Computational Fluid Dynamics

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Lecture no. # 31

Discretization of Convection-Diffusion Equations:

A Finite Volume Approach (Contd.)

In the previous lecture, we introduced some concept of how to discretize a convection diffusion problem. And we discussed with the central different scheme, and outline that what are the possible limitations associated with that particular scheme.

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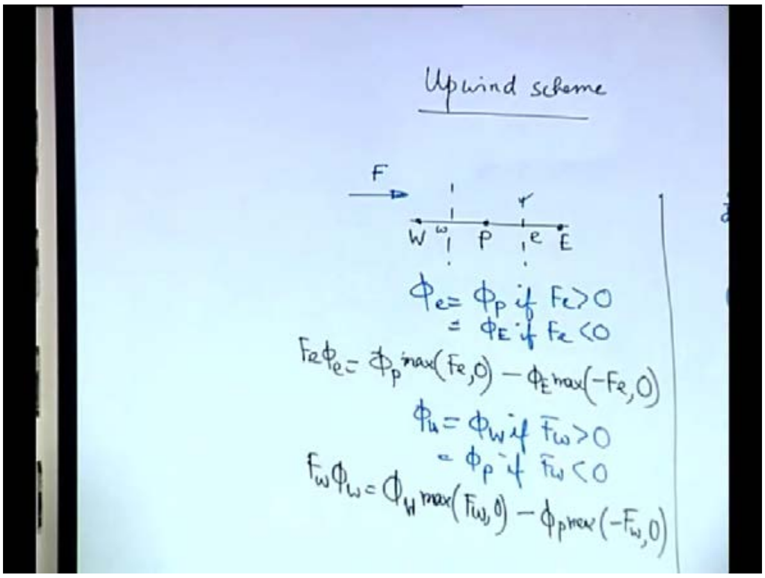

Keeping that in view, we briefly introduced the idea of the upwind scheme, which we will elaborate in today's class. So, if we consider a grid layout like this; the idea of the upwind scheme is to make sure that based on this grid layout, you obtain a discretization which does not violate the basic requirement that all coefficient must be of the same sign. We identified through the central different scheme, that the origin of the problem was associated with the discretization of the advection term. And the upwind scheme tries to deal with it in a somewhat different way.

Since, the main problem of the central different scheme was prominent, when the diffusion was tending to 0, that is when the advection was very strong. In the upwind scheme, we try to address that particular case when the advection is strong; that is you are having a predominantly unidirectional transport. So if the fluid flow is occurring from left to the right, that is F is greater than 0. So we can say that F small e is equal to F, sorry phi small e is equal to phi P, if F e is greater than 0; and equal to phi E, if F e less than 0.

So the value of the variable at the control volume face is same as is assigned to be same as the value at the up string midpoint; that is what is the profile assumption for the advection term. Of course, you cannot use these profile assumption for the diffusion term, because this is just like a piece wise constant profile, so it will not have any first order derivative. I mean it will have the first order derivative as 0, so it will not contribute to the diffusion term.

Now, it is possible to write these two together in a combined expression. Remember that if we discretise the governing equation; so d dx of rho u phi is equal to d dx of gamma d phi d x. If we discretise it, that means if we integrate it with respect to x; from small w to small e. Then it becomes rho u phi e minus rho u phi w is equal to gamma d phi d x e minus gamma d phi dx w. So, that means in terms of our symbol F is equal to rho u, and d is gamma by delta x.

So using that symbol, the left hand side is F e phi e minus F w phi w. So, we do not just require phi e, we require F e phi e, the product of this. So, we can write F e phi e is equal to what? Is equal to F e, now if we write this statement by combining this two; see phi e equal to phi P, if F e is greater than 0.

If we write it in this way, where max (a,b) is a function which returns the maximum of the two, which returns the greater of the two. It is a very simple function, I mean traditionally this function was introduced with a consideration that in in in in tradition people use Fortran as a programming language for numerical computation; and in fortran there is an inbuilt function for calculating this one. Of course, it is such a simple thing to evaluate that there is perhaps no need for an inbuilt function, the such a function can be generated easily.

But the origin of introducing this was based on the fact that, the Fortran inbuilt function could be used for evaluating this. Now, if you see let us consider these two cases separately; phi e, let us consider F e greater than 0. When F e is greater than 0, then max of F e and 0 is F e. So this becomes phi p into F e, when F e greater than 0 max of minus F e and 0 is 0; so this term becomes 0. So F e phi e becomes equal to F e phi p, that means phi e equal to phi p, if F e greater than 0.

If you consider F e less than 0, then max of F e and 0 is 0. And max of minus F e, and 0 is minus F e; so minus F e into minus phi e becomes F e into phi e. So, F e into phi small e becomes F e into phi capital E, if F e is less than 0. In other words phi small e equal to phi capital E, if F e less than 0. So, this expression combined the effects of both F e greater than 0, and F e less than 0. Similarly, let us see what happens for phi w - phi small w is equal to what? Phi capital W, if F w greater than 0 is equal to phi P, if F w less than 0. So, F w phi w - what is this? This is phi w max F w 0.

