Computational Fluid Dynamics

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Lecture No. # 30
Discretization of Convection-Diffusion Equation: A Finite Volume Approach

So far, we have discussed about diffusion type of problems; that is problems where fluid flow effect is not important. Next, we will move one step forward and discuss about certain types of problems, which are called as convection diffusion problems. These are problems where fluid flow is important; now a big issue is there that, if fluid flow is important, where from do you solve the flow field, that is, if the flow field is not given to you, where from do you obtained so that obviously is the is the representative of a special class of problem, where, you need to solve the fluid flow equations, which for our case, will be the Navier-Stokes equation and the continuity equation.

Now, for this particular discussion, we will assume that somehow from some source, we know what is the flow field; and based on that, we will be solving other scalar fields in a convection diffusion problem, so that will be the agenda for today's discussions. Now, when we say that we are interested about a convection diffusion problem, what we essentially mean.

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So let us say, let us recall a physical situation, let us say that you have a flat plate like this, and you have a free stream of fluid coming with a velocity u infinity and temperature T infinity; let us say that the wall of the plate is heated to a temperature, which is greater than T infinity. Now when the fluid comes in contact with the plate, what will be the physical mechanism of heat transfer here? So, first you have to cross a barrier, the heat has to cross a barrier, over which there is no fluid flow, that means the first layer of fluid, which is in contact with the solid boundary, this layer is stationary, by virtue of the no-slip boundary condition.

Now if the heat has to go from the wall to the outer stream, it has to cross this, and because this layer of fluid is not mobile, the only way heat can get transferred across this in by conduction. So, there is a mechanism of conduction, by virtue of which, you have the transport of heat from the wall to the mobile layers of fluids; and then when the heat reaches the mobile layers of fluids, there are two mechanisms by which it is transferred; one is still by conduction, because the fluid - the bulk fluid is also conducting, but also by virtue of fluid flow; so heat gets transported from one place to another place in the bulk fluid with the fluid flow itself; and that is called as advection.

So in the first layer conduction without advection in the outer layers, conduction plus advection. So in totality, the mode of heat transfer here is by virtue of conduction and advection together; and this is known as convection. When we talk about a problem of heat transfer, we call as conduction, which is a transport, which is driven by the negative of the gradient of temperature. Similarly if you are talking about mass transfer, you are talking about the transport of a variable, say concentration; a transport of a variable, which is a function of a gradient of a scalar variable, which is concentration; negative of the gradient of a scalar variable, which is concentration so transport of heat by conduction has an analogy in a mathematical sense, with the transport of mass by diffusion, because transport of mass by diffusion, the rate of mass transfer is proportional to the negative of the concentration gradient that is by fix law of diffusion.

So in general, this type of transport we call as diffusion, where the transport is a function or is directly proportional or the flux rather is directly proportional to the negative of the gradient of the scalar variable, which is driving the flux; so that is called as diffusion. So when we say a convection diffusion problem, it means that there is diffusion, and there is advection, and the problem may be transport of momentum, transport of heat, transport of mass like that. Now when we say transport of mass, we have to keep one thing in mind; continuity equation also talks about transport of mass; so what other aspect of transport of mass we are considering, when we talk about a convection diffusion problem.

So in a convection diffusion problem, we are talking about a transport of mass, say in a multi component system. So if you have two components A and B, the transport of A in the mixture A plus B or transport of B in the mixture A plus B, those are governed by the change of concentration of A in the mixture and concentration of B in the mixture; and for that, one has to solve for species transport equations or species conservation equations, which conserved individually A and B. So the total mass is conserved by the continuity equation, but the individual constituents, they are also conserved in their mass, so mass of the individual components in the absence of any any generation of any new species, the individual mass of… The mass of the individual components will be conserved; in in case of generation of any species, that also can be taken into account through the same formulation with the help of a reaction or a source term. So it is possible to accommodate the variation of the mass, fraction or volume fraction or mole fraction, whatever is the unit in it, in which you express concentration of individual species in a mixture, and that is the role of of a species conservation equation.

