Computational Fluid Dynamics

Prof. Dr. Suman Chakraborty

Department of Mechanical Engineering

Indian Institute of Technology, Kharagpur

Lecture No. # 34

Discretization of Convection-Diffusion Equations:

A Finite Element Approach (Contd.)

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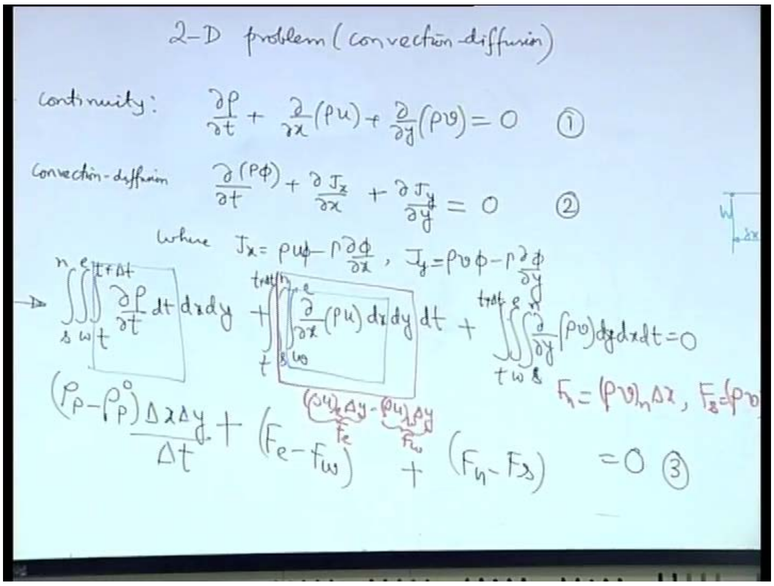

In the previous lecture, we started deriving the two-dimensional discretized forms of the convection diffusion equation by considering an unsteady problem. The governing equations were the continuity equation, and the convection diffusion transport equation. And we define various variables as J x and J y as shown here in the board, and we first integrated the continuity equation with respect to the control volume chosen, and from that we obtain the following equation rho p minus rho p not delta x delta y by delta t plus F e minus F w plus F n minus F s equal to 0.

Where F the quantities capital F represent sort of flow strength across various phases of the control volume. For example, rho u e delta y represents the flow rate through the east phase rho into u is the flux of mass that multiplied by delta y into one, because it is a two-dimensional problem. So, the third dimension width is one. So, delta y into one is the phase of the corresponding east side of the control volume. So, that represents the flow rate, similarly all other terms also represent the flow rate. Now, with this equation in mind this we call as let us see equation three, we will now discretize the convection diffusion equation that is equation number two.

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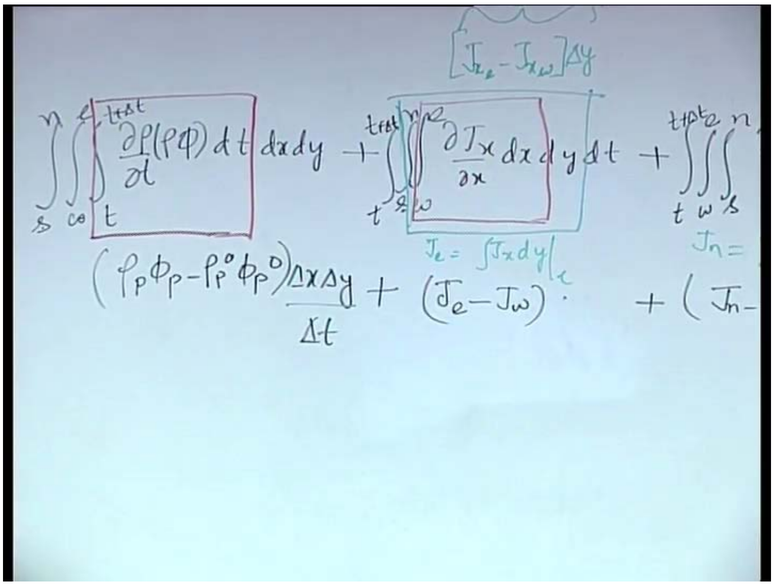

So, what we do we integrate dt dx dy, let us put the various limits of integration t to T plus delta t remember we are doing fully time implicit discretization that will be reflected in the next steps (( )). So, first we integrate the time expression here and what we can assume we can assume a piecewise constant profile for both rho and phi over each control volume. So, rho p phi p minus rho p not phi p not into delta x into delta y for evaluating the next terms first we consider this integral. So, that will become J x at e minus J x at w, then next what we do we consider that integrated over y. So, we have J x e minus J x w into delta y for this particular part of the term this we call as J e minus J w where what is J e integral of J x dy or J x into delta y.

So, to say at e similarly, the same at small w is J w. So, the definition of the J is very similar to a one dimensional problem except you have the previous J multiplied by a delta y. So, it becomes plus J e minus J w into delta y into delta t is there plus J n minus J s into delta x into delta t that is equal to zero.

So, delta x delta y are already considered in the definitions of J therefore, you do not have again a repeated consideration of delta x and delta y. So, likes likewise like J e J n how it is defined integral of J y dx at the phase n. Now you can again divide both sides by delta t as you did for the continuity equation. So, the discretized equation will come as this.

Let us say this is equation number four. Equation number one and two were the continuity and the convection diffusion equation. Equation number three is the discretized continuity equation, and equation number four is the discretized convection diffusion equation. Now you can see here that an additional variable density has appeared rho p. So, you have to eliminate rho p from these second equations.

