Computational Fluid Dynamics

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Lecture No. # 33
Discretization of Convection-Diffusion Equations:
A Finite Volume Approach

Till now we have come across several convection diffusion discretization schemes; for example, the central difference scheme, the unwinding scheme the exponential scheme and the hybrid scheme. Now, we have seen that in the hybrid scheme it is very much faithful in terms of a qualitative expression of the exponential behavior, but it switches off the diffusion term a bit quickly.

So, beyond peclet number equal to 2 or mod of peclet number equal to 2, so to say by considering both the positive and negative sign a e by d e becomes equal to 0. In reality, the term is switched off to 0 for a peclet number which is somewhat greater than that to accommodate for that. What one can do is, one can still avoid the exponential calculation.

That exact exponential calculation will give that corresponding trend, but as we have seen that the exponential calculation is computationally expensive. So, instead of doing the exponential calculation one can make a curve fitting of the exponential behavior through a power law type of formulation and that is known as the power law scheme.

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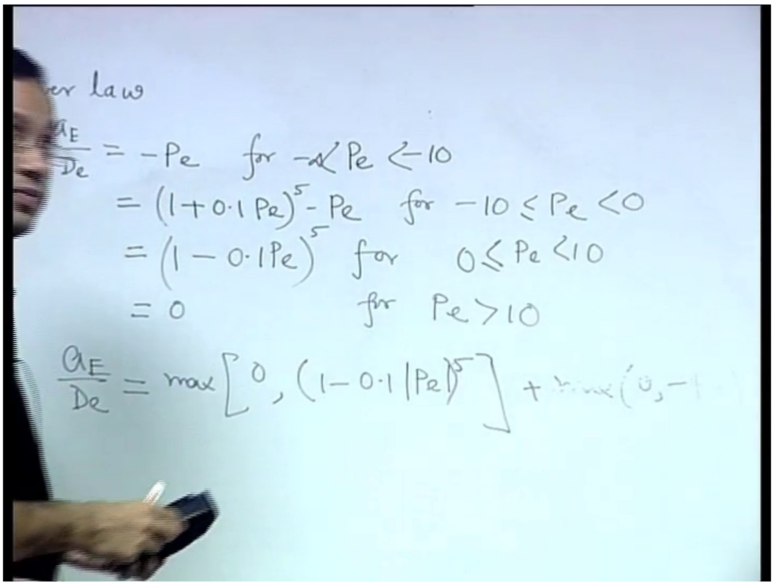

So, let us just write the corresponding dicretized version of the power law. So, it is this, it is this power law described as follows a e by d e is equal minus p e for p tends to minus infinity or even between minus infinity to negative number which is large enough minus 10 is 1 minus 0 point 1 peclet number to the power point 5 for peclet number between 0 to 10 and is equal to 0 for peclet number greater than 10.

So, instead of considering peclet number equal to 2 as a switching of parameter peclet number 10 is considered as a switching of parameter the exponential behavior is such that it lies down to 0 for the corresponding argument tending to 10 in terms of magnitude. So, now, where from this formulae come.

These are essentially the curve fitting of the exponential behavior. So, if you try to represent the exponential behavior in the form one plus a into peclet number to the power b then by using method of least squares you can find a equal to 0 point 1 and b equal to 5 not exactly this, but very close to this 1s. So, that is a numerical exercise we will not go into that numerical exercise because, our objective is to understand from where it comes and to make use of it and to know that why it is important.

So, we have to remember that exponential scheme would have otherwise worked fine, but because exponential calculation is expensive we are going for alternative hybrid is not a bad alternative, but it switches of a e by d e to 0 at peclet number equal to 2 you want to switch it off to a larger at a larger peclet number value say 10 and that is done in conjunction with power law formulation where basically you do not have to calculate exponential behavior it is just to the power 5 means 5 times of multiplication that is the whole calculation which is computationally much much more inexpensive than an exponential calculation. So, that is the motivation behind power law scheme.

Now, you can combine all these to write a single expression a e by d e equal to max of 0 1 minus point 1 mod of p to the power point 5 plus max 0 minus p e. So, what we can see let us consider an example when you have these range that is between minus infinity to minus 10 this part will only be important this part this will be 0. So, it will be minus of p point 1 mod p e to the power 5 yes whole to the power of 5 whole to the power of 5.

