**CFD APPLICATIONS IN CHEMICAL PROCESSES**
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**Week-05**
**Lecture 25: Finite Volume Method**

Welcome everyone with another lecture on CFD applications in chemical processes. We are discussing finite volume method where we have gone into the details of its formulation and implementation with various examples. We have also seen a discretization or differencing scheme specifically is the central differencing scheme by which we have mostly used, we have in fact solved couple of problems, started with a steady state thermal diffusion and then with a source turn, then with convection And also we have seen advection diffusion problem.

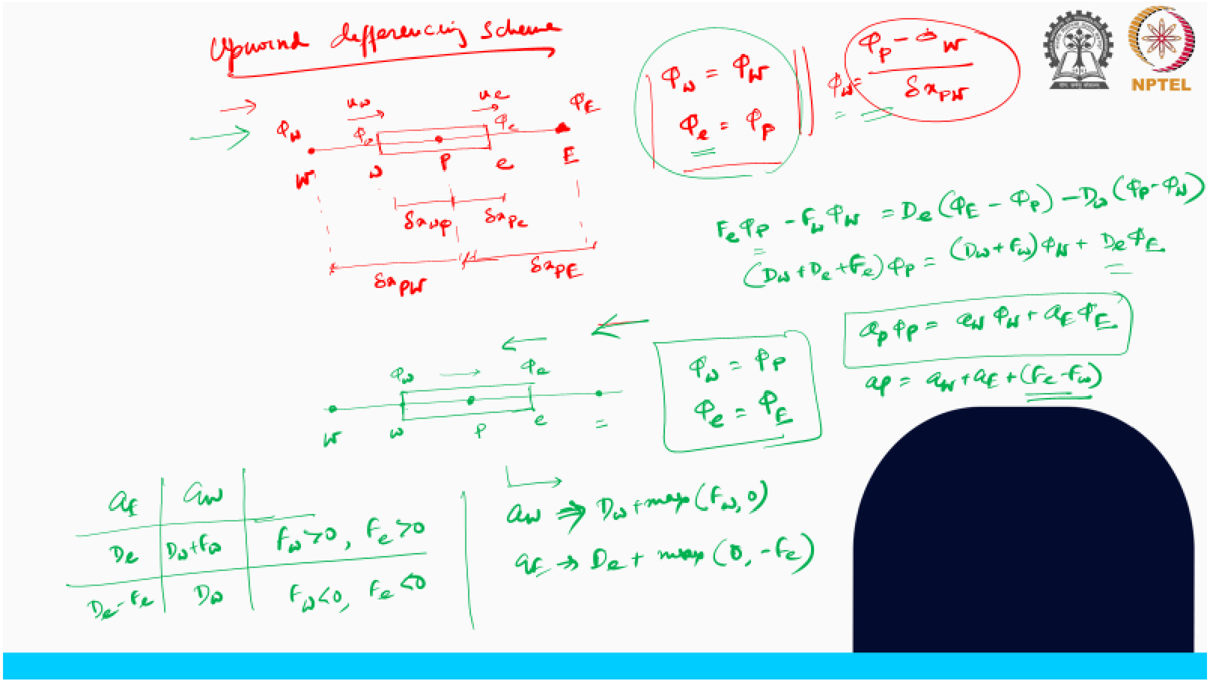
So, and while discussing it, we also discussed the pros and cons of central differencing schemes and what appropriate or good discretization scheme the qualities it should have. It should contain those qualities, those are that I mentioned earlier, say the boundedness, transportiveness, and the conservativeness. So depending on that, and also realizing the drawbacks of central differencing scheme with coarser grid, because it couldn't adjust the flow directionality with the coarser mesh, Because of the cell pickling number has to be with a restricted number, that criteria has to be satisfied. Otherwise, the quotient miss for the central differencing scheme couldn't be used.

There are development of various other differencing schemes. I will mention here couple of the names for your research interest or if you are interested in details you can go into those schemes the literature of it in details. But we will briefly mention them because we have to also go into the other topics. And as I told you in one of the lectures that itself finite volume method can be covered in a 12 week course. But we are here to give you an overview of the different modeling strategies that we will do with the finite volume method.