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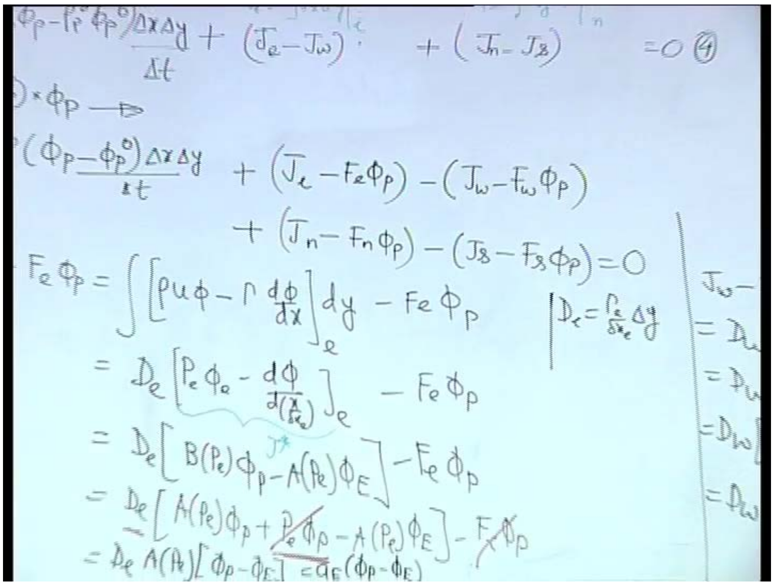

So, how you can do that you can subtract equation three multiplied by phi p from equation four, then rho p phi p minus rho p phi p. So, phi p will be eliminated. So, if you do that you have rho p not into phi p minus phi p 0 into delta x delta y by delta t that is the subtraction of the first two terms, plus J e minus F e phi p minus J w minus F w phi p plus J n minus F n phi p minus J s minus F s phi p equal to 0.

So, other than unsteady term you can see that the other terms have four different groups these are similar ones. So, let us calculate the first group J e minus F e phi p that will give us an indication of what will be the discretization of the remaining groups. So, J e minus F e phi p J e is integral J x dy at e. So, rho u phi minus gamma d phi dx minus F e phi p. Now, you can non-dimensionalize this one remember we are calculating at the small e phase. So, appropriate length scale is delta x e, we are calculating at here this is small e small w small s and small n. Now with that using that as an appropriate length scale we can have a diffusion straying D e physical to gamma e by delta x e, if you divide both if you divide the both of these terms by D e and multiply by d e. So, it will be D e integral of p e phi e minus d phi dx by delta x e dy minus F e phi p.

See this is what this is nothing, but the J star. So, in this D e what we can do. So, this part is nothing, but the J star the non dimensional J p phi minus d phi by d non dimensional x, this we define as J star or a non dimensional J. Now, what we can do is we can also. So, when we have defined D e is equal to gamma e by delta x e that was a 1 dimensional problem in a two-dimensional problem, we can define D e in a bit of a different way this we can multiply by delta y. So, this is the total diffusion strength, because this is like part unit area and delta y into 1 is the area perpendicular to the direction of the propagation of the diffusion flux. So, to if we do that then, what we can write it in this way, we can write this as D e into J star at e that integral of dy that is delta y that has been accommodated in this D e term.

So, next what we can write J star as d phi B of p e B phi i minus A phi i plus 1, what is i you are considering the phase small e. So, what is i and what is i plus 1 i is p and i plus 1 is capital E. So, B phi p minus A phi e minus F e phi p remember the argument p is p based on delta x c you can write B as a plus speckle number. So, D e a of p e phi p plus p e phi p minus A of p e phi e minus F e phi p. Now you see carefully look into this term D e into p e is F e F e into phi p and minus F e into phi p these 2 terms get cancelled.

So, it becomes D e into A p e into phi p minus phi e. So, that is equal to small a E into phi p minus phi e where small a E is D e into capital A. That is the dimensional co efficient and A of p can be written in terms of A of mod p depending on the scheme you choose. So, you can see that it is perfectly generalized you can select a particular scheme and accordingly substitute the expression of A of p here.

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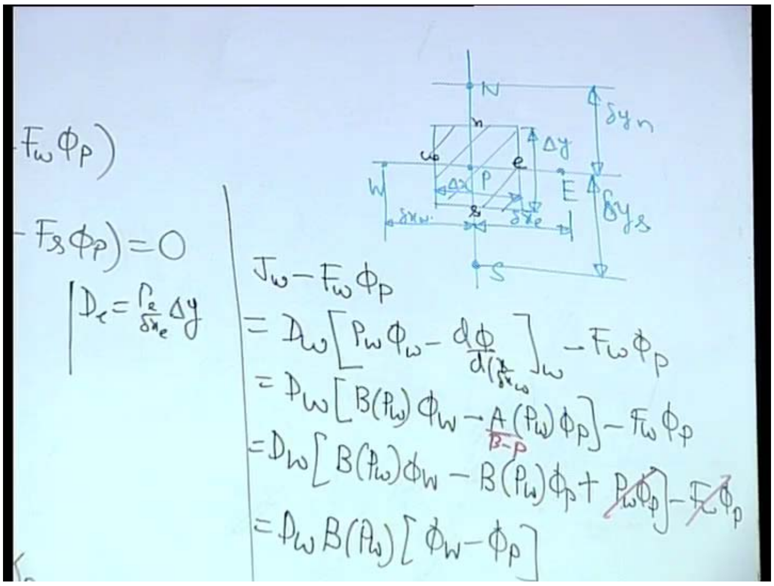

Similarly let us consider one more term may be J w minus F w phi p. So, let us try to skip a few steps try to take a lesson from this one and try to write. So, instead of D e it will be D w p w phi w minus d phi dx by delta x w w minus F w phi p. So, this is D w this is J star at small w. So, B p w phi capital w minus a p w phi capital p minus F w phi p.