So, what we can see from here is that if you go for different ranges all the different ranges can be accommodated through this common formula for example, if you consider the range of between minus 10 to 0. So, between minus 10 to 0 mod of peclet number is minus peclet number and this term will dominate over this term.

So, this like the hybrid scheme where you replace the linear part by this power part it is it is almost like that and max of 0 and minus p is minus p. So, this minus p for the peclet number between minus 10 to 0 between 0 to 10 you have max of 0 and minus p is 0 and therefore, max of these 2 is this 1. So, 1 minus point 1 p to the power 5 and for peclet number greater than 10 both of these have max 0. So, the net result is 0; therefore, all these ranges can be summed up by this single integrated formula.

Now, what we want to see next is something as follows. What we want to see next is that how we can utilize the understanding that we have developed. So, far for the calculation of the coefficient in a generalized frame work. So, till now we have considered several different schemes and the schemes different schemes have given rise to different coefficients.

Now, what we want to see is that if you have a generalized description of the corresponding convection diffusion scheme then that generalize description how it can be utilized to represent all the scheme, but in a generic form not in the specific form; that is, no different formula for a central different scheme or a unwinding scheme or a power law scheme, but a unified formula or formulations where expressions of different terms will be different for different schemes, but the formulation is general and the formulation is not different for different schemes.

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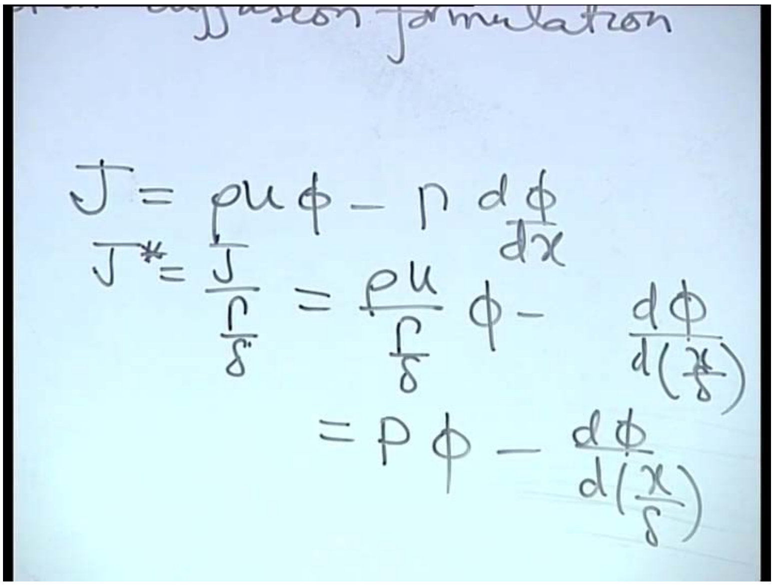

That we call as a generalized formulation generalized convection diffusion formulation. In the generalized convection diffusion formulation what we want we want to consider that there are 2 grid points i and i plus 1 there is an interface and there is a flux through the interface we want to represent this flux in terms of the values of the variable at the grid points by considering both advection flux and diffusion flux which is something that is consistent with any of the convection diffusion formulation.

So, remember that j is rho u phi minus gamma d phi d x to make it generic what we will do we will consider a non dimensional j. So, we will consider j star as by some of j by gamma by delta you can see that j has rho u phi; that means, f into phi we have to divide f by d to get the peclet number. So, that d is gamma by delta some gamma diffusion coefficient by some length scale. So, this becomes rho u by gamma by delta phi minus gamma d phi or gamma is canceled; so, d phi d x by delta.