Let us just verify, if F w greater than 0, then the first term will only be there; so F phi small w becomes phi capital W. And if F w is less than 0, then the first term is not there, second term F w sorry, phi w becomes equal to phi p. So these two are the consolidated or I would say concized forms of the profile assumptions corresponding to phi e, and phi w for the advection term. We have a choice of choosing a different profile assumption for the diffusion term, and we indeed have to do it; there is no other way, because this profile cannot be used for the diffusion term, it cannot capture the radiant in the diffusion term.

So for the diffusion term, what we can do we can still maintain the central difference scheme, because that was a scheme, where without the advection term - the diffusion term discretization created no problem with the piece wise linear profile assumption between the grid points.

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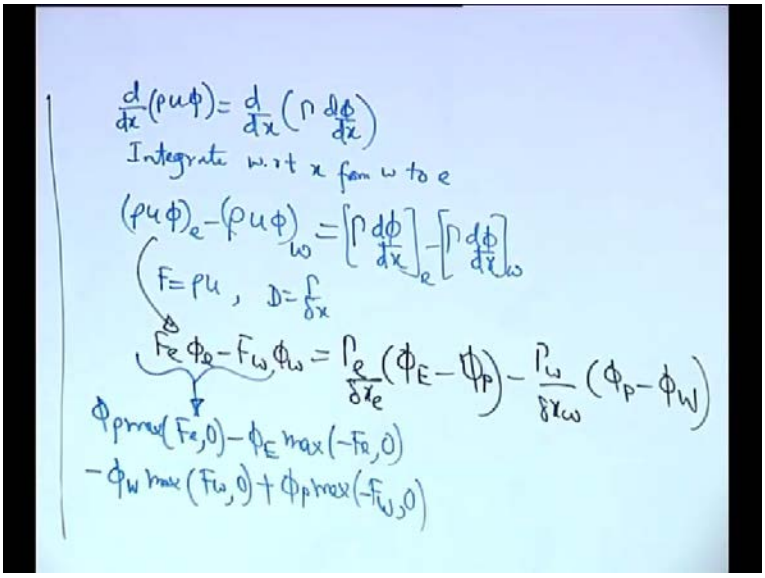

So if you do that, then what we get? So, let us write the left hand side in in place of this one, we have F e phi e as phi P max F e 0 minus phi E max minus F e 0. Then minus phi w max F w 0 plus phi P max minus F w 0.

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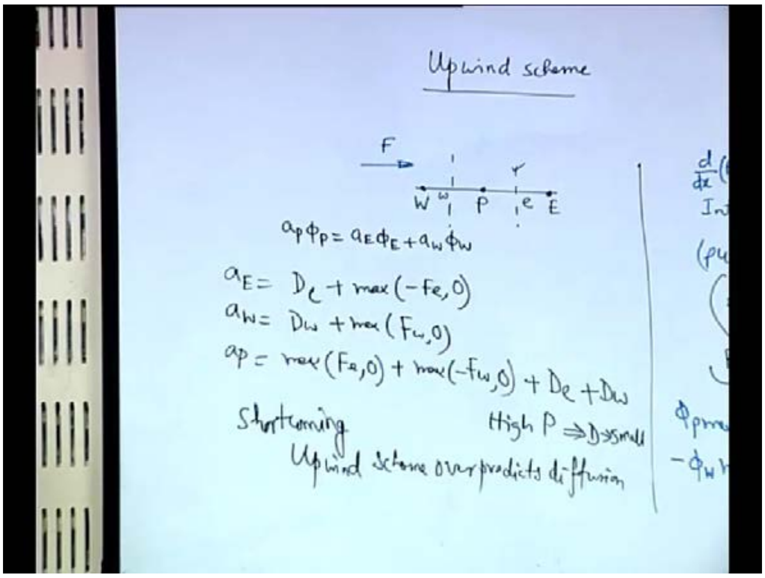

So this we can organize as a P phi P is equal to a E phi E plus a w phi w. So, to use the symbol D, we can use we can call this as D e, and we can call this as D w. So what we can do? We can write a E equal to, what is a E? We can take the coefficient of phi E on the other side plus there is a D e on the other side. So, D e plus max minus F e 0, what is a W? D w plus max F w 0; what is a P max F e 0 plus max minus F w 0 plus D e plus D w. One can non-dimensionalized the coefficients, you can see how do you non-dimensionalized the coefficients the right hand side, you can whatever is there if you divide it by D. Then a E by D is 1 plus max of minus (p e,0), where p is the peclet number based on the length scale delta x t.

So in different books people use different styles, either you use a dimensional form of the coefficient or non-dimensional form of the coefficient by dividing it by the D, dividing the original coefficient by the corresponding D, diffusion state. So by looking into this, we can observe one important thing; that all coefficients must be of the same sign, because D, D w are all positive. And max of these two they will always return something which is at least 0, because if F e is greater than 0 this will return 0; if F e is less than 0 it will return minus F e which is greater than 0.

