CFD APPLICATIONS IN CHEMICAL PROCESSES

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Week-05

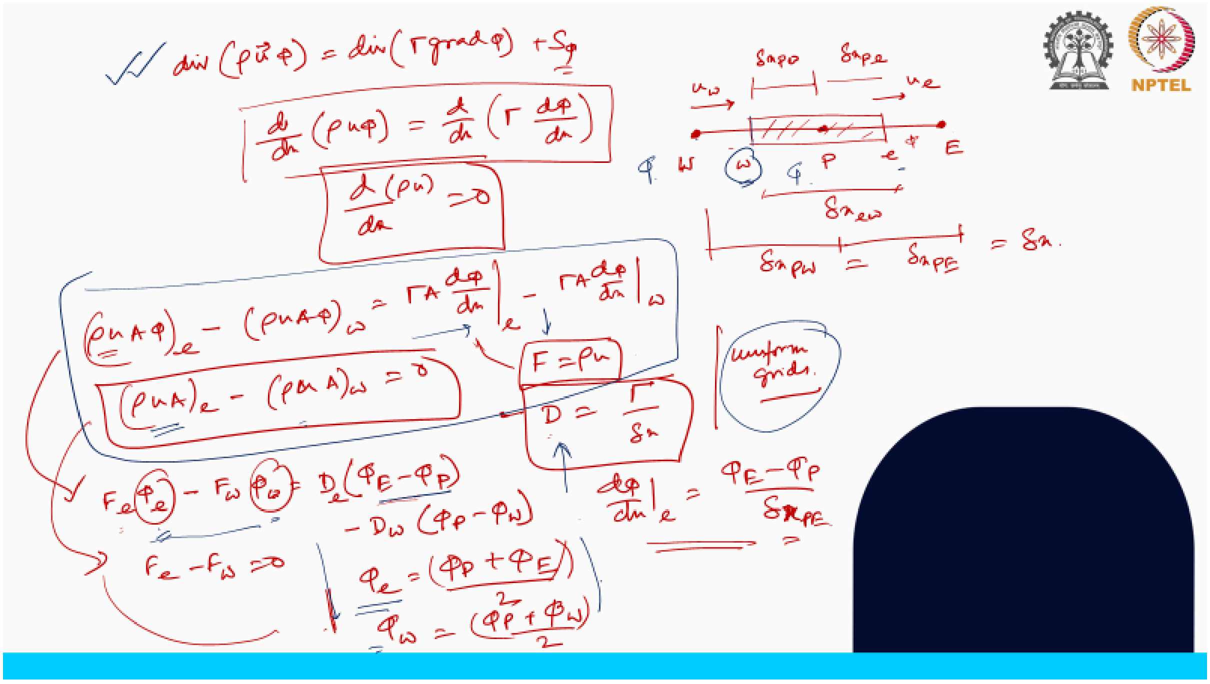
Lecture 23: Finite Volume Method

Welcome everyone in the NPTEL certification course on CFD applications in chemical processes. I am Arnab Atta. Since the last couple of lectures, we are discussing about finite volume method, its implementation. Couple of examples we have seen with one dimensional cases, including steady state equations. All the examples we have seen till now are for the steady state operation or the steady state governing equations that we have seen, particularly taking an example of the temperature profile. We have seen the cases of steady state heat conduction.

We added a source term later on it and with it and then we have also seen the pin-fin problem where we had convection. We started the last class with an example of advection along with the diffusion. So the problem or the governing equation that we started was is we mentioned that it is say having a generic expression that is given here. And for one dimensional case, for the sake of simplicity, what we have done is that we have discretized this equation as per our previous understanding.

And for uniform grid particularly, we defined two terms or the two variables. One is f that takes care of the rho u or the convective part. we also had D which is the diffusive part that is gamma divided by delta x where delta x is the control volume size or the grid size. So, now based on this we came till this part that we had to estimate this phi e on the east face and the phi at the west face those were there which we estimated as a simple arithmetic average which is the easier to take into consideration.

So, when we now include all these discretized form in the governing equation from where we came. So, this set the thing that we get is essentially is having a form that is f e by 2 phi p plus phi e minus f on the waste phase phi w by phi p is equals to, because this is the phi E and phi W that we have considered, it is the simple arithmetic average of the two neighbor nodal points or the grid points. So, for example, for the waste face, this property phi is essentially the average of what is phi W here and phi at this T location. And then on the right hand side of this expression, we already had approximated in terms of phi E and phi P by the central differencing scheme or different differencing scheme that we had discussed earlier.

