CFD APPLICATIONS IN CHEMICAL PROCESSES

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Week-05

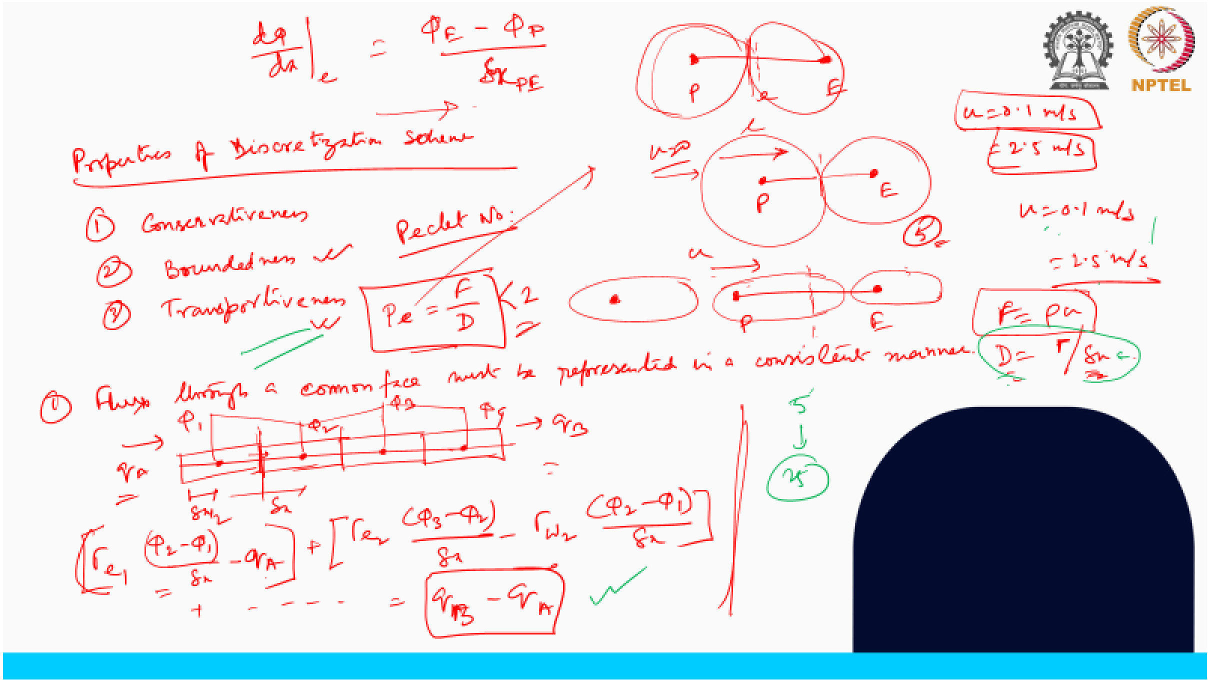
Lecture 24: Finite Volume Method

Hello everyone, welcome back once again with another lecture on CFD applications in chemical processes. and particularly in the topic of finite volume method that we are discussing. In the last class, I showed you one example where we discussed the importance of grid independency more clearly than the grid independent result or the grid independency test because we are not able to capture the correct physics. that the governing equation was telling with the given boundary condition and the numerical values that were provided.

So, what went wrong definitely the number of grids can help us. Now, there are other aspect that I discussed briefly while touching on the discretization that what could possibly the source of those kind of errors. One error is certainly the coarser grid, the distance between the two nodal points that actually played the role. At the same time, there are the discretization scheme which introduces such error. Remember, we used the central differencing scheme in those processes, in those examples.

Because what we did when we tried to convert this d phi by dx term at any particular phase, what we did, we took phi e minus phi p divided by the delta x or the delta x e e, the difference between those two points. Now, that is actually fine when or say the point that we have is that what we call the influence of two neighbor points. So, this means that when we are estimating at this face east face for point P and point E, we are assuming that it has the equal influence from both the sides of the neighbor points.