Now, you have to eliminate phi F w phi p here. So, now, what you can do is instead of this a you can write this as B minus p. So, D w B p w phi w minus B p w phi p plus p w phi p minus F w phi p, where we have written this a as B minus p. So, now D w into p w is F w into phi p that F w into phi p term gets cancelled out. So, you are left with D w into B p w into phi w minus phi p it is straight forward to find the remaining two terms which are exactly similar as these two terms. So, when we assemble these equation finally, what is the form that we will get.

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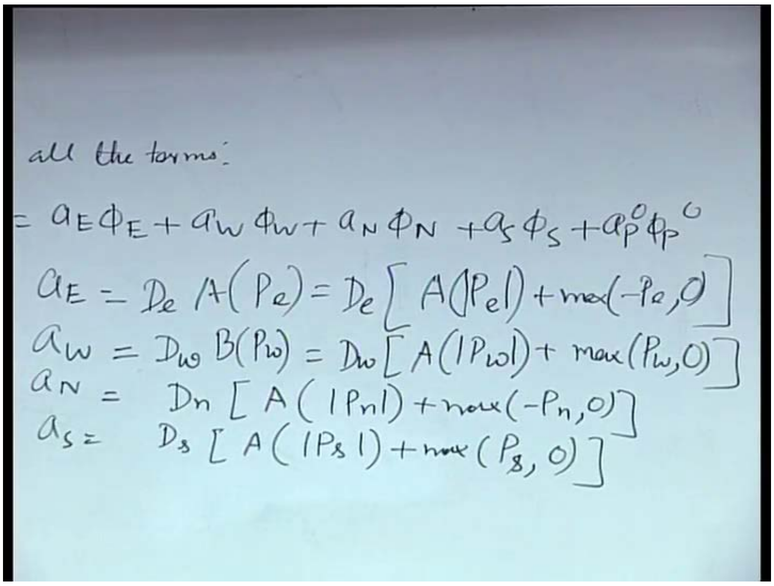

So, assemble all the terms you will get a p phi p is equal to a E phi e plus a w phi w plus a N phi N plus a s phi s plus may be a p 0 phi p 0 plus there is no source turn here. So, out of this how can you define what is a E for example, in this particular form where from it has come it has come from the multiplier with phi e what was that D e into A of mod p. So, this is D e into not mod p A of p e . So, this is D e A of p is A of mod p plus max minus p e 0.

Similarly, a w D w into B of p w that is D w into A of mod p w plus max p w 0 just check the formula for B that we derived in a previous lecture that will give the corresponding expression of B of p in terms of A of mod p similarly, you can write what is a N just let us write a n and a s quickly. So, a N is D N A of mod p n plus max minus p n 0, a s is equal to D s into A of mod p s plus max p s 0. Where p n is speckle number based on delta y n p s is speckle number based on delta y s.

So, we have seen a two-dimensional discretization and in the two-dimensional discretization we have generalized it in term of A of mod p where the expressions of A of mod p are same as that those which we have derived for the one-dimensional case. Now. So far whatever we have discussed it has given us a clear idea of the kind of policy or the kind of strategy that we can take to generalize the formulation of a convection diffusion problem once we have that generalization the next question is will the convection diffusion discretization what for all problems.

So, we have seen for example, that the central difference scheme has certain constrains in terms of it is applicability with regard to the sell speckle no and. So, on now we will go into the more involved issue concerning the applicability of these particular schemes or two of these particular schemes. So, to say.

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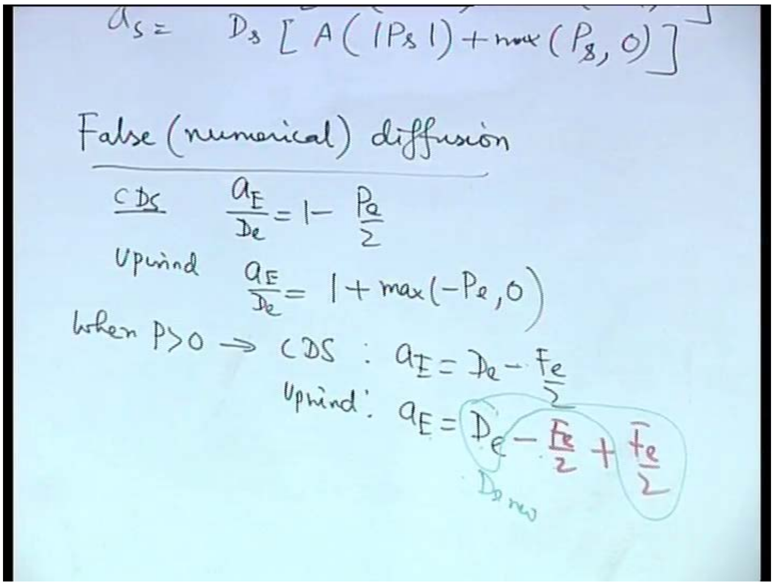

And that issue is known as false diffusion or numerical diffusion. By the name of false diffusion it is apparent that it is a diffusion which is not a physical one. So, it is at extra large diffusion which can be thought of originated as a numerical artifact, that is because of numerical errors or something false quantification of additional amount of diffusion is there where that diffusion is physically not there. So, that kind of situation if it arises then it is told or it is considered that that particular scheme has a problem with false diffusion.

Now, how do we address the issue of false diffusion or what is the correct view, what is the incorrect view there is a bit of a historical prospective about it because like when these schemes when these convection diffusion schemes were developed remember that the original view point of this false diffusion was not based on the entire sequence of development that was available to the community. So, the for the first time when people thought about it was for the first time when people faced a contradiction when the upwind scheme was thought of as a remedy to some of the problems which the central difference scheme was used to give us.

So, traditionally the finite difference community was happy with the central difference scheme. Now suddenly after some research people realize that well fine the central difference scheme had its own problems some of which can be could be taken care of by the upwind scheme and that sort of gave threat to the central differencing community.

