that there has been some improvement with the fixed number of meshes. For example, for five numbers of meshes in the previous problem, if you have done it with the central differencing scheme and then with the upwind differencing scheme, you would see the result has improved.

So, similar to the mesh-independent result, you should also have the discretization scheme-independent solution. So now the point becomes the velocity-pressure coupling. So till now, whatever we have considered, the velocity field was known at every point or wherever we are

considering. That is why the velocity at the phases we did not need to calculate or estimate earlier. But the point is, say, when we have even a steady-state flow, what you see is that

Let's write it for the two dimensions, similarly for Y momentum, we will have SV part, and I have the continuity part equals zero. So, what we can see from this set of equations is that all the things here are essentially all the three equations are coupled, okay?

If my velocity field is not known, if we knew the velocity field, then this set would be solved like we have done earlier. We do not have any problem, but since we do not know, it requires this simultaneous solution of the velocity and the other scalar, for example, here is the pressure. Now, the point is, all the examples we have seen earlier, what we considered is that the scalar values are stored on the nodal points or the centroid of the control volumes or the grid points or the nodal points that we have done.

So, when we considered this control volume, the centroid of it, we considered that all the scalar properties are stored here. And accordingly, we estimated at the cell faces or the mesh faces. Because these are my grid points, and for 2D grid points, I will have a more complicated structure. Now, if we also consider here that along with

Velocities are also stored at the nodal points, then for some cases there may be certain problems. Say, for example, the scalar quantities along with the velocities are stored at the nodal points. So, in that case, what would be the problem? Say I have a formulation which is for a domain, and in this domain, say I am considering this as my point P. So, I will have a control volume which is this. Okay. Now, consider somehow in this domain.

So, this is my west-east. This is my south, and this is the north point. Now, consider somehow I have an oscillatory pressure profile where I have, or the velocity profile where I have, say, the scalar quantities that I have here. Say this is, at this point I have 100, this one is also at 100, and here I have a value which is 50. Similarly, in the north point I have a value of 100, at the south I have a value of 100, here I have 50, here I have 50, this is also 50, this point is also at 50. Okay, so if now we look into this and try to estimate

So, say this is my real case, that is the actual field. But if I had to estimate it, okay, if I had to estimate it based on our previous understanding of what could be the pressure profile or the velocity profile or the fields that we are calculating here. In that case, what we could have done is say here, so del P by del X. If we do so, it is essentially for this cell: this is the east, this is the west face, P E minus P W by delta X. And since we do not know P E and P W, we would write P capital E plus P capital P, the arithmetic average of these two points, minus P capital P plus P capital W divided by two.

For this one and this one, divided by delta X, which, if we simplify, would give P E minus P capital W divided by 2 times delta X. And now, if you look at this, the actual field, this is based on our previous understanding that this is how we could have done it. But actually, we have a value which is defined as 50 in the domain. As per this estimation of the finite volume, the discretization that we have done, the central differencing, what we see is that here we have P E minus P W of these two nodal points divided by two delta X. Okay, so this is one delta X, this is one delta X. And it essentially results in zero because we have 100 here and this is 100 here.

Which means that causes some problem. That it will not actually give me what is actually there. So such kind of oscillatory pressure profile would not possibly be exactly calculated or exactly estimated. So how to overcome such a scenario? We will discuss this next week, in the next class, and we will continue from here. We'll see how this velocity and pressure couplings are sorted and how this problem can be overcome.

With this, I stop here and thank you for your attention.