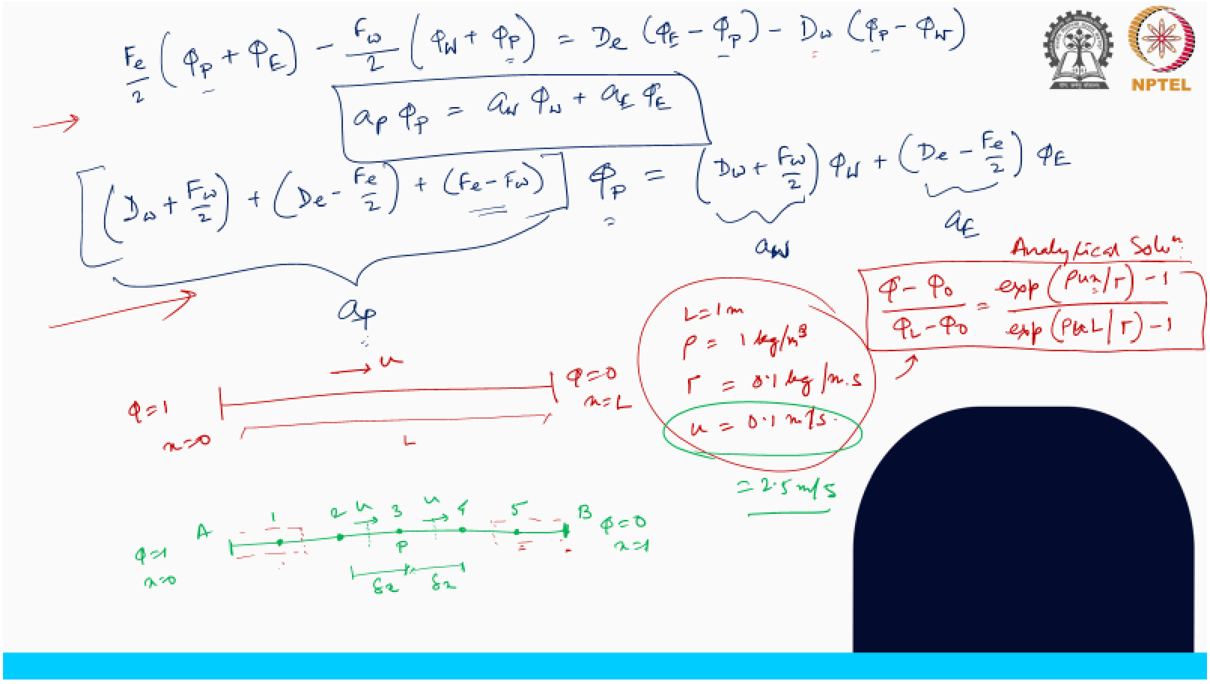


So, similar to that here, we have taken this as phi E minus phi P divided by delta X and this delta X divided the gamma divided by delta X is the capital D. So, those are written here. Now, again similar to our previous examples What we will do here, we will segregate the coefficients of phi p, phi e, phi w to have the same form or the similar form of a p phi p is equals to a w phi w plus a e phi e. In this form, we will try to write it or we will try to rearrange this equation.

And then what will happen is it would be something like this that we have once we find out all the coefficients of phi p and take it on the left hand side by 2 plus dE. F e by 2 plus F e minus F w. Remember F e minus A w is 0 because this here what we see that this is F e and this is essentially F w. So, f e minus f w is essentially 0, but we are keeping it here because we will have this form complete. So, this multiplied by phi p is equals to phi w plus y e. So, once we rearrange this expression, we find that this is my a p, this is a w and this is a e. So, we get the coefficients of a p, a w

which is capital W and AE. Now, for all the nodal points, the same formulation remains as it is. Now, depending on these values that we have in the problem statement for the velocity field, for the diffusive coefficients, etc., we will find out what are the coefficients of AP, AW and AE. And accordingly, we can develop that set of algebraic equation we have seen earlier and we solve it for the phi P. So let's take an example that say we have

a flow problem where phi is 1 at x is equals to 0 and phi is 0 at x is equals to L. Now, if I have L is 1 meter, the flowing fluid rho has a density of 1 kg per meter cube. the diffusive coefficient is 0.1 kg per meter second and say this velocity I know is 0.1 meter per second. So, what would be my phi profile as we go along this length that is L. total length is L which is 1 meter. Now, similar to our previous example, what we will do?