So in other words, similarly you will have max of minus F w, 0; so and max of F w, 0 max of F e, 0 also will implicate similar thing. So, what we can conclude is that at least the problem of having some coefficients with different signs than other coefficients, will not aggregate, will not be there at all. So this upwind scheme is physically consistent. Now despite being physically consistent, there are still some short comings with this scheme. What are the short comings? Short comings, when you use the upwind scheme, you tend to use it for a case when there is a strong unidirectional transport.

Advection transport, when it is dominating it tends to make a transport unidirectional whereas, diffusion tries to have a multi directional transport. So, diffusion effect of diffusion is something where a disturbance propagates in all possible directions; whereas, advection primarily is oriented along the direction of the flow. So, if there is a predominant predominant direction of the flow.

Now of course, advection also may have multiple directions, if the flow is not unidirectional; if the flow also has components in several directions, but if the flow is predominantly unidirectional, then the advection transport will be predominantly unidirectional. So, when you have a strong flow in one particular direction, then if there is a counter diffusion also in in the opposite direction that will not be important, because eventually the transport will be governed by the dominant unidirectional advection.

Now in that case, if it is a dominant unidirectional advection, the diffusion term should be 0; diffusion term should be small, but still in this particular scheme, the diffusion terms are discretized by using the central different scheme, therefore for high Peclet number. When the diffusion term is, the diffusion term is small, if not ten into 0 at least small; even if it is small, that is not omitted in this particular scheme, because the diffusion term is still retain, and it is discretised in the standard central difference way.

So this scheme can predict diffusion, when there is very little diffusion, because this scheme is essentially meant for working very nicely for a case, when advection dominates much more than diffusion. And even then keeping that physical aspect in mind, we implement that only in the advection term, but not in the diffusion term. So, that it shows that the upwind scheme over predicts diffusion.

So there are situations, in which upwind scheme may be conveniently used, but one has to be careful about these particular shortcoming of the upwind scheme, that it over predicts diffusion in a sense that, when diffusion is supposed to be negligibly small. Even under that case, it tries to represent the diffusion in a different way. And that makes it, over predict the effect of diffusion than what is the actual case in the physical situation.

Nevertheless the upwind scheme is expected to behave in a more physically consistent way, then the central different scheme for any arbitrary Peclet number. If you keep the cell Peclet number within the limits, that is cell Peclet number is less than two in terms of its magnitude. You will see that the central different scheme works perfectly well. So if you has, if you have to use a central different scheme you have to be careful about that. In the upwind scheme, we need not be careful about such restrictions, and still it works in a physically consistent sense. So to see the how the upwind scheme works in different problems, let us try to work out an example.

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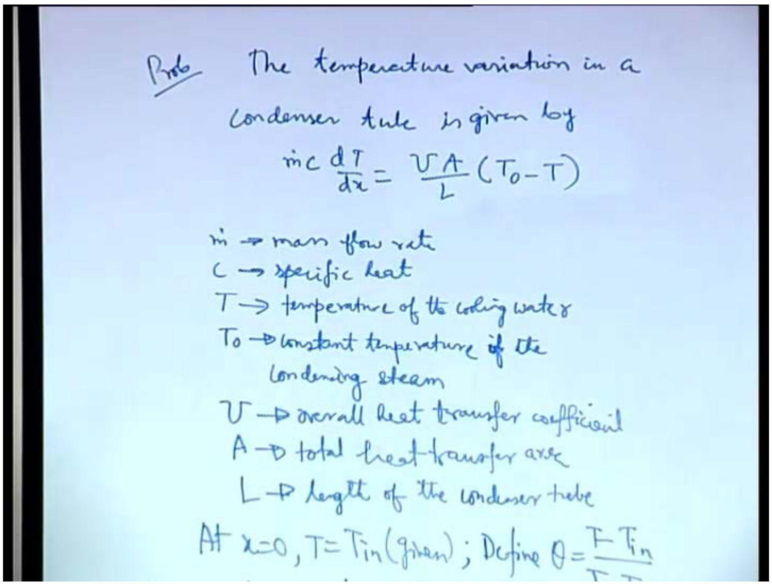

The example is as follows: The temperature variation in a condenser tube is given by m dot c dT dx is equal to UA by L, T 0 minus T, where m dot is the mass flow rate, c is the specific heat, T is the temperature of the cooling water. T 0 is the constant temperature of the condensing steam. U is the overall heat transfer coefficient. A is the total heat transfer area, L is the length of the condenser tube. These are the meanings of different symbols.

Now at x equal to 0, T equal to T in which is given inlet temperature. Then define a non-dimensional temperature theta equal to T minus T in by T 0 minus T in, and the non-dimensional length y equal to x by L, obtain theta as a function of y. Numerically taking only five grid points using upwind upwind scheme, also compare with the exact solution you may take AU by m dot c equal to 2.

So, the physical problem as you know that what is a condenser in a power plant, in a thermal power plant; for example, you require to condense the steam; so to do that, you have some cooling water, and the steam in effect of heat transfer with the cooling water, rejects it to the cooling water, and gets condensed. So, the temperature variation in a condenser tube for the cooling water is given in this by this formula m dot c dT dx, where x is the axial coordinate of the condenser tube, that is given by… So, U A by L into T 0 minus T; so whatever is it is basically a heat balance.