So, this sphere of influence is equal on this phase where we are estimating this gradient. This could be true if my problem or the given problem statement is diffusion dominated. because think of a point that something is coming from point P towards this face and also from an equidistance point on the east side. So the property values, their influences are equal that can happen if I have a purely diffusion problem. The values are propagated towards this face are equal from both the neighbors if there is only diffusion but there is no advection from any side.



So where this U is zero. But that is not the case for the problem that we solved earlier and particularly when we increased from u of 0.1 to 2.5 meter per second even for 0.1 meter per second although there is some convective motion or the advective motion but still we were able to predict or capture the actual physics with 5% error with 5 nodal points but when we have a strong influence of advection, what happens is that then this influence becomes something like this.

Although I have point P here and E, from the west side, whatever is there that would influence most this neighbor P point and from point P, to this side, whatever we have would also be propagating something like this. So this influence area would be something like this when we have a very strong advective motion that in the direction to the east from point P. If this happens, this would be distorted. The area of influence would be distorted like this.

So the point that we are estimating here, actually it is mostly influenced by point B without any influence of point E. But that we are not able to capture when we do this central differencing scheme with coarser grid. Which means there must be some criteria or a selection criteria or say discretization characteristics that dictate the choice of such discretization schemes. So that means what are my criteria that can be dictating that if we have multiple discretization schemes, which one to choose?

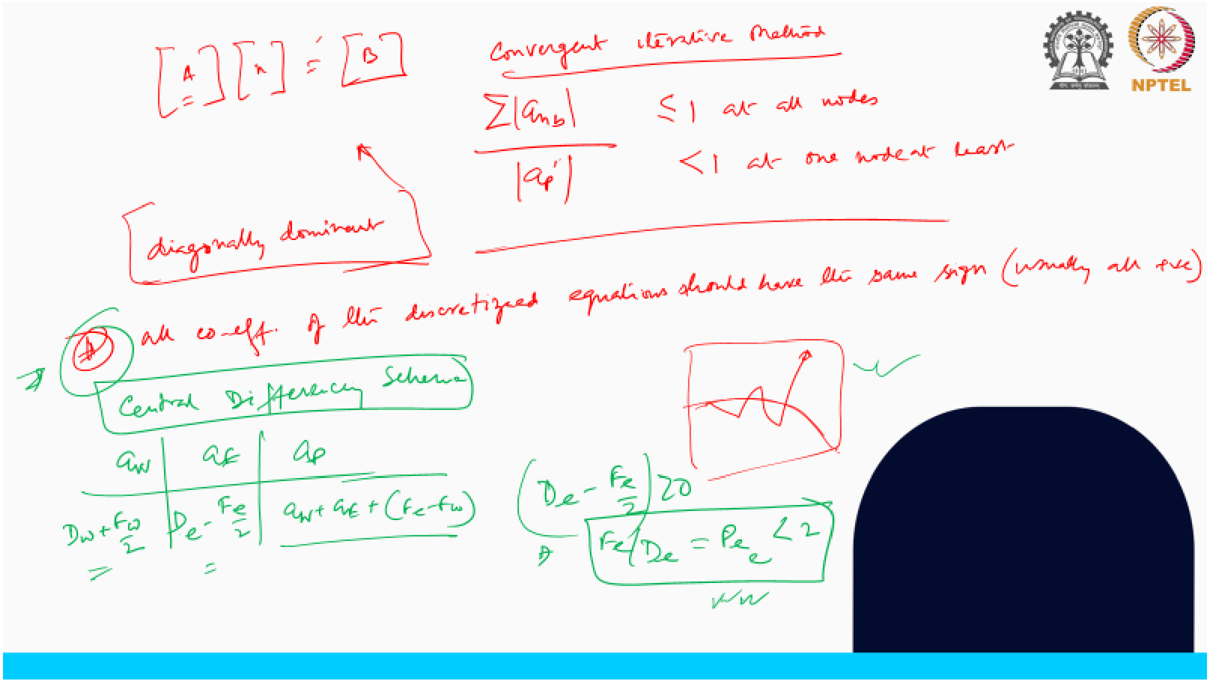
Those criterias are the properties, I would say, the properties of discretization schemes The one is definitely the conservativeness. Second is the boundedness. And third is the transportiveness. Conservativeness means that the flux through a common phase must be represented in a consistent manner. Your chosen discretization scheme should represent the flask that are going through or passing through. So if I have this control volumes, if I have, say the quantity comes in, QB going out from this. So if you have some gradient that you are calculating at this, say, the faces of this two control volume, then if you have here phi A and this is phi B, or say phi 1 and phi 2,