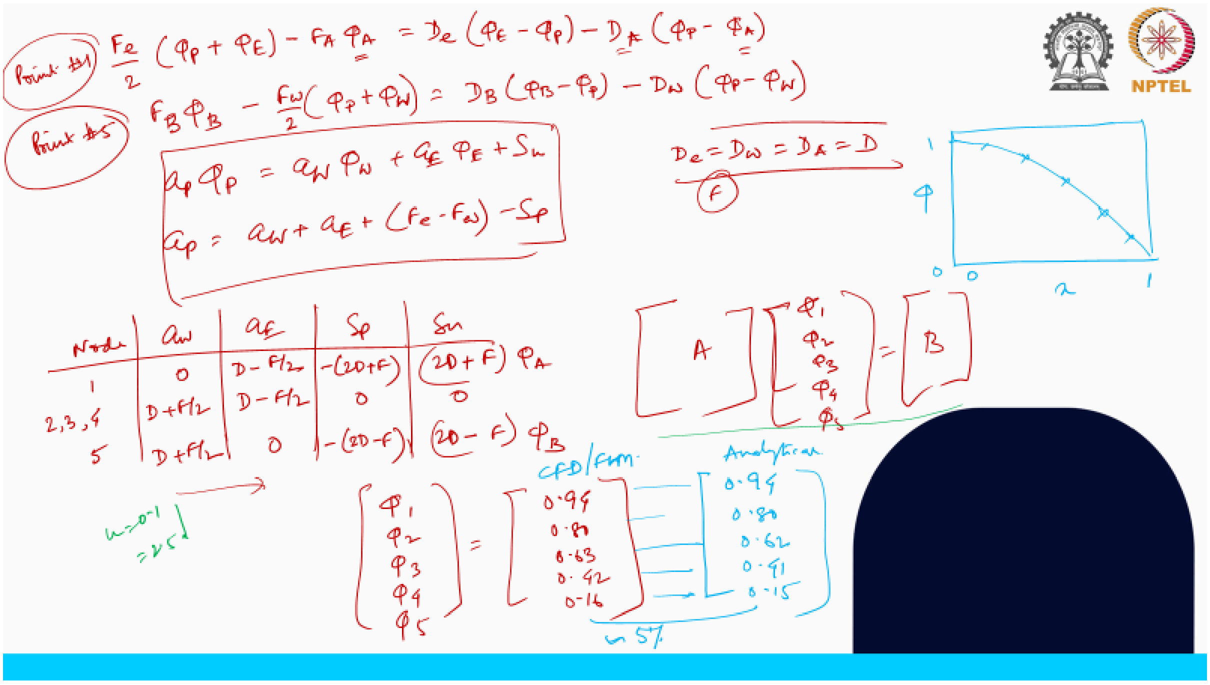


The first step would be that we divide this domain into say for example, here say I have point one, two, three, four, and five nodal points I have. So then what I have is that along all these points, so this is one, two, three, 4 and 5. This is my boundary condition a and b, where phi is equals to 1 at x is equals to 0, where phi is equals to 0 at x is equals to 1. Now, here this distance is essentially delta

So it is equispaced we have considered or we consider here is the equidistant points the nodal points are here. So what we have now if these are my faces say I consider point 3 as my point P. So if these are my faces so what I have the U values are the U for the flow domain we know the value of U. Now, for this problem there also exists an analytical solution which is pi minus pi 0 divided by pi L minus pi 0 is equals to by gamma minus 1, this is L minus 1. So, for various you can find out the value of phi at that particular x location.

Now this, the reason of writing it, this is the analytical solution so that we can verify or cross-check our finite volume prediction after we solve it and we will cross-check that how much accurate our predictions are based on the five nodal points we have considered here. So here, for this problem, the same development of governing equation, discretization, et cetera, remains. And in this case, we already have done this. Okay. And so similar to this, our previous understanding, what we will have is that first and the last point would require our special attention or bit slight deviation from this generic development because for 0.5, we have the boundary on the east side and for 0.1, we have the boundary condition at the west side. So, for those two points, what I can write or this you have already seen, if A phi A is equals to because this is the point where we do not have the waste boundary, formerly waste point, but we have the boundary condition which is phi A, phi P minus phi A. So, we directly also similar to that previous case. So, here instead of waste, there is no waste for point 1, but the boundary condition.