So, whatever is the heat rejected heat rejected from the steam to the cooling water, that gives raise to a axial change in increasing temperature of the cooling water, at steady state. So, this is the rate of increase of temperature of the cooling water, and this is the heat that is done from the steam to the cooling water.

Now, what is given is at x equal to 0 at the inlet that temperature of the inlet is given, and you have to find out the temperature distribution along the length of the condenser tube, using an upwind scheme; with some non dimensional coordinates y equal to x by L, and non-dimensional temperature theta, define as follows.

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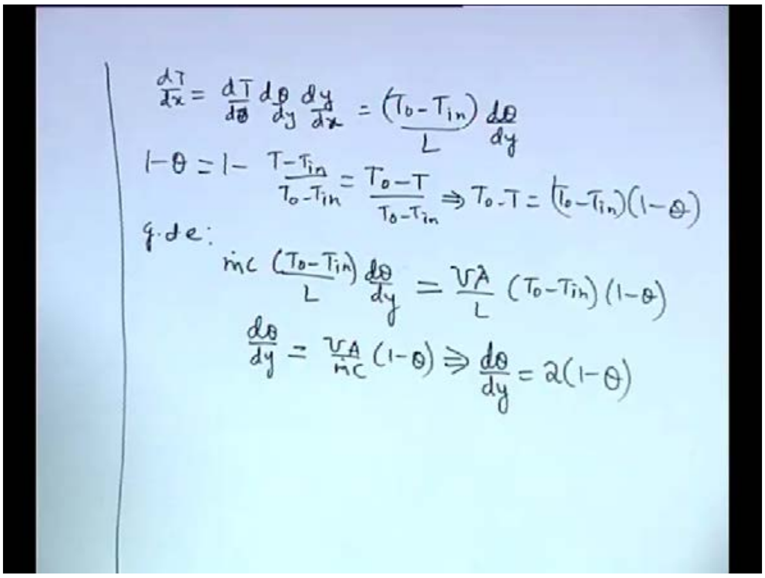

So, let us try to non-dimensionalized this equation first. So, first is dT d x, dT d x is dT d theta d theta dy into dy d dx. So, dT d theta is T 0 minus T in, and dy dx is 1 by L, so T 0 minus T in by L into d theta d y. And to calculate T 0 minus T effectively you can do that by using 1 minus theta. So, 1 minus theta is equal to 1 minus T minus T in by T 0 minus T in. So, it is T 0 minus T by T 0 minus T in; this means T 0 minus T is equal to T 0 minus T in into 1 minus theta. So, the governing differential equation becomes m dot c into T 0 minus T in by L d theta dy is equal to UA by L into T 0 minus T in by 1 minus theta. So, that you get d theta dy is equal to UA by m dot c into 1 minus theta. So, what is given is UA by m dot c equal to 2. So d theta dy is equal to 2 into 1 minus theta. Now, this has to be solved by using an upwind scheme, that means using the first the convection diffusion framework.

Apparently this does not look like a convection diffusion problem, I mean these are certain situations, where one has to apply just a bit of a common sense. In my experience, I have seen that one one such a problem is given to a student; a student is puzzled, because there is no diffusion term. And it does not appear to be a convection diffusion problem, it is actually a very simple very simple version of convection diffusion problem, where there is no diffusion. So here, you have the advection term, as if the velocity is one. So if you consider, let us try to compare it with the prototype of a convection diffusion equation one-dimensional.

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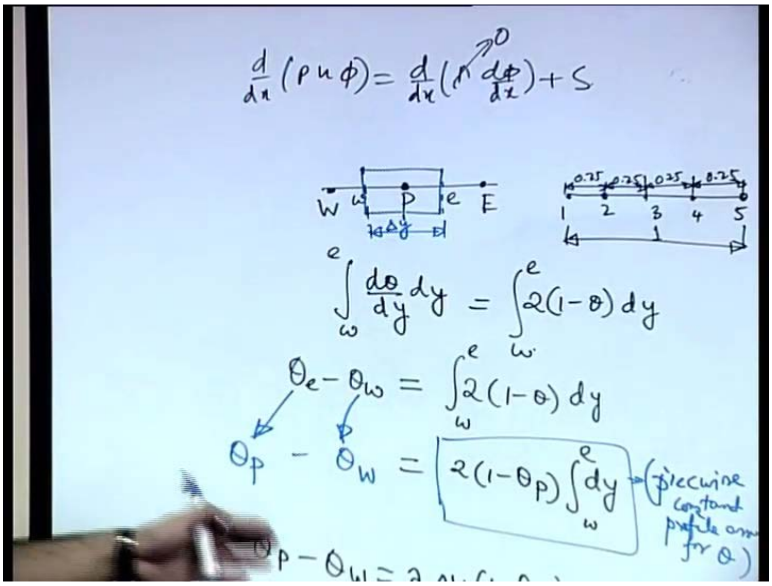

So, one-dimensional convection diffusion equation is what? d dx of rho u phi is equal to d dx of gamma d phi dx plus S. If you have a problem, where u is constant, that is u is say uniform. So rho into u, where u is of a uniform profile; say you have a plug flow, where you have uniform velocity profile. And you say, and and say you have also uniform density. So, rho into u if that product is a constant that will come out of the d dx; so it will become basically d phi dx, just like d theta dy. Here gamma is equal to 0, so this term is not there - there is no second order derivative term, and the remaining term can be a source term. So it is a convection diffusion problem, where you have some advection term, no diffusion term, and one source term. So with that analogy, let us try to discretize it.