Or one of the implementation strategy is the finite volume method. So considering the drawbacks of the central differencing scheme, later people came up, the researcher came up with the discretization scheme called the upwind differencing scheme. Now in upwind differencing scheme what happens is that Instead of taking a two point average, what it does, say if I have a control volume of this size, where I have this is as east node, east face, this is the west face, and I have other nodal point capital E and capital W on this phase.

So, what we estimate is the UE and UW at the phases. These distances say for the sake of simplicity again our equidistance delta x small ew and this is the point p small ep delta x p small e this is the distance delta x capital ep and the distance between point p and this nodal point So, based on this what we did in the case of central differencing scheme is that while calculating the flask at this faces we took the central differencing, we applied the central differencing and we applied the Taylor series expansion.

and its truncated form in between P and E. But here, if the flow is from west to east or from left to right, okay, so what the upwind differencing scheme considers that this phi w, small w, the west face, what we are estimating at different phi values, E and phi w, at the faces because that we have to approximate by this finite volume method and with the central differencing scheme we have seen earlier how we considered that. But here what we consider is that if we consider its upstream value the value of phi at a nodal point where it is known and at the nodal points we generally know the value of phi. because it either comes from the boundary condition or from the initial condition.




So, phi small w at the face is basically phi capital W and phi E is basically phi P is the upstream point. So, phi E the east face has its upstream point P and the west face has its upstream point point, waste point which is capital W. So, this is the thing that we do in upwind differencing scheme. And then we replace these values in the formulation that we did similar in the case of central differencing scheme. That means, the steps of converting the volume integral to area integral and from there writing the step remains same.

Only point we change this phi small e and phi small w that we did in the case of central differencing scheme like this. This was the approximation for phi w at the waste phase by the central differencing scheme. Instead of that, we consider here the upstream point value. Because if you remember the sphere of influence, the discussion that we did for the case of the drawback of the central differencing scheme, which actually is circumvented by this differencing scheme. So it actually takes care of the flow directionality.

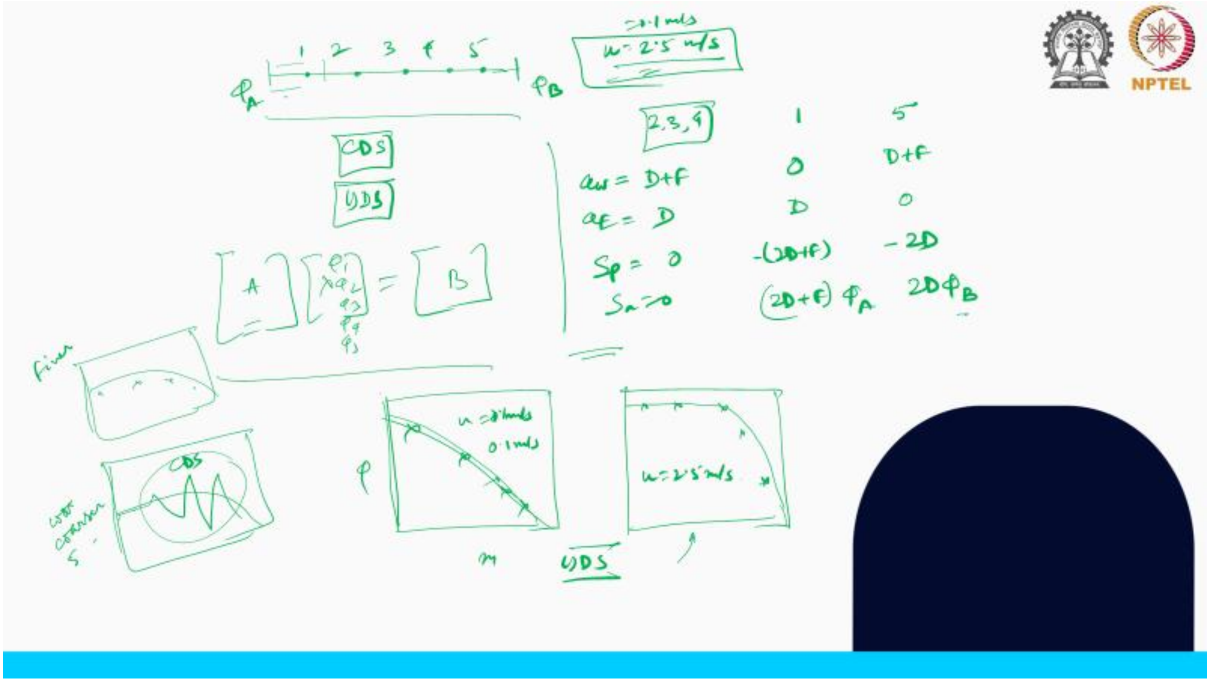
And so when this happens, when the flow is in from left to right, In the same case, if the flow happens from the right to left, so if the flow direction is from this way, so if I draw it once again, So all other thing remains same, the distances and all. And say now here the flow is in this direction. So in that case, my phi w would be phi p because the flow is happening from right to left.