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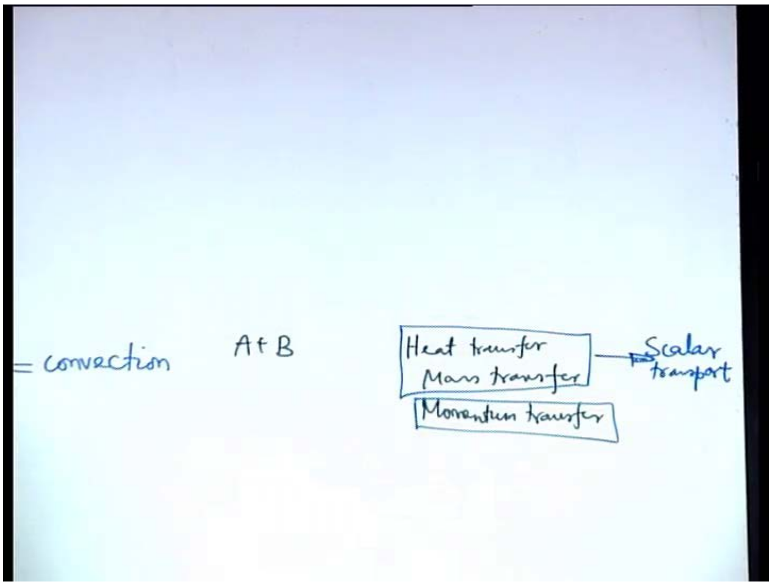

So we have we have come across examples of heat transfer and mass transfer, where the governing equations are of convection diffusion type. Momentum transfer also is of convection diffusion type; momentum transfer equations are basically the navier-stokes equation, but we will not put that in the same framework as the convection diffusion equations, that we are discussing currently. Why? The momentum equations have certain additional complexities; in the momentum transfer equation, in the source term, you have a special independent variable called as pressure; you have negative of the pressure gradient as the source term; whereas you do not have an explicit governing equation for pressure, so that kind of situation is not there for the heat and mass transfer problems that is number one.

Number two is the heat transfer and the mass transfer equations in in in the in the language of partial differential equation, they are linear partial differential equations; whereas, when you consider momentum transfer they are non-linear partial differential equations, so if you say in more simple terms in the heat and mass transfer equation, why they are linear, because you are they are linear in in terms of the variable that you are solving; so if you are solving a heat transfer problem, it is linear in terms of temperature, because the corresponding other variable velocity, it is a different variable which you can prescribe independently.

In the momentum equation, you have product of u with u, u with v, so all these terms make the momentum equation non-linear; we have earlier discussed about this issue. So when you have the momentum transfer equation as a non-linear equation, it cannot exactly be solved in the same framework as that of the linear equations, until and unless you employ special iteration techniques, to convert or to absorb the nonlinearity. So you require special iterative techniques to absorb the nonlinearity - number one; and to accommodate for the fact that you have a pressure gradient as a source term, where you do not have an explicit governing equation for pressure, so you have to make a formulation for that; so momentum transfer equations are to be discussed in a separate perspective than the heat transfer, mass transfer or a general scalar transport equation. In this particular chapter, we will discuss about the heat transfer, mass transfer or in general, any scalar transport equation, where advection and diffusion affects are important; and these equations, we will broadly term as the convection diffusion equations.

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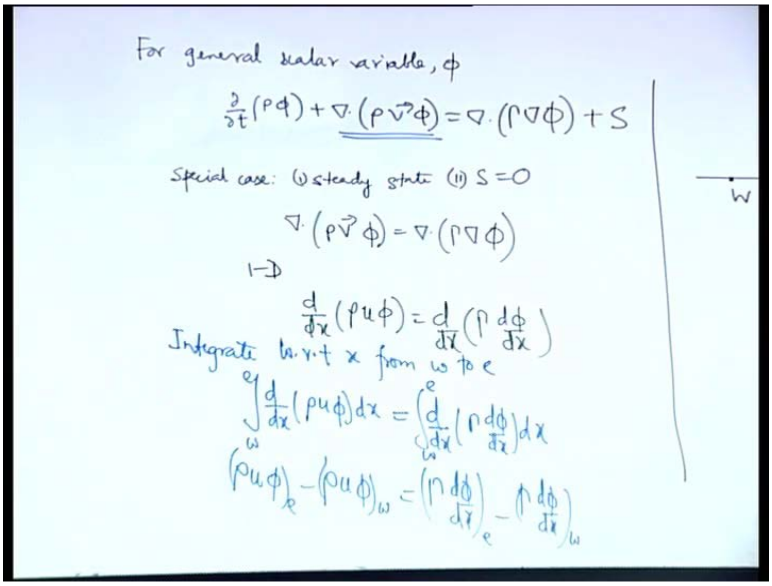