So, physically what you are doing, you are asked to use 5 grid points; so let us take 5 grid points uniformly spaced 1, 2, 3, 4, 5. What is this total length y? Non-dimensionally one, because y is x by l. Remember we are not using x as a coordinate, we are using y as a coordinate; so this total length is 1. So individually these are 0.25. So this point P is a representative of any of the interior grid point say 2, 3, 4, whatever. Now, what will be the first step in the finite volume method, we will integrate the governing differential equation over this control volume. The dimension of this is delta y, if it is uniformly space, then this delta y is same as the 0.25; if the control volume faces are located at the midway between the grid points. So, we integrate d theta dy with respect to y from small w to small e.

So, theta small e minus theta small w equal to this integral. Now, when we evaluate this integral, first let us write this, and then we will evaluate the integral in the next step; when you evaluate this integral, you need to make a profile assumption for theta as a function of y. So, what profile assumption can you take for theta as a function of y. You can take piecewise constant within the control volume, because this does not require any derivative calculation for theta. So, if you take the piecewise constant profile assumption for theta then, it becomes 2 into 1 minus theta P into integral of dy from small w to small e. Because it is a constant, it comes out of the integral. So, piecewise for theta, that is for this particular term, but not the left hand side. Left hand side also is some constant, but that constant is not a unique choice; it depends on the flow direction, because it has to be based on the upwind scheme, that is what is part of the question.

So in the upwind scheme, what is the flow direction here? Positive y or negative y or what? So here, you have just like as if rho u equal to 1; so that means u is positive, so you have effectively a flow in the positive y direction. So, what is theta e? Theta e is theta p right, so you can easily make out depending on the flow direction; theta e is is up stream grid point value theta p, what is theta w, theta capital W.

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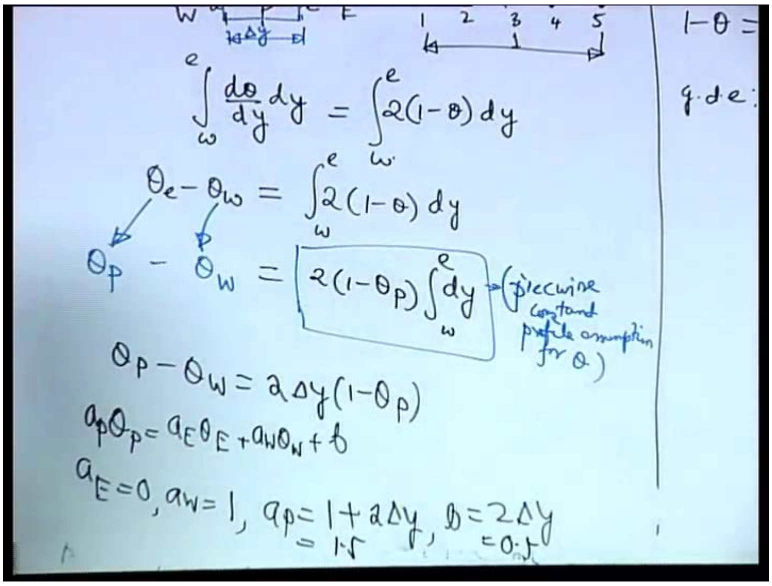

So, if such problems are there do not always try to have a formula based solution of the problem, think of max, what you will write and all those things. In those are for formal statements of the algorithm ms, but when you are solving this problem just like by manual calculations, you can use your justice, your basic understanding of what is the upwind scheme to substitute the corresponding values.

This reveals that you really understand, what is upwind scheme, rather than just remembering the formula of the upwind scheme. So, when you write it in this way, so you have theta P minus theta W is equal to 2 into delta y into 1 minus theta P. So this is of the form a P theta P is equal to a E theta E plus a W theta W plus b. What is a E, a E 0, what is a W? 1. What is a P? 1 plus 2 delta y, and what is b? 2 delta y. Again, you see that, never keep certain things like a magical formula like a P is not equal to a E plus a W here. So, because in many examples, you have a P is equal to E a plus a W, there is a tendency to think that, that should be the common case rather than the exception; that is that is not obvious. Depending on whether there is a source term present or not, and the may be few other factors, whether there is a unsteady term or not and so on, you can have a P which is different from a E and a W.

So, there is nothing wrong with having an a P, which is different from a a E plus a W. So with this, now you can write the or you can find out the numerical values delta y is 0.25; so 1 plus 2 into 0.25 that is 1.5, and b is 0.5.