So, when it gave a threat to the to the central differencing community the central differencing community tried to assess the upwind scheme on the basis of their own prejudice of the central difference scheme itself as if it is the standard benchmark and with respect to that standard benchmark they commented that the upwind scheme is having some false diffusion or artificial diffusion, how they on what basis they commented remember that in the central difference scheme a E by D e is one minus p e by two central difference scheme in the upwind scheme a E by D e is equal to one plus max minus p e 0. So, when p is greater than 0 central difference scheme gives a E is equal to D e minus F e by two and upwind scheme gives a E is equal to D e. So, this can be written as D e minus F e by two plus F e by two.

So, if you compare the central difference scheme with the upwind scheme it might appear as if this D e is augmented by a F e by two to have the same formula as that of the central difference.

So, augment D e with D e plus F e by two that this new D e d e new. So, it becomes D e new minus F e by 2, which is same as the formula of the central difference scheme. So, if you cast the upwind scheme and the central difference scheme in terms of the same formula which is not logical, but if you still try to do that you find that as if you have an enhance diffusion coefficient in the upwind scheme which is the original diffusion coefficient plus F e by 2 and this was originally told as the origin of a numerical artifact in terms of an additional diffusion of F e by 2.

We can clearly understand that this logic has a fallacy because this logic presumes that the central differencing scheme provides a benchmark formula in which you have to cast all the convection diffusion coefficients, but the central differencing scheme has its own problem to understand where lies the problem of false diffusion is it just the choice of the scheme or it is something much beyond the choice of the scheme. Let us try to consider a problem.

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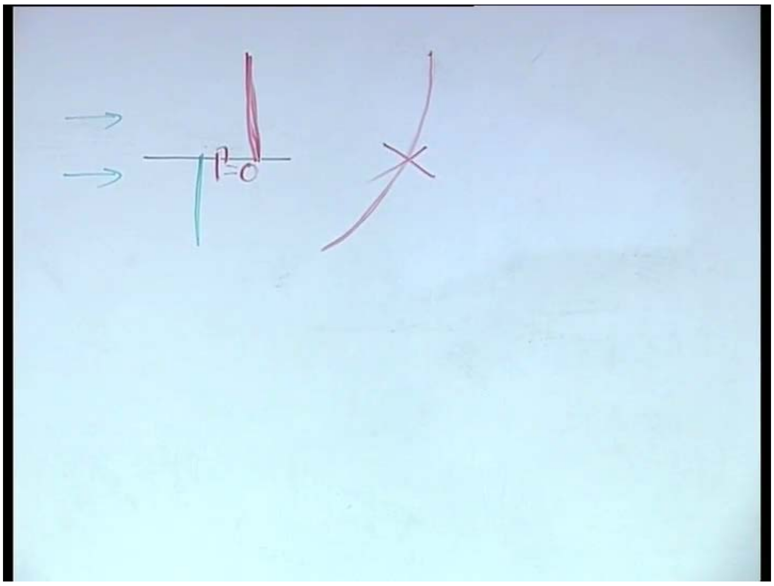

Let us say that you have two streams of fluid one with this temperature uniform temperature profile that is the upper fluid and another is another uniform temperature which is the lower fluid, and these fluids are flowing along positive x direction and let us say that the diffusion coefficient between these 2 fluids is 0. That is the they the effects cannot mix.

So, if they cannot mix what will happen that temperature profile is expected to remain this uniform for the top fluid and this uniform for the bottom fluid, if they were allowed to mix there would be something like it may be not exactly this, but an effect where you have that temperature of the lower fluid increasing a bit and the temperature of the upper fluid decreasing a bit and there. So, that because they are mixing with each other, but this is not the correct case when diffusion coefficient is equal to zero. So, when diffusion coefficient equal to zero, this is a predominantly one dimensional problem.

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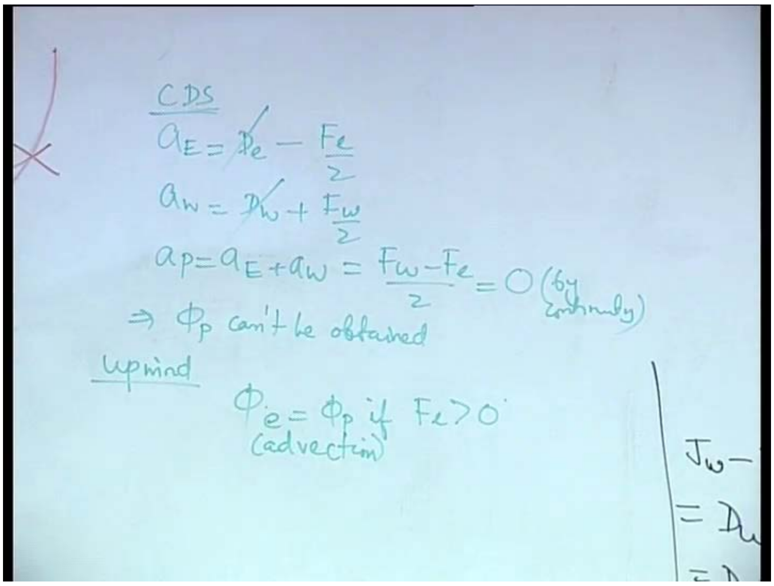

So, you have a E consider the central difference scheme a E is equal to D e minus F e by 2 a w is equal to D w plus F w by 2. So, when the diffusion coefficient is 0 these terms are not there. So, a p is equal to a E plus a w, that is F w minus F e by 2 and this is equal to 0 by continuity; that means, phi p cannot be obtained because to get phi p you have to divide the right hand side by a p. So, it is a division by 0 problems.

So, you are trying to assess the physical situation by considering a scheme as a standard which itself does not work at 0 diffusion strength, on the other hand if you consider a upwind scheme you have phi at small e is equal to phi p if F e is greater than 0. So, at all the upstream points you have the same value of phi the diffusion term will be 0, because the right hand side is the diffusion term which is 0.