So first of all, we will try to see that what is the prototype equation that we are looking for; so for the general scalar variable phi… you have Now that you have the fluid flow effect, so this term which was not there in the diffusion type of problem; now this term will be important; so all these terms potentially can be important, but we will first consider the special case with steady state and source term equal to 0. So the equation boils down to the treatment of unsteadiness and the treatment of the source term, we have already seen how to do that in a diffusion type of problem, and that strategy does not change with a convection diffusion problem; so in a convection diffusion problem, the strategy changes, because of the inclusion of the advection term, and that is why we consider this very simple prototype, to see that what what are the discretization strategy.

So the next simplification, we can make by considering it as a one-dimensional problem, the whole idea is that in general, we can develop significant insights, physical insights on the problem by looking into the one-dimensional variation; and we can use that insight for solving multi dimensional problems or two-dimensional problems or three-dimensional problems. So if you consider a one-dimensional problem, this will become d d x of rho u phi is equal to d d x of gamma d phi d x. Now when you are having this particular equation, which you are interested to solve; the next question comes that what would be the method that you are interested with.

So we have already seen that the finite volume method has a lot of flexibility, in terms of solving the transport phenomena equations - numerical solution of the transport phenomena equations; wherever the fluid flow appears, it becomes more and more useful, and so from this stage onwards towards the end of this particular course, we will be more emphasizing on the use of finite volume methods for solving the concerned problems; and we will be illustrating this particular solution of this particular equation strategy to the use of the finite volume method. Now if you are interested to use the finite volume method here, you need to have a grid layout.

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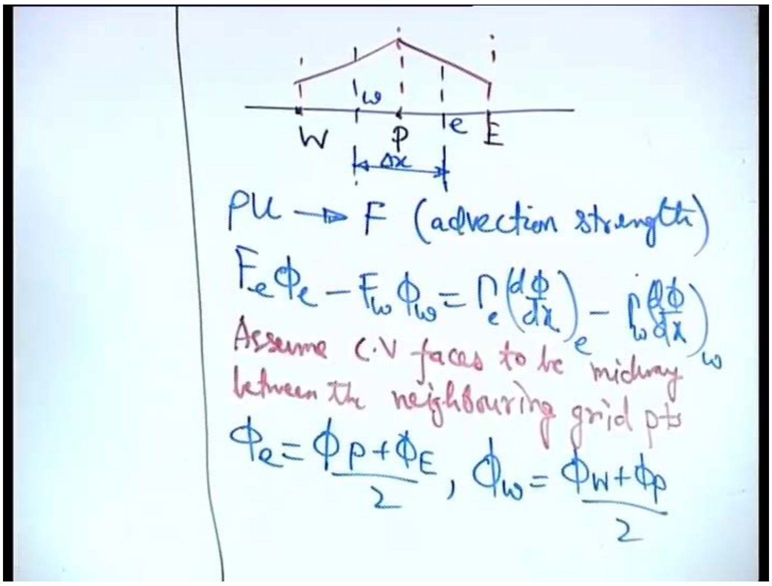

So let us consider a grid layout like this; and the size of the control volume has delta x. So what will be the first step for solving this equation in a finite volume environment, you have to integrate the governing differential equation over the control volume that spans from small w to small e; so integrate with respect to x from small w to small e; if you do that, let us write the corresponding formula form small w to small e, and this one also form small w to small e. So this becomes rho u phi e minus rho u phi w is equal to gamma d phi d x e minus gamma d phi d x w.

It is interesting to note the variation of rho u, remember that when you have a fluid flow, you must have a corresponding velocity field satisfying the continuity equation. So here in case of this one-dimensional problem with steady state, the continuity equation is d d x of rho u equal to 0; so if you integrate with respect to x form small w to small e, what you will get is rho u e minus rho u w equal to 0. Now what does it represents; what does rho into u represent; rho into u into area, what does it represent; it represents the mass flow rate; so rho into u represents mass flux that is rate of mass flow per unit area normal to the direction. So what it essentially says is physically as follows that whatever is the rate of mass flow out is same as the rate of mass flow in, so the rate of mass flux out is same as the rate of mass flux in, the areas are the same.