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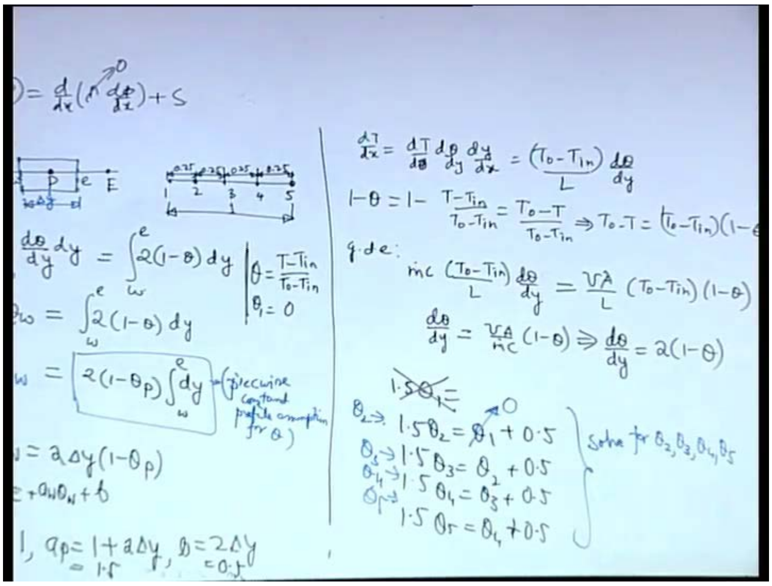

So, what are the equations. So, for the first equation a P phi P sorry a P theta P. so a 1, all a P's are 1.5; so 1.5 into theta 1 is equal to… There is nothing there is nothing called as theta W here. When you write it for the grid 0.1, there is nothing for the waste of the grid 0.1. So, you really do not have to write any equation for grid 0.1. And that is true also from a physical sense, because you are given the temperature at the grid 0.1. So, you need not write any additional equation for grid 0.1. So, you start with the grid 0.2; so 1.5 theta 2 is equal to a W is 1 that is equal to theta 1 plus 0.5 right.

Then 1.5 theta 3 is equal to theta 2 plus 0.5, 1.5 theta 4 is equal to theta 3 plus 0.5, 1.5 theta 5 is equal to theta 4 plus 0.5. Out of this theta 1 is known; what is theta 1? So theta is, what is the definition of theta T minus T in by T 0 minus T in. So theta 1 is 0, because T is equal to T in. So then you have a system of four independent algebraic equations with four unknowns - theta 2, theta 3, theta 4, and theta 5. So, you can solve for using any method for solution of systems of algebraic equation. That I leave on you as a simple exercise, you can solve for theta 2, theta 3, theta 4, and theta 5.

Again you can see that, it is like this problem has a physical sense that it has a marching type of nature; so at the inlet if you specify the value you can march along the positive x direction, and get the subsequent values. So this is like an initial value problem, where the coordinate x acts like the time coordinate. So, as if at initial x is like initial time you have specified something, and you are calculating the things at subsequent times;

subsequent times are like subsequent x's. So, you have a one way or a unidirectional coordinates system which is like a time like coordinate system, and here the special coordinate system acts like a time like coordinate system.

Now, so you march from left to right, whatever is the value at the left depending on that you get the corresponding value, values at the right. How you can check it from these these equations; so you can clearly see that these equations, although they appear to be a system of algebraic equations, these may be solved explicitly one after the other. Like if you can calculate theta 2 from here, then theta 3 from here, then theta from here, and then theta 5 from here. So the scheme is knowing theta 1 you calculate theta 2, knowing theta 2 you calculate theta 3, knowing theta 3 you calculate theta 4, and knowing theta 4 you calculate theta 5.

So, as if you are marching along theta, knowing 1 theta you are calculating the next theta. So, you basically do not require to have an overkill by employing any method for solution of systems of algebraic equations; it is just like calculating one after the other. So, it is it is effectively a marching type of scheme, and because it is a first order differential equation - first order initial value problem, it requires only one condition, the initial condition which is at y equal to 0 or x equal to 0; there is no condition necessary at the other end. So you can go on doing it, to increase the length, you can get a subsequent solution. So, as if it is like, this is T equal to 0, this is T equal to some delta T, T equal to 2 delta T, T equal to 3 delta T like that. So the physics has a similarity with the similarity of a time dependent problem; the mathematics also has also a similarity in a way, this is like a initial value problem. Now, let us quickly work out the exact solution, and see that whether the numerical solution replicates that in some way or not.

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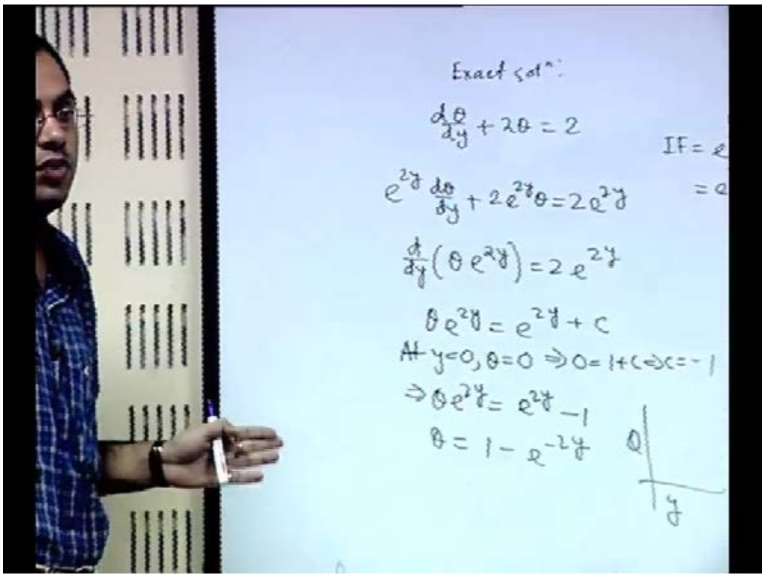