So this is the upstream direction from where the flow is coming. So since the upstream direction is this, from right to left. So the assumption of this point, the scalar variables or the values at this point or this phase is equals to the Phi P, capital P. And Phi small e at the east phase is essentially Phi capital E of this point. That is the from where the flow is or from that side or the direction the flow is coming.

So, this is the upwind differencing scheme. So, we replace these values in the formulation and then we solve the problem. Now, while doing so, what happens? The formulation, it becomes something like this. So, when we try to write it, the formulation that happens is FE, phi P, okay, minus Fw, small w and phi capital W, because here you look this phi E, the east face has been replaced by its upwind point,

considering the flow is happening from left to right, is equals to dE phi E minus phi P minus dw phi p minus phi w. So we try to find out the expression of phi p the coefficient of phi p which would look like something like this. So the point is, after replacing these values or with the Appoint Differencing Scheme, we can find out again, similar to the Central Differencing Scheme, with a similar strategy, the expression of Ap phi p

is equals to AW phi W plus AE phi E just like we have done earlier where AP is AW plus AE plus FE minus FW because this is the continuity part which is essentially 0. Once you do this, I will skip this part. I want you to go to the formulation of the previous one. And in place of phi w, small w is equals to this, which is the central differencing scheme. If you replace that with the upwind differencing schemes, what you should find is that the coefficients would be AE and AW.




Now here for the generic formulation, we will put a criteria in which direction flow is happening. That means if I have FW greater than zero and FE greater than zero, I will have a generic set of expression. or if the flow is happening from right to left, that means this is this, then I will have another generic formulation. So when the flow is in, so generally we consider this is the positive direction, positive X direction. When the flow is happening in the positive X direction, the AW coefficient you should find out

or you should land up with this value. And AE is DE. Okay. In case the flow is reversed, in that case, what I will have or we will have is that DE minus FE. So essentially, AW is will be in generic those who try to write the CFD code is the maximum value between W and zero and AE similarly would be DE plus max of zero and minus FE.

Accordingly, automatically the code will understand the direction of flow and that kind of wiggle formation would possibly be reduced. And then what we'll do, we will solve the same previous problem that we considered earlier where we have this one meter long domain with five points with five points and velocity of 2.5 meter per second with all the previous properties that we did earlier. So in that case, remember, we still have a boundary conditions or two boundary conditions that we have to incorporate. So, when you do this generic formulation like in the central differencing scheme, what we have basically a generic formulation for one nodal point 2, 3 and 4, similar to the central differencing scheme.

For that, what I have, what we have is that this is the coefficient would be for AW and AE would be D again considering uniform diffusion uniform properties throughout the domain. SP you would find out 0 and SU is 0. But for node 1 and node 5 or the control volume 1 and control volume 5 you will have For control volume one, you will have no waste phase.