So, it is purely on the basis of advection remember in the upwind scheme in the left hand side you have the advection term represented by upwind and in the right hand side diffusion term represented by the central difference scheme. So, here because the diffusion coefficient is 0 right hand side is there no more. So, only the advection term is the dominating term is the influencing term only that term. So, phi e is equal to phi p if F e is greater than 0 that means, all the subsequent stations will have the same temperature along x. So, this profile will not be disturbed.

So, whatever is the change this type of change is not possible because this profile will remain intact and the solution will be there. So, in the limit as diffusion strength tends to

0 the upwind scheme does not the central difference scheme does not work, but the upwind scheme gives a corresponding physically consistent solution still there might be a problem with false diffusion, but that problem can be assessed by aligning the flow in a different orientation let us try to do that.

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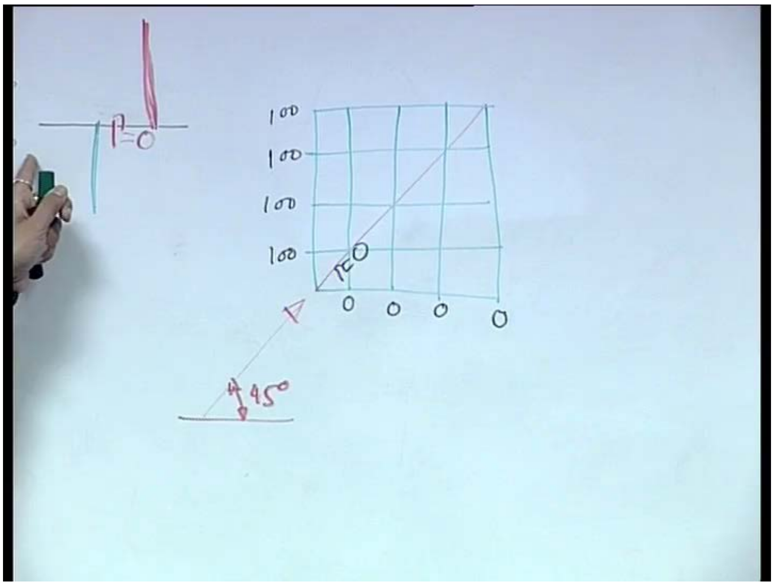

Now, let us say, that we are considering the same problem, but the flow is now incline at an angle 45 degree with the x access. So, it is a incline flow like this instead of flow along x access it is 45 degree with respect to the x access. And let us consider a problem domain like this, let us say that on one side of this flow orient flow direction you have the temperatures as 0 degree centigrade 0 0 0 and on other side it is 100. So, these are the boundary conditions, on one side on the side below it is 0 on other side the side above it if you just consider this as below and this as above on other side it is 100. So, let us try to calculate the values of temperature at the other grid points assuming that the diffusion coefficient is 0. So, the same problem, what we have done we have now oriented the flow in a manner incline to the grid orientation that is the only change that we have made.

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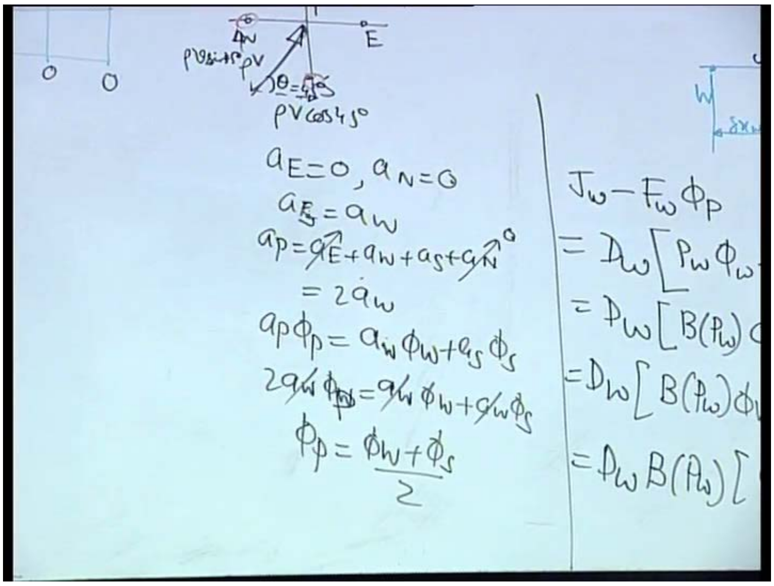

Now, let us consider the grid layout this is the point p e w n s the flow is coming in this way. So, what will be the corresponding coefficients which if you use the upwind scheme out of these four w e n s which two will be effective. W and s right because those represent the upstream directions if you reserve this flow into components let us say that this is rho v this angle is 45 degree. So, this is rho theta equal to 45 degree. So, this is rho Cos 45 degree this is rho v sine 45 degree. So, with respect to this flow this is the upstream grid point with respect to this flow this is the upstream grid point.

So, you have a E equal to 0 a n equal to 0, because Cos 45 degree and sine 45 degree are the same you have a s equal to a w, remember we are using the upwind scheme instead of using the formula we are directly using the concept of upwind scheme to do it quickly, then a p is equal to a E plus a w plus a s plus a n considered as steady state problem. So, a E a and a N are 0. So, this is 2 a w and your governing equation discretized equation is a p phi p is equal to a w phi w plus a s phi s others are other terms are 0. So, 2 a w phi p is equal to a w phi w plus a w phi s all these are all a w. So, phi p is equal to phi w plus phi s by 2. So, let us see what is the implication? Implication is very interesting.