So, d theta dy plus 2 theta is equal to 2. So, you can multiply both side with an integrating factor e to the power integral 2 dy; so e to the power 2y. So e to the power 2y d theta dy plus 2 e to the power 2y theta is equal to 2 e to the power 2y. So d dy of theta into e to the power 2y is equal to 2 e to the power 2 y. If you integrate this theta e to the power 2y is equal to e to the power 2y plus constant of integration. So, at y equal to 0, theta equal to 0; which means 0 is equal to 1 plus c that is c equal to minus 1.

So, you have theta e to the power 2y is equal to e to the power 2y minus 1; so theta is equal to 1 minus e to the power minus 2y. So, it is like an exponential decaying, sort of temperature profile. At y equal to 0 theta is 1, theta is 1 minus 1 that is 0, sorry it is exponentially increasing, because it is a it is a cooling water, so it is getting heat from the steam, and its temperature is increasing. So, at inlet it is 0, and then subsequently it will be greater than 0.

Now, I leave it on you as an exercise, you make a plot of this theta versus y, analytical solution, and you make a plot of theta versus y, it is numerical solution using the upwind scheme, and compare. How they agree or disagree with each other, and give your comment on the possible reasons of agreement or disagreement. Now, we have seen two schemes by this time for convection diffusion problems; one is a central different scheme, another is the upwind scheme and we have seen merits demerits of both. So, now it may be of interest to see that if you have a simple one-dimensional problem, then what is the analytical solution, and how do these schemes compare with the analytical solution. The reason is that the analytical solution can give us a clue of possibly a better profile assumption, then the profile assumption that we get, that we have used for the central differencing scheme, and the upwind scheme.

You may always argue and say, that if that is analytical solution, that is the correct solution. So, why do you require a profile assumption based on that; the reason is that the analytical solution is for a very simple version of the problem that we will consider for more complicated problems, the solution does not remains to be that, but that at least that can give a qualitative indicator of how the profile assumption may be taken, at least we we can compare that how does it fair in perspective of the two schemes - two interpolation schemes or like the two profile assumptions based on the central difference, and the upwind scheme that we have seen so far.

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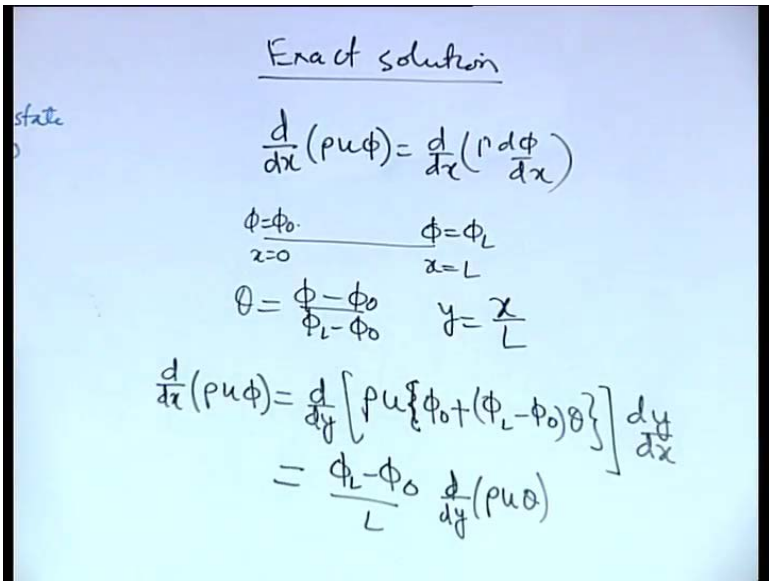

So, exact solution. So, the governing differential equation is d dx of rho u phi is equal to d dx of gamma d phi d x. What are the assumptions? One-dimensional steady state, and source equal to 0. Let us say that this equation is to be solved between x equal to 0 to x equal to L. The boundary condition is phi equal to phi 0 at x equal to 0, and phi equal to phi l at x equal to l. It may be convenient, if we rescale the variables that is let us define a new variable say phi bar or may be theta phi minus phi 0 by phi L minus phi 0. In this way, you can have a scale variable which is constraint to be between 0, and 1; and a new variable y as x by L, that is constraint between 0 to 1.

So, d dx of rho u phi is equal to d dy of rho u in place of phi you can write phi 0 plus phi L minus phi 0 into theta; d dy of this into dy dx; d dy of rho u into phi 0 is what? d dy of rho u into phi 0 is phi 0 into d dy of rho u. It is as good as calculating d dx of rho u, because y can be rescaled to x. So it is basically as good as evaluating d dx of rho u into some constant; by continuity equation d dx of rho u is equal to 0. So, this term will not be there, and dy dx is 1 by L; so it becomes phi L minus phi 0 by L into d dy of rho u theta.