and for here if you have phi 3, this you have say phi 4. So, this is delta x by 2 and all these are delta x. So, the point is whatever comes in that is going out and that must be represented at this control volume faces consistently. So in this case, if I try to write that phi gamma E1 for the first control volume, so phi 2 minus phi 1 divided by delta X minus QA. This is my balance for the first control volume. This thing comes in, this thing goes out from this phase.

Plus for this phase, when we do by this analysis, the same analysis by E2, phi 3 minus phi 2 divided by delta x minus. So this is for the 2 represents the second control volume, phi 2 minus phi 1. Now this is the part that comes in from 1 to 2. delta x and similarly you write for 3 and 4 and you must find out after solving this part or if once you simplify this part this must be equals to QB minus QA that is the net quantity. So if this is satisfied, once you write such analysis for the, now this is here we have done this central differencing scheme and we will find out for this case that it is indeed this is conserved.

This is the property that we say the conservativeness of this point, of this discretization scheme. In the second case, what we have is called the boundedness criteria. Now, typically for this problem or whatever we have seen, there is what we do is that this is the matrix that we solve at the end or after formulating it. Now it is that we have a sufficient condition when there is a sufficient condition for the convergent iterative method. And that is the summation of this coefficient that we have divided by a p prime

which is including or this source term is essentially less than equals to 1 at all nodes and less than 1 at 1 node at least. If this criteria is satisfied, then we will have a stable solution. What it does? It actually imparts, because this A is essentially containing all these neighbor points. So this, once this is satisfied, what it results is that a diagonally dominant solution. diagonally dominant matrix, which are bounded by the boundary values and the criteria is that all coefficients of this discretized equation should be, so all coefficients of the discretized equations should have the same sign. all positive. If that doesn't happen, then we have this Weigel formation that we have seen in one of the predictions earlier. That although my exact solution was like this, but then I had this kind of a Weigel formation.



If this criteria, this boundedness criteria is not satisfied. So the third point is the transportiveness that I illustrated here is that this directionality of flow and corresponding influence of the neighbor point that has to be taken care automatically by this discretization scheme. And that is actually dictated or understood by the parameter which is called the dimensionless number called the Peclet number. So this Peclet number that is the ratio of the convection coefficient and the diffusion coefficient tells us the nature of the problem

And also it must account this discretization scheme that we should use must take care of this directionality of the flow. That it is current in this direction. So the points that are there on the east side would be influenced by east west neighbor points. So transportiveness is essentially that means the adapting or the characteristics of adapting the directionality of the flow or the flow direction that it picks up very quickly or understands and also implements this criteria that whether my problem is diffusion dominant or the convection dominant.

If these are satisfied by a discretization scheme, that would be perfect or the ideal for that particular problem. And that is why you will find several discretization schemes that are given in any commercial CFD solver that you should choose from apart from their default values. So the point is we have seen that central differencing strategy and the magnitude of its error or the order of accuracy. The second order discretization scheme previously we have seen is having the order of accuracy to the second order. So for this problem, once we calculate this Peclet number for the last problem, when we had this U is equals to 2.5, okay?