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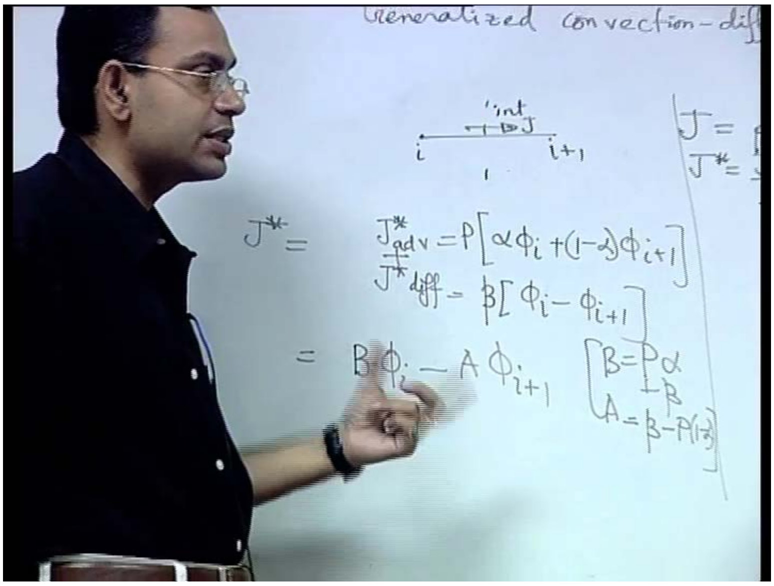

So, this is peclet number into phi minus d phi d x by delta. So, clearly the first term is advection flux non dimensional second term is diffusion flux non dimensional now if you consider j star advection the advection flux is proportional to phi; that means, we can say that the advection flux is proportional to the value of phi at the interface to be more specific now phi at an interface may be expressed in terms of phi at i and phi at i plus 1 depending on the scheme that you are using it will be some weighted average of phi i and phi i plus 1 no matter whatever if the scheme you use.

You dump the effect of the interface as the weighted function of phi i and phi i plus 1 if it the central different scheme it is half half otherwise you can have different weights. So, this is you can write alpha into phi i plus 1 minus alpha into phi i plus 1 where alpha is that weighting parameter J star diffusion we have seen that the diffusion flux is proportional to the negative of the gradient of phi; that means, essentially the difference in phi between the points i and i plus 1. So, it is like beta into phi i minus phi i plus 1 where beta is another coefficient and the j star total is equal to sum of these 2.

So, you can see that it is nothing, but some constant into phi i minus some constant into phi i plus 1 these constants we give the name b and a where b and a both are the functions of peclet number because b and a will contain alpha and alpha contains peclet number. So, b and a are not absolute constant, but these are the parameterized functions of the peclet number that we must remember.

So, every time we will not write b as a function of peclet number or a as a function of peclet number we will keep in mind always that b and a are the functions of peclet number . So, you can find out what is b for example, b is p alpha plus beta and a is beta minus p into 1 minus alpha by comparing these expressions. Now, once we express this in terms of b and a. So, no more alpha beta these are important now everything we will be expressing in terms of b and a.

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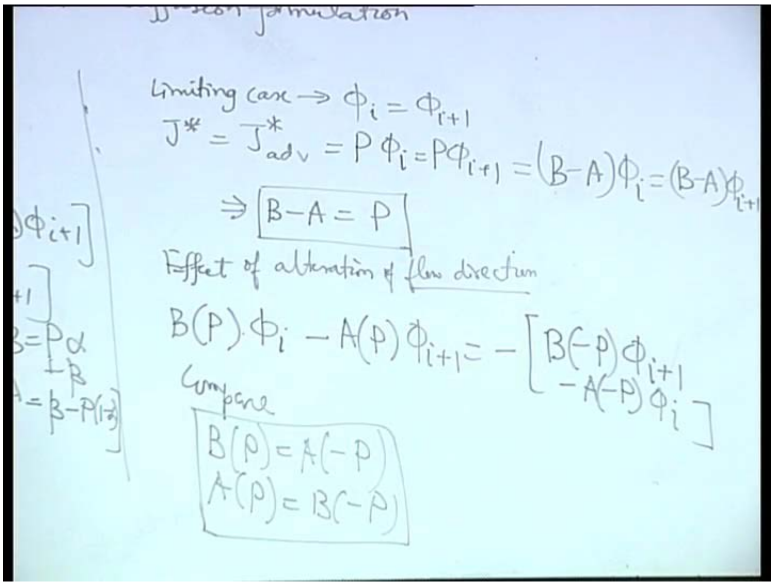

Now, this relationship should be satisfied even in very limiting cases. So, what are the limiting cases we can consider let us consider limiting case when phi i equal to phi i plus 1 then what is j star j star only will be j star advection diffusion is 0 and z star advection phi i equal to phi i plus 1 means it will be p phi i. So, it is p phi i is equal to p phi i plus 1 also from the general formula it will be B minus a into phi i or b minus a into phi i plus 1.