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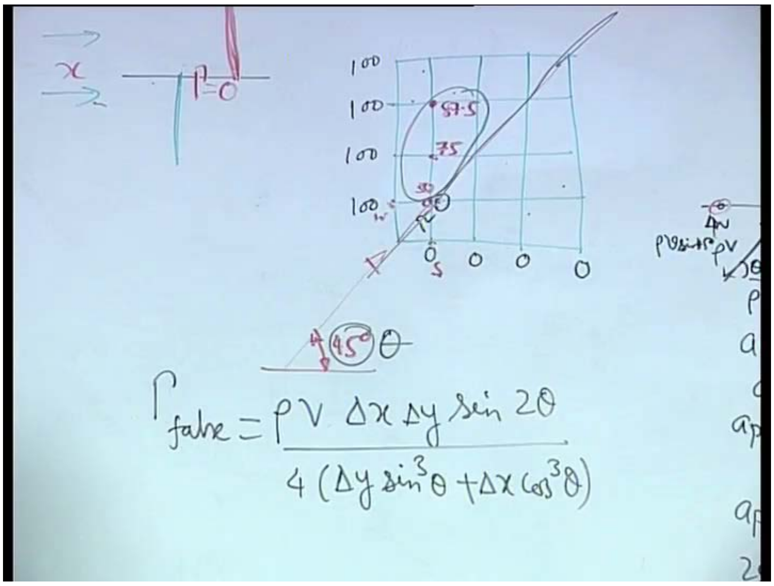

So, this is like w this is like s. So, this point will be 100 plus 0 by 2. So, this is 50 this is 50 this is 100. So, this will be 75, 100 plus 50 by 2 then, this is 100 plus 75 100 75 by 2 what it is 87.5. So, you can see that what you expected you expected that on one side of the diagonal temperature will remain as 100 on other side it will remain as 0, because there is no diffusion across it, but that is violated now you are having a false diffusion because of which there is a gradient in temperature in this side.

The same problem could be avoided if your x access was oriented along this just like this case, actually it is a camouflage it is a same problem only the access is misoriented physical problem is the same that is you have 1 line on 1 side there is a temperature on another side there is another temperature and there is 0 diffusion across that, here we have just inclined the problem nothing else.

So, what you can see here is that now you have a false diffusion. So, what we can infill out of this that there is a false diffusion which can be attributed to what which can be attributed not to the particular scheme as such, but the misorientation of the grid lines with the flow direction. So, this angle theta is the contributor to the false diffusion. So, that is the correct view point of the false diffusion it is not.

So, much on the scheme of course,, the scheme has some role to play and one can try to improve upon that, but more importantly it is the orientation of the dominant flow direction with the grid lines, if that is misoriented that can give rise to these problems and. In fact, one can calculate a false diffusion coefficient we will not go into the details of that, but just we will just give you an expression.

So, it can be shown, that you can have a corresponding expression for the false diffusion our objective here is not to prove it, but to see that what we can get from this expression in this particular expression. So, this is an expression for a false diffusion coefficient gamma is a diffusion coefficient. So, this is not a correct diffusion coefficient, but a numerical artifact just like this and we can see that it is a function of this angle theta. So, it is maximum when sine 2 theta is 1 that is theta is equal to 45 degree. So, when the flow is oriented in a bad manner that is it is misaligned with x misaligned with y and maximum misaligned with the combination.

So, intuitively that is theta equal to 45 degree where the misalignment with both of these is a sort of equal and you can of course,, minimize the false diffusion coefficient by reducing the grid spacing delta x delta y these types of things. So, this formula gives us a clue it is not important for us to remember the formula, what is important for us is to understand that the false diffusion is governed by this angle theta which is very important. So, if you make this angle theta equal to 0 the false diffusion coefficient is gone that is when the flow is oriented along the gridlines.

Now, what can you do to minimize the false diffusion effect considering that the flow orientation is something which is not in your hand of course, if you know the predominant flow direction you can orient your grid choice accordingly, but in a complex problem you do not have a single predominant flow direction and it is very difficult therefore, to orient the grid lines in a in a in a particular way which will minimize the false diffusion.

So, what is the way out, the way out may be to have some other types of differencing schemes which are a bit more I would say bit less prone to false diffusion than the upwind scheme itself. So, you can tackle it by considering the improvement of the scheme or the grid layout in a way that it is oriented in a manner which is oriented in the direction of the flow. Now, predominant direction of the flow is very difficult to get in complex problems.

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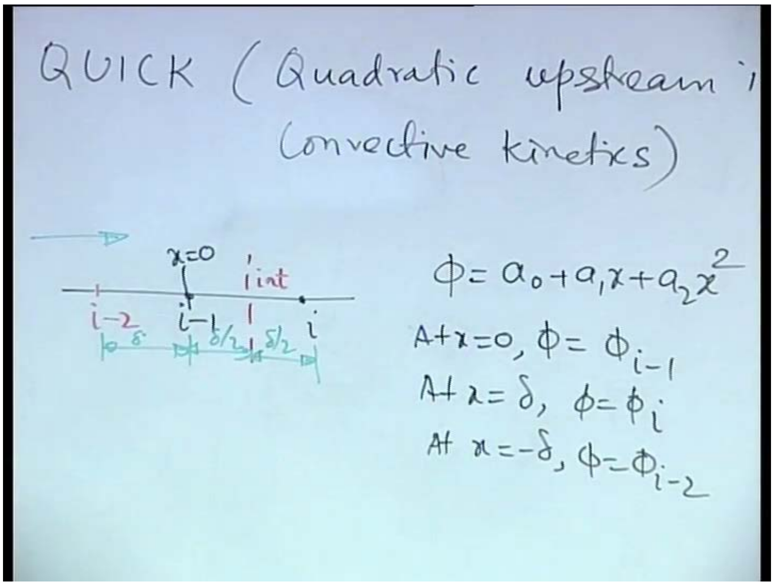

So, we try to go for an improved scheme and that one such scheme we will give an example, that is called as quick scheme. So, its full form is quadratic upstream interpolation scheme for convective kinetics that is the full form of the quick scheme. So, what it tries to d if you j have a grid point i minus 1 and a grid point i and this is the interface where you are interested to calculate the flux then what it takes is if this is the flow direction it considers a quadratic interpolation that is a quadratic profile assumption instead of a linear profile assumption a quadratic profile assumption. So, a linear profile assumption required how many points 2 grid points quadratic will require 3 grid points.