And Peclet number is defined is essentially F by D. So it is the Peclet number. We discussed this non-dimensional number at the very beginning in the introductory lectures. So this Peclet number, that is this convective property divided by the diffusive property here. If this is less than 2, then it is seen that the central differencing scheme works pretty well for the problem that is given.

So, for the problem if you are able to calculate this Peclet number and if you see that it is I mean Peclet number based on this definition, if you see that it is less than 2, then you can safely use central differencing scheme for your problem. So, what happened? that when we had u is equals to I mean why the central differencing scheme worked for u is equals to 0.1 meter per second, but did not work for 2.5 meter per second.

If you replace the numerical values in f by 2 because f is rho u and d is diffusion coefficient divided by the delta X. Now this delta X is essentially the grid size, if you remember correctly. And F is purely based on the flow property, the velocity field and the physical property of the flowing fluid. This D here, is also having the diffusion coefficient divided by the delta x. Now, this delta x is user defined.

So, for the problem statement that we have seen earlier, when u was 0.1 meter per second, if you calculate this Peclet number for 5 grid points, the reason I am saying the 5 grid points because that dictates this delta x. this delta x for 5 grid points if you had a length of 1 meter you get the delta x for that particular delta x if you calculate the Peclet number with u is equals to 0.1 meter per second you would see that the Peclet number is indeed less than 0.2 this less than 2 and that is why it worked for you and why this number comes to because for the central differencing scheme if you look at the coefficient you would see that aw that we developed was and this is AE plus AW plus FE minus FW.

So this was our development or we derived this. Now, if you see this point, this criteria of boundedness that I have should have all coefficient of the discretized equation of the same sign and possibly or usually all are positive sign. If you look at this coefficient, you see that AW is indeed a positive value. But the chances of AE being negative is there until and unless this DE minus FE by two is greater than zero always.

And that leads to the criteria that Fe by De is equals to Peclet number on the east side must be less than two. So for that problem that we had, if you see that U for 0.1 meter per second with five nodal points that defines the delta x, we have the Peclet number satisfying this criteria for all the faces. But when we increased it to 2.5 or 25 times increment of it, keeping the same delta x, that is the five nodal points, we actually are not satisfying this criteria for implementing central differencing scheme.

And that is why we had this kind of a wiggle formation. So it is clear to you that if you choose the default value or if you choose any particular discretization scheme, you must be aware of its limitation. or its applicability. And that is why several other discretization schemes are usually given. So to overcome, so this central differencing scheme is perfect in terms of conservativeness. If you put the criteria of boundedness, you will have its applicable range. but it miserably fails in transportiveness.

What transportiveness? For this problem that we have understood that, okay, even if it is 2.5, now what you have in hand to reduce or to come into this applicable region is that reducing the value of delta x. That means you are refining or making the grids finer from the coarse value. And that is why it works for 5 to 25 when we increase it to 25 or 20 number of nodal points. Because then this delta x becomes very small and we have the d value much larger.

So, the Peclet number becomes or comes within the applicable range which is Peclet number is less than two. So if with the, so because once you increase the E value of U, that means you are moving from diffusion dominant problem to the convection dominant problem. And convection comes with the flow direction. So that means if you make the grids finer and finer or

then you can use the central differencing scheme, which is very robust, has the accuracy of the second order, and it complies with the conservativeness criteria. And everything looks very fine there. But that increasing the number of grids comes at the cost of computational time and computational resources. So therefore, there are alternate or alternative discretization schemes that are also available or the differencing schemes that are also available, okay, which we will discuss in the next class, couple of them. There are several, but I will just mention two or three names and we'll see how it works.

And then we move on to the pressure and velocity coupling because whatever we have discussed till now considering like this problem the velocity field is known to us. But in most cases or in fact several cases that the velocity field is also to be calculated along with this other scalar variables or the scalar properties like the pressure and or temperature. So on this note, I will stop here today. And in the next lecture, I will come up with the other differencing schemes that can replace central differencing scheme. Thank you for your attention.