So, by comparing this expressions we can write b minus a is equal to peclet number this is a very very important relationship between A and B no matter whatever is B and whatever is a their difference is always that peclet number that is a thing. Next is let us try to see that what happens if we alter the flow direction if we the flow direction before altering the flow direction. So, effect of alteration of flow direction. So, effect of alteration of flow direction if all the values are the same if all the values are the same what we expect is j star will be reversed because of reversing the flow direction.

So, b of p minus sorry b of now we are writing as a function of p because on reversion of flow direction B of p becomes b of minus p p peclet number becomes minus p only reversing the flow direction, but not the magnitude and all other quantities are remaining the same. So, b of p phi i minus a of p phi i plus 1.

So, this will be negative of the transport with the reversed direction. So, with the reversed direction now b p will become minus p in place of phi i it will become phi i plus one because now the transport is from i plus one to I remember when you are writing B phi i minus a phi i plus one transport is from i to i plus one now if you reverse the flow transport is from i plus 1 to i .

So, B of minus p into phi i plus 1 minus a of minus p into phi i. So, if you compare both sides you will get B of p is equal to A of minus p and A of p is equal to B of minus p. So, this is another set of interesting relationship between A and B with this relationships let us now try to see that how we can make a plot of a and b we have to0 also remember what is the relationship between this capital a capital b and our various coefficient a p a e a w the which have been defined for the non the dimensional form of the corresponding dicretized equation.

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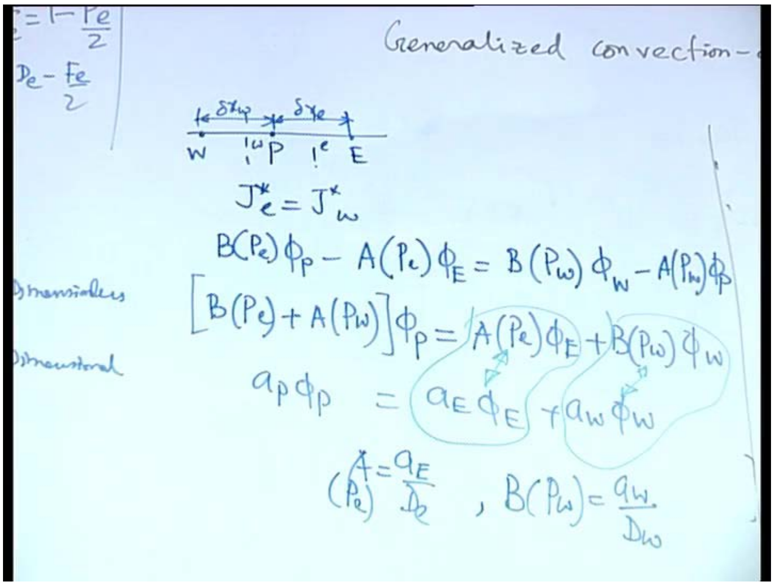

So, if you write or if you dicretized your equation by considering these grid points you have j star e equal to j star w. So, j star e is b phi p. So, b of p e phi p minus a p e phi e this is j we star and what is j w star. So, remember this peclet number is based on which length distance between p and e that is delta x e that is the delta length scale that was used for the general description between i and i plus 1 here i is p and i plus 1 is.

Similarly, when you consider j w star. So, then what will be the corresponding length scale for the peclet number delta x w. So, it will become p w where p w is the peclet number based on delta x w p w into phi w minus a p w into phi p. So, b p e plus a p w phi p is equal to a p e phi e plus b p w phi w this is the dimension less form. Dimensional form a p phi p is equal to a e phi e plus a w phi w. So, which term comes from which this term these 2 term are equivalent only the dimensions are different these 2 term are equivalent only the dimensions are different and how you can convert one to the another remember when you had a e.

Let us consider the central difference scheme for example,. So, you have a e by d e is equal to 1 minus p p e by 2 what is was 1 minus p e by 2. So, you can see that a e equal to d e minus f e by 2 this is the example central difference scheme. So, you can convert a e to a dimensionless form by dividing it by d e then it becomes 1 minus d e by 2. So, 1 minus p e by 2. So, parametric function of peclet number.