So, another grid point i minus 2 located upstream. So, at the interface 2 grid points at the upstream end and 1 grid point at the downstream end. So, that the scheme is capable of considering not just the upstream grid point effect, but also the downstream grid point effect. So, it can be of thought of as a sort of improvisation of the up winding scheme or a higher order up winding schemes. So, to say.

Now, let us say that this distance is delta by 2 this is delta by 2 and this is delta let us fix up origin of the coordinate system somewhere let us say this is x equal to 0 and let us say that we consider phi as a 0 plus a 1 x plus a 2 x square this is a quadratic profile. So, our objective will be to find out a 0 a 1 a 2 in terms of phi i minus 2 phi i minus 1 and phi i. So, you have at x equal to 0 phi equal to phi i minus 1 at x equal to delta phi equal to phi i and at x equal to minus delta phi equal to phi i minus 2.

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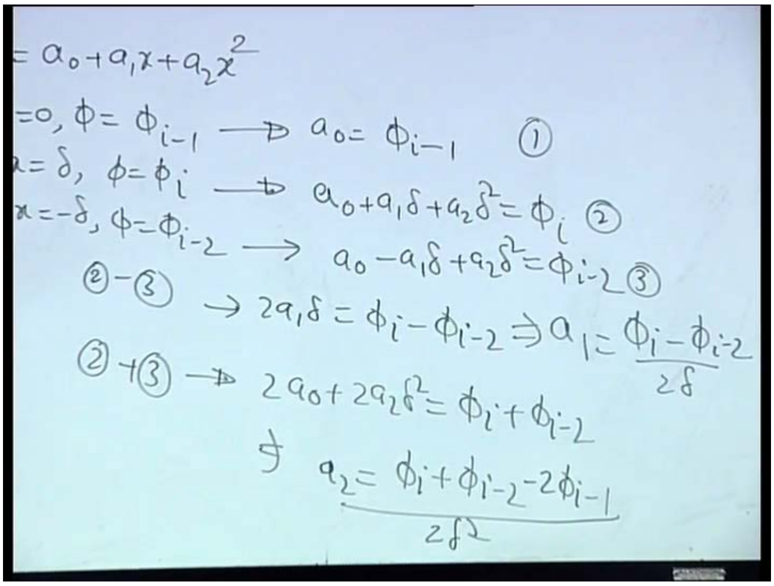

So, from here we can write a 0 is equal to phi i minus 1 then from here we can write a 0 plus a 1 delta plus a 2 delta square is equal to phi i from here we can write a 0 minus a 1 delta plus a 2 delta square is equal to phi i minus 2. Let us say, this is 1 this is 2 this is 3 now you can subtract. So, 2 minus 3 then you will have 2 a 1 delta is equal to phi i minus phi i minus 2. So, a 1 is phi i minus phi i minus 2 by 2 delta and you can add 2 and 3 2 a 0 plus 2 a 2 delta square is equal to phi i plus phi i minus 2. So, a 2 will be phi i plus phi i minus 2 minus 2 a 0 means minus 2 phi i minus 1 by 2 delta square. So, what you require you require phi at the interface that is after the interpolation you require.

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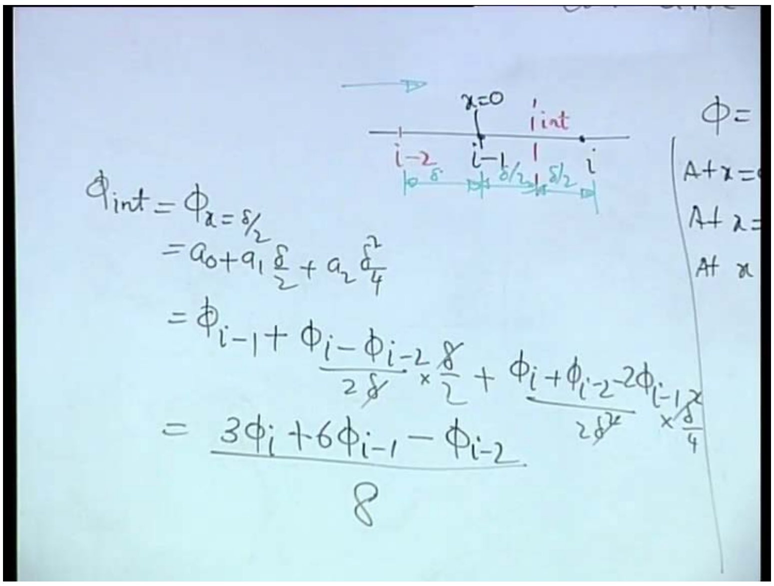

So, what is phi at the interface that is phi at x equal to delta y 2. So, that is a 0 plus a 1 delta by 2 plus a 2 delta square by four. So, that is phi i minus 1 plus a 1 delta by 2. So, plus phi i minus phi i minus 2 by 2 delta into delta by 2 plus phi i plus phi i minus 2 minus 2 phi i minus 1 by 2 delta square into delta square by four. So, this delta square and delta will cancel. So, it will be 8 in the denominator how many phi i are there you have here you have if you take 8 then this is four into 2. So, 2 phi i then plus 1 phi i 3 phi i then phi i minus 1 here you have 8 minus 2. So, six plus six phi i minus 1 and phi i minus 2 here you have minus 2 and then you have plus 1. So, minus 1. You can see that ultimately it is a waited combination of i i minus 1 and i minus 2 sum total of the weight 3 plus 6 minus 1 is equal to 8.