Now, because rho into u represents a mass flux; it also is an indicator of the strength of advection. So if you are considering the advection flux of the variable phi, if you are considering the advection flux of the variable phi, then rho into u is the mass flux that times phi is a rate of transport of the phi with the fluid flow. So the advection flux is proportional to rho into u and therefore, the this strength of this term rho into u is an indicator of the strength of advection in a convection diffusion transport. So this we call as F in a symbolic form, which we call as advection strength higher the value of rho into u stronger is the advection or the transport of the variable by virtue of fluid flow.

Now, so the left hand side is F e phi e minus F w phi w, these are small e and small w, is equal to gamma d phi d x e minus gamma d phi d x w. Now what would be the next step? You have to express these quantities in terms of algebraic values of the variable phi at the main grid points capital W, capital P, capital E like that. So to do that, you require a profile assumption; so the most common profile assumption that we can take here is a piecewise constant, but if you take a piecewise constant profile assumption, then you cannot calculate d phi d x that becomes 0. So piecewise linear profile assumption something like that.

Next for example, we consider that the control value faces are midway between the grid point so that we can write in simple algebraic expressions; so assume control volume faces to be midway between the neighboring grid points; if you do that that essentially means that small w is exactly midway between capital W and capital P, small e is exactly midway between capital P capital E like that. So then if it is a linear profile then phi small e is equal to phi capital P plus phi capita E by 2; if it is a linear profile and if it is a midway, it is just the half of the sum of that two neighboring values; similarly, phi small w is equal to phi capital W plus phi capital P by 2; the discretization of the right hand side, we have already seen through the diffusion type of problems, the same applies here as well and together with the left hand side and right hand side, we can write the final discretized equation; so what we can write?

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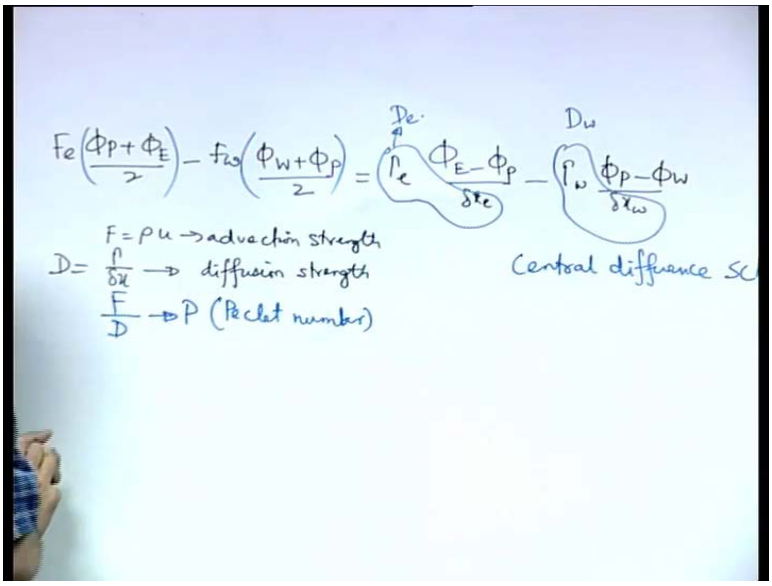

We can write F e into phi P plus phi E by 2 minus F w into phi W plus phi P by 2 is equal to gamma e, then d phi d x at E is equal to phi E minus phi P by delta x e, where delta x e is this dimension similarly, this dimension is delta x w. So minus gamma w into phi P minus phi W by delta x w. Just we have as we have seen that F, which is rho into e is advection strength gamma by delta x, which we call as D in terms of the symbol is a diffusion strength.

Let us take some examples, let us consider a… Let us divert a little bit and take from examples of heat transfer and momentum transfer and mass transfer to see that what do we mean by these advection strengths and diffusion strengths?