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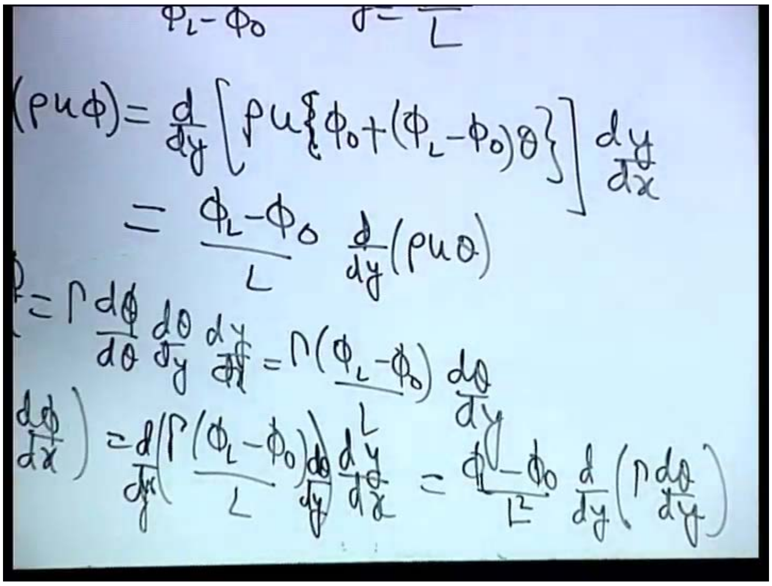

Next, the right hand side d dx of gamma of the first let us calculate what is gamma d phi d x; this is gamma d phi d theta d theta dy into dy dx. d phi d theta is phi L minus phi 0; so gamma into phi L minus phi 0 by L into d theta dy. So, d dx of gamma d phi d x is equal to gamma into phi L minus phi 0 by L into d dy of that into dy dx. So, this is phi L minus phi 0 by phi L into d dy of there is another L square; so there is one d theta dy inside; d dy of gamma d theta dy. There is another one d by L, because dy dx is 1 by L.

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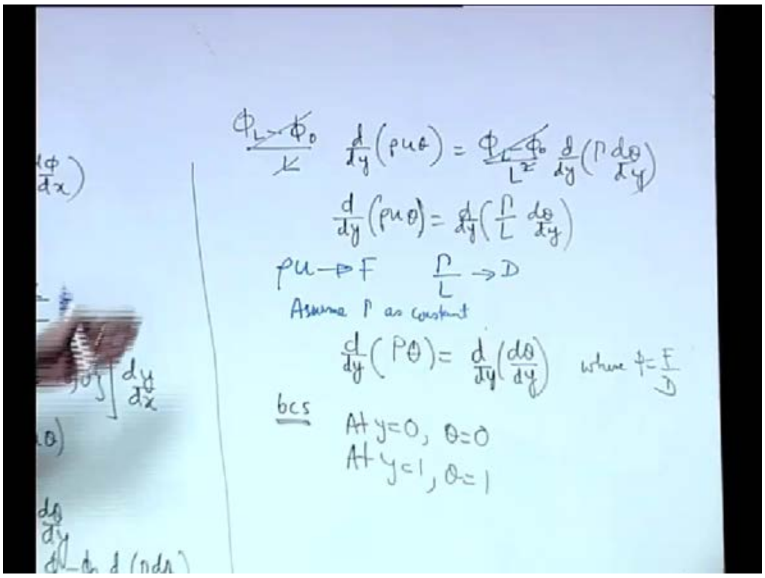

So, phi L minus phi 0 by L into d dy of rho u theta is equal to phi L minus phi 0 by L square into d dy of gamma d theta d y. We can cancel phi L minus phi 0, and one of the l's, so we can write d dy of rho u theta is equal to d dy of gamma by L d theta d y. From our previous discussions on physical ground rho u is equal to the advection string F, and gamma by L is the diffusion string D, because d dx of rho u equal to 0, rho u is a constant; that is F is a constant, but there is no guarantee that D is a constant, because gamma may be a function of x.

But if you assume that gamma is a constant, then you can treat this as constants; assume gamma as constant, just for simplicity. You can write d dy of P phi sorry this should be theta right, P theta…Is equal to d dy of d theta dy, where P is equal to F by D. So, this is the non-dimensional form of the equation, and you see that very elegantly the peclet number has appeared, so that the solution can be parameterized, in terms of the peclet number. And what are the boundary conditions? At y equal to 0, you have theta equal to 0, because phi is phi 0; and at y equal to 1, theta equal to 1, because phi is phi L.

So, we will leave this problem definition up to this here. And in the next class, we will try to obtain a solution of this one, and from that we will see that whether this can be used as a profile, this solution can be used as a profile assumption; indeed there is a scheme for that which is known as exponential scheme. And we will study there that scheme in our next lecture, thank you.