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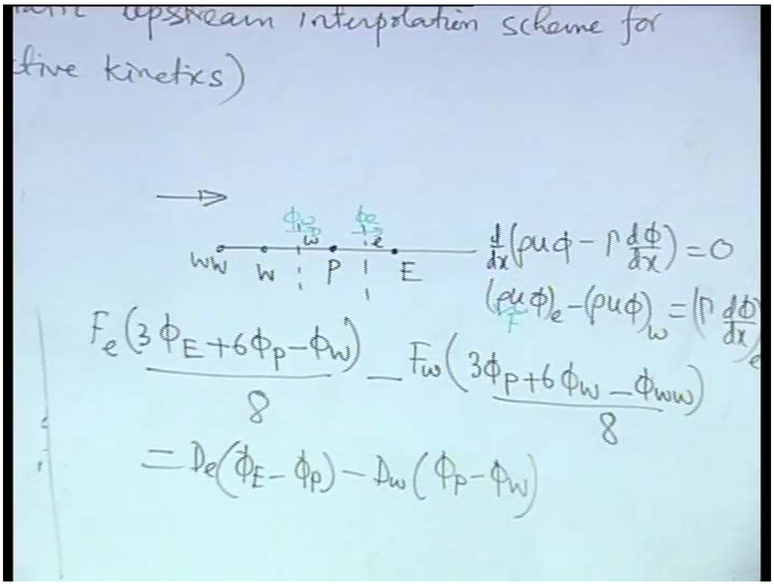

So, based on this consideration let us try to write a discretization. So, p e w let us consider a one dimensional problem and let us say that this is the flow direction. So, if this is the flow direction now let us writes the corresponding discretized equation. So, you have rho u phi dx of rho u phi minus gamma d phi dx equal to 0. So, if you integrate it with respect to x rho u phi at e minus rho u phi at w is equal to gamma d phi dx at e minus gamma d phi dx at w.

So, you require phi at small e remember rho into u equal to F. So, the first term is F e into phi at small e. So, with respect to small e i minus 1 is p i is e and i minus 2 is w. So, 3 phi E plus 6 phi p minus phi w by 8, minus now you require phi small w. So, you require another upstream point. So, that conventionally is given a name w w. So, it is another upstream point just equidistant. So, then you have F small w into now 3 phi p plus 6 phi w minus phi w w by 8.

So, this is the advection term profile the diffusion term profile you can still take the piecewise linear profile because the whole problem was associated with the representation of advection term. So, diffusion term you can write D e into phi e minus phi p minus D w into phi p minus phi w. Where D e is gamma e by delta x e and D w is gamma w by delta x w. So, remember one very important assumption is that quadratic profile for the advection term and piecewise linear profile for the diffusion term. So, not the same profile for the advection and the diffusion term.

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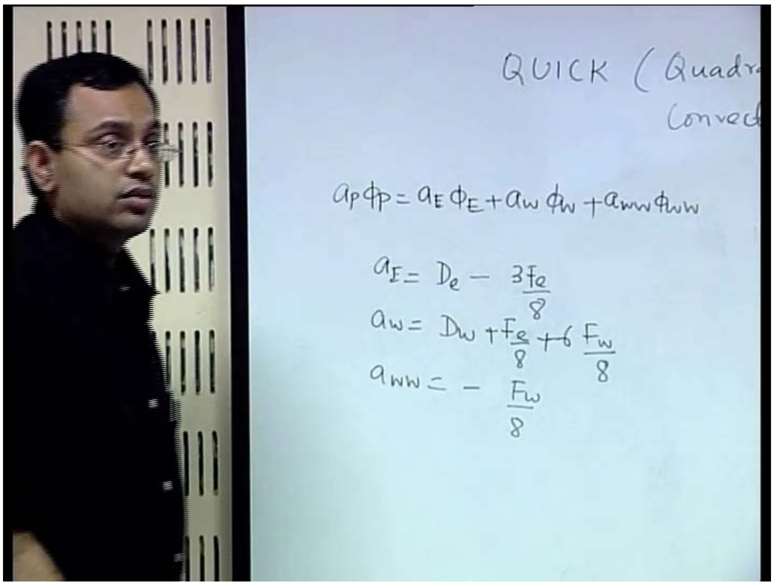

So, if you now assemble these terms you will get an equation of the form a p phi p is equal to a E phi E plus a w phi w plus a w w phi w w there is no B here. So, what is a E d e. So, if you consider the right hand side here it is a D e minus 3 F e by 8 what is d a w D w plus F e by 8 then plus six F w by 8 a w w is equal to minus 8 F w by 8 and. So, on.

So, you can clearly see immediately that this scheme has a problem that all coefficients will not always be of the same sign. So, if you have D w F e and F w all positive which we have considered in this problem then only a w is guaranteed to be positive neither a E nor a w w is guaranteed to be positive it depends on the relative advection and diffusion strength relative F e and D e and a w w is always negative only F w by 8 that is fine. So, we can see that this particular scheme try to rectify a problem, but has created a different problem.

So, it is like having a medicine where the medicine is trying to take care of a disease, but having another side effect. So, the diseases of false diffusion it tries to take care of false diffusion, but in the way it incur the possibility of having all coefficients not of the same sign and that could give rise to physical inconsistent solutions.

So, we can summarize that it is not a trivial to choose a particular scheme perhaps choosing a simple scheme is better and once one chosen a simple scheme it is important to take care of the fact, that you satisfy the basic rules which are corresponding to a correct action of the discretized equation.

So, we stop with the convection diffusion equations here and from the next class we will start discussing on how to solve the fluid flow problems of the Navier-stoke equations because till now we have solved the convection diffusion equation by assuming the flow field is known, but where from the flow field is known it has to be solved from the fluid flow equations that is the couple continuity and the momentum equation, that we will take up in the next lecture. Thank you.