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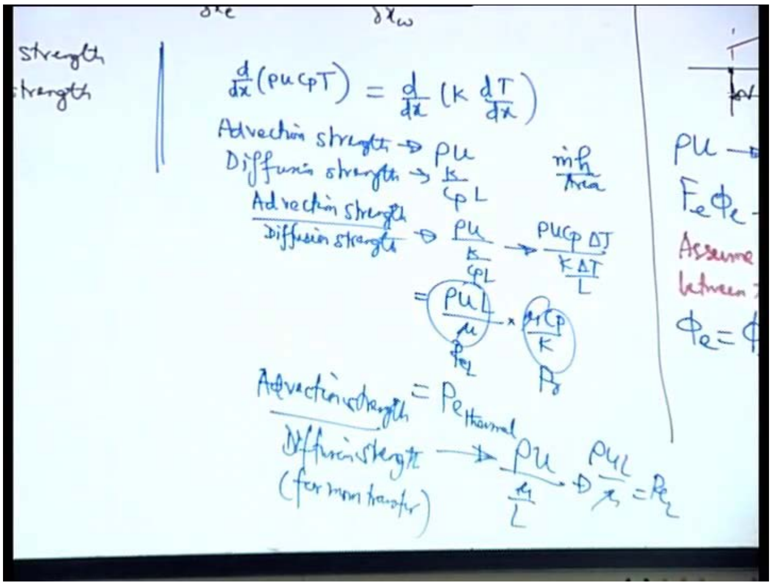

So let us say that we are interested about a heat transfer problem; so d d x of rho u C p T, so what is the advection strength - rho into u; what is the diffusion strength - here gamma is k by C p; so k by C p divided by some say, let us consider some length L, where L is the characteristic length here delta x is the characteristic length in a numerical solution which is may be the grid size; so here L is a characteristic length governing the physical variation within the problem. So for example, for a flow through a channel it can be the hydraulic diameter something like that. So advection strength by diffusion strength.

You can just write it in a different way so that it actually looks like advection strength by diffusion strength in the physical way, we understand a heat transfer problem. So you can write rho u C p into some delta T divided by k into delta T by L. So what is the denominator? The denominator is the conduction flux k delta T by L, where delta T is a characteristic temperature difference; conduction is the mechanism of heat diffusion, so this is the conduction flux, and the numerator is the advection flux of the thermal energy. So C p into the delta T is like what, is the enthalpy, is the specific enthalpy; so it is like the mass flow rate into the specific enthalpy per unit area. So the m dot into h by area; m dot is rho into u into area that into specific enthalpy is C p into the characteristic temperature difference. So it represents the rate of advection of thermal energy or the rate of transport of thermal energy by virtue of fluid flow, and it represents the rate of diffusion of that.

So indeed rho into u by gamma by delta x represents the advection strength by diffusion strength that we can verify through this example. So if you now write it in this way, you can write it as rho u L by mu, where mu is the viscosity, and that multiplied by mu C p divided by k; so we know that this is the Reynolds number and this is the Prandtl number. So this product is called as thermal Peclet number.

In heat transfer you have studied about Peclet number, but that is not the generalized description of Peclet number, that is the thermal Peclet number. You can have similar Peclet number for momentum transfer, for mass transfer and so on; so in general, we will call advection strength by diffusion strength as Peclet number. If it is in the context of a heat transfer problem, it is thermal Peclet number; if it is in the context of a mass transfer problem, it is a corresponding mass transfer Peclet number; if it is a momentum transfer context, then let us see what it is, advection strength by diffusion strength for momentum transfer.

So advection strength for… The momentum equation advection strength is always given by rho into u; what is the diffusion strength; what is the corresponding gamma or the diffusion coefficient for the momentum equation; that is the viscosity mu. So gamma by length, so mu by L, so this is nothing but the reynolds number; so the reynolds number is also a Peclet number. The Peclet number with which you are more familiar is because of your familiarity with the heat transfer problem that is the thermal Peclet number, which is reynolds number into Prandtl number; but Peclet number does not mean reynolds number into Prandtl number that is just a definition of thermal Peclet number.

So in general, Peclet number may be reynolds number, reynolds number into prandtl number, reynolds number into Schmidt number for mass transfer whatever it is; the important understanding is it is the ratio of the advection strength and diffusion strength. And why this number holds the critical or plays the critical role in a convection diffusion problem? It plays the critical role in a convection diffusion problem, because in a convection diffusion problem what is important is, what is the relative strength of advection and diffusion. If advection strength in a limiting case becomes negligible as compare to the diffusion strength, it becomes as good as a diffusion type of problem.

On the other hand, there may be such a situation where the flow speed is such that advection far, far over weighs the diffusion strength; and then that is another limiting condition. The real situation may be somewhere in between these two; so we are interested about the relative strength of the advection diffusion F by D, which we call as P, which is the Peclet number in general.