So, that is why we have written that it is the diffusive part or the diffusion coefficient for point A and the phi A. So, this is for point 1. For point 5, we have FB multiplied by phi B because we do not have the east point for nodal point 5, but we have the boundary condition phi B minus phi p plus phi capital W is equals to dp phi b minus phi p minus phi w. So, this is for 0.5, this is for 0.8. And why we are doing this?

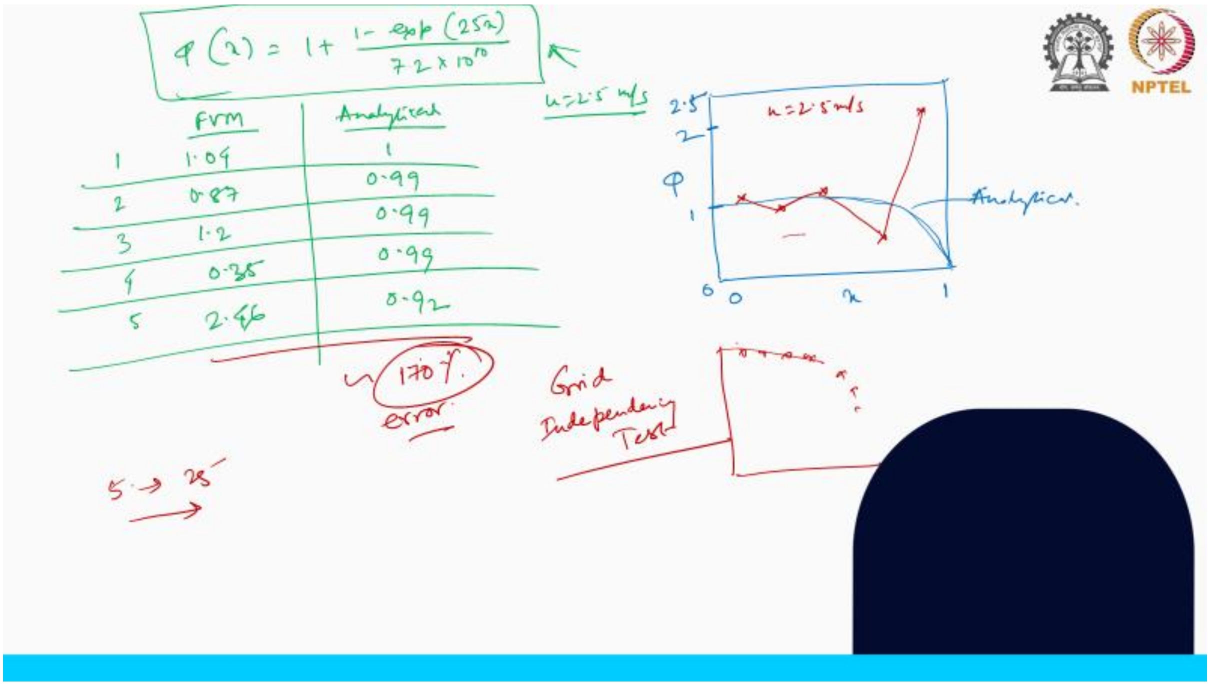


Because we are trying to have a generic form of this equation so that we can write it similarly for others. Where AP is equals to AW plus AE plus the continuity form because that is 0 that has to be conserved minus SP. So, in this form, if we write the previous expression, this one as well as these two nodal, the extreme nodal points, then for the node 1, I have AW, AE, SP and SU. I can find out the coefficient for 1 for 0.234 because those would be common and for 0.5. So, I find the coefficient for 0.1 for node 1 phi w, we do not have a w, but a e is d minus f by 2.

Once we rearrange And we will find out that the coefficient of AE would be D minus F by 2. So here what we are further assuming is that DE is equals to DW is equals to D is equals to D.

So all the values are uniform throughout the domain. And so the F. So D and F are uniform throughout the domain. There is no change in density.

as well as the velocity profile throughout the domain. So, in that case the coefficient after rearranging which you should do and you find out such coefficients would be there for 0.1, for 0.2 we have f by 2 d minus f by 2 sp is 0 and su is 0. Now, remember here there is no source term, but these are appearing for the first and last nodal point because of this rearrangement of the coefficients. So, this also has this form the last point the nodal point 5 minus 2D minus f and it would be 2D minus f multiplied by 5B.