So AW would be essentially zero. Okay, AE would be D. SP would be 2D plus F. And this would be 2D plus F into boundary condition, phi F. For 0.5, AW would be D plus F just like the 0.234, AE would be 0, SP would be minus 2 times D and this would be 2D phi B, the boundary condition. The same problem that we did with the central differencing scheme, now we'll do with the upwind differencing scheme. This would be the formulation where I have skipped several part because we are doing it for the several times and I hope you have gotten the idea so that you can come

till this part with the matrix formulation where I will have this part where A would be the coefficient matrix. This is the phi 1, phi 2, phi 3, phi 4, phi 5 for the five matrix points and B would be the other matrix where we have the other all known parts. And then if you solve this problem by any method. What you would realize that then in the case of instead of say earlier problem which was 0.1 meter per second, where the central differencing scheme predicted somewhat decent result, the upwind differencing scheme also would give you the similar trend.

Phi versus M. With the same number of points, with the same number of points, when we do it with the upwind differencing scheme for U is equals to 2.5 meter per second, what we will see that it is eventually giving it is giving the similar trend even with the five number of meshes. So what we have, so here this is 0.1 meter per second and this is 2.5 meter per second with the upwind differencing scheme. The real improvement we see in the case of this convection dominated problem when U was enhanced by 25% from 0.1 meter per second to 2.5 meter per second. The central differencing scheme with the same number of nodal points were unable to give us the result. The result was in that case, if you remember, this was supposed to be the analytical result. But in that case, we have such vehicle formation with the central differencing scheme with five nodal points or the five grid points. but with the coarser mesh, that means if we consider five nodal points as the coarser mesh, with that, because I told you that if we had increased that number of control volumes or the number of nodal points from five to 25 or five to 20, this result by CDS even would give us the similar trend as of the analytical solution.


So this was the fine mesh or the finer mesh and this was the coarser mesh. Five nodal points was the coarser mesh. So for this mesh CDS, the central differencing scheme was unable to predict or to match the analytical result or the actual physics. But the upwind differencing scheme nicely captures the trend, but again with improvement, with finer meshes, the results would also be further improved. So how much is the improvement?

If you want to know that quantitatively, you have to solve this part that I have given you by replacing the numerical values. and what you should get that five equispaced points or the five equal size control volumes, what you should get that for node one, for node one, two, three, four and five, the finite volume method by the upwind differencing scheme would be having this value against the analytical solution. Where analytical solution is one for nodal point one, here it is 0.99 and this is also 0.99.

For nodal point three, So, this is basically x is 0.1, this is x is 0.3, 0.5, 0.7 and 0.9. So, these are the x values at this distance from the left hand side boundary condition. At nodal point 3, the value we have say 0.992, so all these are 0.99, so 0.999 again. For 0.4 you would find 0.952 and here 0.999 and then at this you have 0.714 and here you have 0.918. So the maximum deviation happens at the last point and that deviation is in the range of 22%.

Whereas in the case of central differencing scheme, it was much pronounced and also not only that, because the graphical solution or the graphical plot would give us that it was not able to capture the physics itself, the trend. Capturing the trend means capturing the physics what is happening inside the domain. But in this case clearly visibly this upwind differencing scheme is capturing the physics correctly and also it is accurate for most of the points except the last point where it is deviated by 22%. So in this case that means again with the refinement of the grid we can achieve more accurate solution. So that accuracy depends on the number of grids as you go finer and also with the number of increasing grid points you can understand

The thing that I told repeatedly is the computational demand or the computational power demand increases. Computational resources, everything you would require in more exhaustively as the grid becomes finer. And accordingly, you have to set your wish list that how much accurate result you would require with the stipulated time. or the set time that within this duration or I cannot waste much time on this if I have 10 percent accuracy I am fine with it then accordingly the mesh you have to refine but remember again the point the importance of grid independent result or the grid independency study because a minimum number of grids are required in order to capture the physics otherwise your CFD predictions or the finite volume method predictions would go wrong.

So with this, I will stop here today. And again, with the next lecture, we'll briefly take you through the other differencing schemes that are available, the higher order differencing schemes. And then we will move on to the velocity pressure coupling. That is extremely essential because we discussed that all the cases we have discussed illustrated till now considering the velocity field is known. What happens when it is not known?

We will discuss that in details in the next lecture. Thank you for your attention.