So in place of gamma e by delta x e we will write it as D e, in place of gamma w by delta x w, we will write it as D w. This particular scheme considers a piecewise linear profile between the grid points and the grid points are centered around the neighboring grid points, and this is the central difference scheme; so if you use a central differencing approach using the Taylor series expansion in the finite difference method, you will arrive at the same equation.

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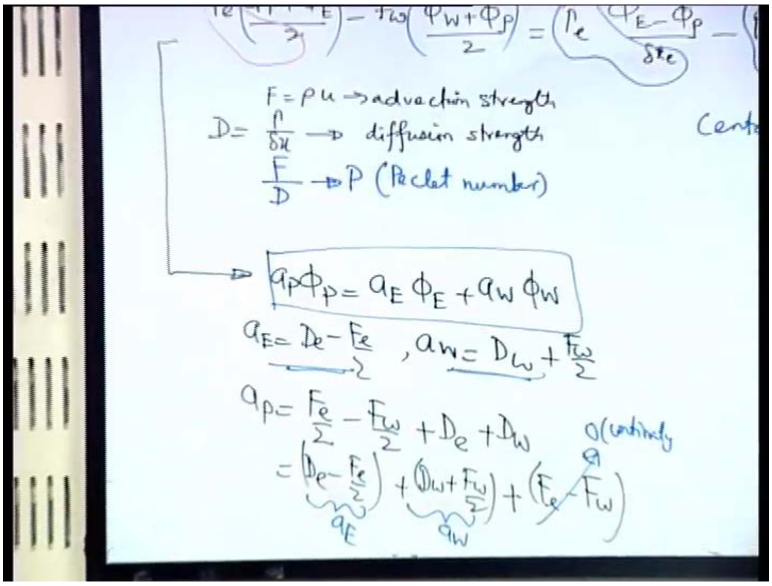

Now let us arrange this equation in the form a P phi P is equal to a E phi E plus a W phi W plus b there is no b here, because we have not considered any source. (37:14 to 37:26) So what is a E - a E is D e minus F e by 2; you can easily find it out the coefficient of phi E here it is D e, and in the left hand side it is F e by 2, so if you take both in the right hand side, it is D e minus F e by 2; then what is a W, D w; so here it is minus and minus make it plus d w plus F w by 2; and what is a P; so what you can see here, a P will be… In this side you have F e by 2 minus F w by 2 plus D e plus D w.

Now this you can write as D e minus F e by 2 plus D w plus F w by 2 plus F e minus F w. Why you write it in this way, because you are interested to write a P as a function of a E and a W, this is a E and this is a W when you add these two, to make an adjustment to come back to the same equation, you have to add F e and subtract F w. So this is a E, this is a W and by continuity equation this is equal to 0, because continuity equation says that F e equal to F w.

So in one-dimensional problem, the central difference scheme boils down to this final expression, where you have a E and a W given as these ones; and a P is equal to a E plus a W. Now let us try to make an assessment of this scheme, so the next agenda is assessment of the central difference scheme.

We have to keep in mind that while making the assessment, eventually we have to relate the assessment with the Peclet number, because you can see that it is the relative strength of the diffusion and advection that will play a key role towards the values of the difference coefficients, that is relative strength of D e with respect to F e, relative strength of D w with respect to F w like that.

The other important issue to note is that this Peclet number is not the any global Peclet number, this is the cell based Peclet number, so the length scale for this Peclet number is some delta x, where the delta x may be delta x e delta x w like that, so these are this is called as cell Peclet number, so Peclet number for each computational cell or it is Peclet number with reference to the computational cells; it is not a global problem geometry based Peclet number.

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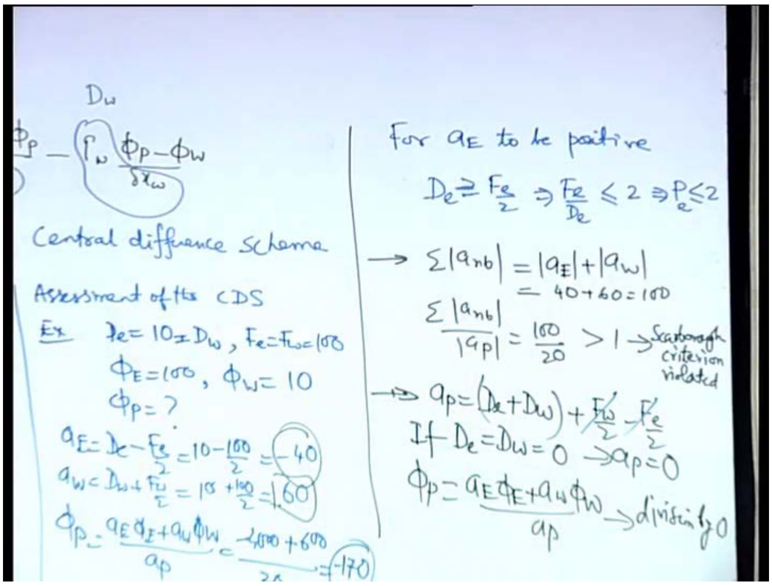