So once we have this and once we replace this numerical values, the properties and the velocity field in this coefficients, what we can find out that we will have a matrix of the values and of phi 1, phi 2, phi 3, phi 4 and phi 5. is equals to further on the right hand side you have the other matrix AX is equals to B you have to find out the X matrix. And if you solve this after replacing this numerical values here what you would find is that phi 1 this is equals to 0.94, 0.80, 0.63, 0.42, 0.16. These are the values you would find.

And then you cross check your result with this analytical solution. This is the analytical solution. So for this analytical solution for each and every value of X at the same location where you have taken this 0.12345, you also get the exact solution for these five values. And if you compare it, the profile would be something similar to this, but this is not to the scale. So, from 0 to 1 in the X, you have the value of phi.

So, if this is 0 for phi and this is 1. So the property that you will have some values like this. The analytical solution would look like this. And this CFD predictions by finite volume would also be similar to that value. So these points, the discrete point that I'm drawing that eventually will fall on this analytical solution curve.

which means these values, the analytical solution. So if I write the analytical solution at these points, the similar values you would be having 0.80, 0.62, 0.41 and 0.15. So that you can see that corresponding values are very much closer to the analytical solution. So this is the CFD, this is the analytical solution. Finite volume method, and this is the analytical solution.

So here, if you compare the maximum deviation happens at this last point, which is in the range of 5%, in the range of 5%. which is great I would say considering that the number of elements that we have taken here is only 5. So, that means this number of grid and if I consider my 5 percent accuracy is acceptable then it works pretty well. Again the same problem can be repeated with 10 number of grids And further this 5% accuracy can possibly be further improved to say 2%, 3% or something like that.

Now, if you redo the same problem, same development, only here the thing that I am asking you to change and practice yourself is that this U value from 0.1 to 2.5 meter per second. That is 25 times increase in the velocity. So this velocity is now increased say 25%, that means it becomes 2.5 meter per second. So for this problem, once you increase it to 2.5, the exact solution,

would be 10 to the power 10, but here till this step the development remains same. the model development. Only the numerical values would change that instead of now u is equals to 0.1, you have u is equals to 2.5. And you solve the problem for five nodal points. Okay, so what you would notice in this case that your nodal point

1, 2, 3, 4, 5, you had your finite volume predictions and analytical result. For 2.5 meter per second, the analytical solution here, I will come to that, but before that, let us write the If you had done the same problem and found this finite volume predictions, the value would be something like 1.04.87, 1.26.35 and 2.46. On the other hand, at the same location, analytical values from this expression would be 1, 0.99, 0.99, 0.99 and 0.92. The result trained would be for this case.

So, again from 0 to 1 here from 0 to 1 if I consider for phi and x and let us say here I give 2.5. So, say my 1 is here. So, this is 1, this is 2. So, the trend, the actual trend would be say, this would be the analytical solution. But your numerical result or the CFD prediction here would be something that would be showing by this and say here 2.5. So you have a complete different profile than the analytical solution for U is equals to 2.5 meter per second.

For the same number of grid, same development, everything remains same. Which means for this point, the last point, you have accuracy in the order of 170% or 69%. huge percentage error. And quite visibly so, that you can see. That you have a complete different profile than the actual physics that is happening inside the domain. Why is so? We will find out in the future lectures. But the point is that means

that this five number of nodal points is possibly that one indication is possibly that five number of nodal points are not sufficient to capture this thing. So your task, you increase the five nodal points to 25 or 10. And you will see that indeed if you increase it to 20, 25, you would indeed capture this trend that is there when you have fine meshing or the fine grids in the problem. That when it is 25 or so, 20 or so, you would then start capturing this physics that is happening in the domain. And this is the importance of grid refinement.

Because you are solving the governing equation by finite volume method, so you are supposed to capture the physics, the flow physics. But with coarser machine, you are not able to do that in your first attempt. So in the next attempt, you must do the grid refinement. And that is why again and again we are highlighting the importance of grid-independency test. So in the next class, we will start discussing about the other aspect that what possibly has gone wrong and whether at all with the coarser mesh

we can capture the trend of this physics that we are not able to do with the coarser mesh. Till then, thank you for your attention.