Now assessment of the central difference scheme, so let us first start with an example numerical example; let us consider that D e equal to 10 is equal to D w and F e equal to F w equal to 100, phi E equal to 100; and let us say phi W equal to10. So we have to find out what is phi p; very simple problem. So let us calculate the coefficients a E is equal to D e minus F e by 2, so 10 minus 100 by 2 minus 40, a W is equal to D w plus F w by 2 10 plus 100 by 2 is equal to 60. so what is phi P - is a E phi E plus a W phi W by a P. So what is a E phi E minus 40 into 100, so minus 4000 plus a W phi W plus 600 divided by a P is a E plus a W that is 20. So what does it become? Minus minus 1 minus 170, so let us make an assessment of this for problem, we had phi E equal to 100, phi w equal to ten we are interested to calculate what is phi P, in the absence of any source or sink you expect phi P to be between 10 and 100; no matter how complicated the solution is the solution in its physically realistic sense should give something between these limiting values, but here you see minus 170, which is out of bounce.

What is the origin of this problem? The origin of this problem is the negative sign of this coefficient, remember that one of our basic rules was that all coefficients must be of the same sign, but here the two coefficients are of different sign; this is plus and this is minus, and that has created the problem. So why a E was negative, a E was negative, because D e was less than F e by 2.

So for a E to be positive, D e must be greater than equal to F e by 2 or F e by D e less than equal to 2 that is Peclet number based on delta x e less than equal to 2 that means what? That means you have to select your grid size; if you are interested to use the central difference scheme, you have to select your grid size delta x in a way, see what is F by D, this is rho u delta x by gamma. So the cell base Peclet number is according to your choice of the cell dimension; rho u is given by the flow strength, which is already there; gamma is the diffusion coefficient, which is also known to you; only you can play with delta x, so you can keep delta x small enough so that the Peclet number is less than 2. cell base Peclet number - cell base Peclet number with the length scale of delta x e, P subscript e stands for P calculated with the length scale of delta x e that must be less than equal to 2.

So this is the physically inconsistency; next interestingly let us see that how the physical inconsistency gives rises to a mathematical inconsistency. So in this particular problem, what is sigma mod of a n b is equal to mod of a E plus mod of a W that is 40 plus 60 equal to 100; sigma mod of a n b by mod of a P this is equal to 100 by 20, this is greater than 1, so if you recall the Scarborough criteria for the solution in the iterative scheme of the system of algebraic equation that Scarborough criteria is violated.

Again you can see through this example that how beautifully mathematics follows physics. So this problem displayed a physically inconsistency, even if you are not careful enough to capture that when you go in terms of solution of the corresponding system of descritized algebraic equations, you are caught up there by virtue of dissatisfying the scarborough criteria, where mathematically your requirement is disobeyed.

Let us consider another interesting point; if you see a P is equal to a E sorry D e plus D w plus F w by 2 minus F e by 2 so that is equal to a P; now F w and F e are equal, so this is 0. If D e equal to D w equal to 0 that is a problem, always when you are doing a with a numeric dealing with a numerical scheme, take the scheme with extremes, so one of the extremes is that zero diffusion; convection diffusion problem will have always some diffusion, some advection in general, but one of the extreme limits is that the diffusion strength is negligibly small, advection is very, very, very, very strong. So you have a very strong unidirectional flow as an example through which say heat is transferred. So if the diffusion strength is 0, it does not mean that literally diffusion coefficient is 0; what it means is that the relative strength of diffusion with respect to advection is such that you can take it almost equal to 0 as the diffusion strength.

So when you have that, then you have a P equal to 0, and your equation is phi P equal to a E phi E plus a W phi W by a P, so it is division by 0, so it collapses here; that means in the limit of very weak diffusion, the central difference scheme does not work. So we have seen a lots at least, if not lots at least, a quite a few number of significant limitations of the central difference scheme. So we have to figure out that what was the origin of this limitation; the origin was see if the advection term was not there, then with the only diffusion problem, there would have been no discrepancy. We have already used the linear profile and solve the diffusion problem without any discrepancy.

Now with a linear profile, with the introduction of the advection term, we are getting some discrepancy; that means the linear profile has a problem in representing the advection term that is the advection term, where the value of the variable at the face is represented as the average of the value of the neighboring grid points, this is the source of the problem, this is not the source of the problem, because this was already there in the diffusion type of problem, when created no problem; so we have to think of some alternative mechanisms of finding out a profile, which represents the advection term in a physically more consistent way.

So we have to also keep in mind that we can do that, because in the finite volume method we have seen that you can use different profile assumptions for different terms; that means although, you have used a linear profile assumption for the diffusion term, you could use a different type of profile assumption for the advection term; and that different profile type of profile assumption for the advection term is motivated by the fact that it should be such that at least it should not give rise to this physical violation of this physical requirement of all coefficients to be of the same sign; and the physical situation based on which, we can intuitively design one such example, one such example profile variation is as follows. If you see that the case of extreme failure of the central difference scheme is the case where the diffusion strength is 0.

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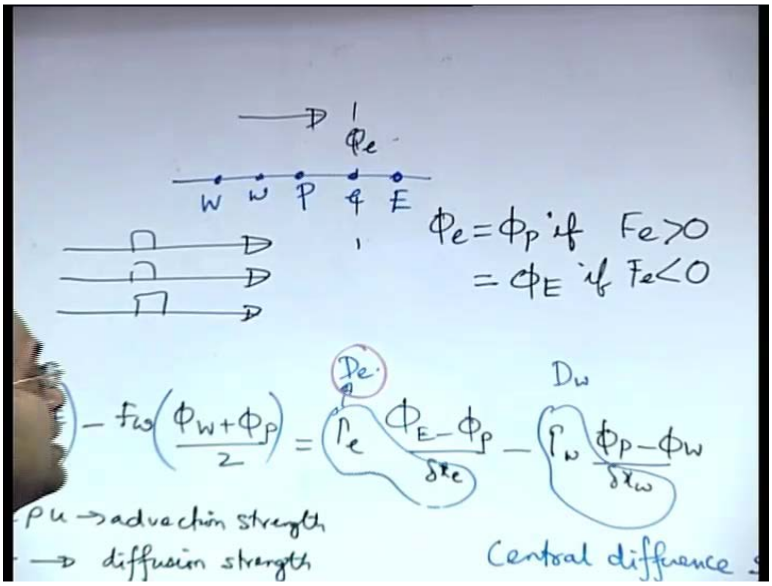

So let us consider such an idealized case where the diffusion strength is 0; if the diffusion strength is 0 or very, very small that then what it means is that the flow strength - the flow is taking along the responsibility of transporting the variable from one end to the other, so the flow strength or the advection strength is the critical issue. So then, if you are considering a grid point layout like this…

If you are having a flow in this direction, then what is phi e, so it has two neighbors; P and E, out of the values of these two neighbors, which value will influence phi e more, phi p, because it is swiping from left to right, so whatever is the value of p by virtue of the very high flow strength, it will try to assign the same value to phi small e; there will be some effect of phi capital E also by virtue of the fact that diffusion is not unidirectional diffusion occurs in all possible directions, but because of the dominant strength of advection that will try to over weigh the effect of the value of the variable at capital E.

So what we can say is that phi e can be equal to phi p, if F e is greater than 0 that is flow is taking place from left to right; on the other hand if flow is taking place from right to left, then phi e is equal to phi capital E that is if the flow is taking from left to right, then phi at small e will be primarily govern by phi at capital E, if the flow strength is very large, if a P is less than 0. So if you make a profile assumption, this is just like a constant piecewise constant profile assumption; if you make a profile assumption of this kind, this particular scheme is called as upwind scheme.

So today we have discussed about the physical basis of the upwind scheme; in the next lecture, we will continue with this; and try to see that when we substitute the upwind scheme in the discretization of the advection term, what different consequence it leads to, and what are the pros and cons of the scheme as compared to the central difference scheme; thank you.