So, from here what we can conclude that a is nothing, but a e by d similar terms only dimensions are not matching one is dimensionless another is a dimensional function. So, you can covert one to the another by dividing a e by d e to get a a of peclet number function of p e peclet number based on delta x e similarly b of p w is equal to a w by d w. So, that is how you can relate those coefficient with a and b. So, since we have studied different co efficient it is possible to have an expression of a and b for different cases and you can make a summary of that.

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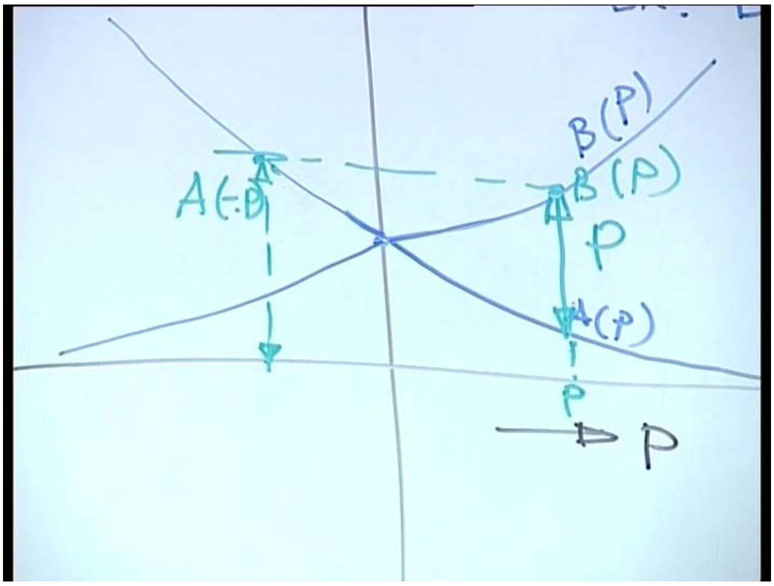

So, for example, you can consider a scheme central difference if you consider a central difference scheme this is equal to p e by 2 upwind scheme what was a e by d e 1 plus max minus p e 0 exponential scheme p e by e to the power p e minus 1 just check whether this are all right we have derived all these earlier hybrid scheme max minus p e 1 minus p e by 2 0 and the power law scheme which we have dealt today max 0 1 minus point 1 mod p e to the power 5 plus max 0 minus p e similarly you can write expressions for capital b which we are not writing here, but it is possible to write in this way.

Just to see qualitatively how you can have a variation of a and b let us make a plot of a and b as a function of peclet number corresponding to the exponential scheme. So, let us plot p e by e to the power p e minus one we have seen that at that plot will correspond to a behavior like this this we have already seen through our previous experience with the exponential scheme.

So, we are considering example of exponential scheme. So, this is a then you have to remember that b minus a is peclet number. So, what we are plotting here we are plotting for a as p by e to the power p minus 1. So, b is equal to this plus p when this tends to 0 b tends to p. It will be something like this when peclet number equal to 0 both a and b are 0 1 in that limit because a is 1 and b is a plus p. So, 1 plus 0 is 0 1 then when you consider the limit as p tends to minus infinity. When p tends to minus infinity b is equal to p plus a. So, when p tends to minus infinity a was tending to minus p that we have seen earlier.

So, that minus p plus p; that means, it will tend to 0. So, you can see that if you draw this properly these are sort of like reflections of 1 with respect to the other. So, this is b of p and the difference between these 2 for any particular p is p itself and why these are sort of reflections of one with respect to the other because we have seen b of minus p is equal to a of p. So, you have b of minus p say this is minus p. So, this is b of minus p this is same as a of p or here is the other ways a of minus p in this graph. So, a of minus p is same as b of p similarly it can be shown it can be seen from the graph that b of minus p is equal to a of p. So, if you consider b of minus p this is b of minus p and this is b of p.

All the important characteristics b minus a equal to p b of minus p equal to a of p and a of minus p equal to b of p are evident from this sketch next what we will do is we will try to generalize it further we have written it in terms of the peclet number, but it is more general to write it in terms of mod of peclet number because the peclet number can change from p to minus p if the flow direction is changed, but if the flow strength remains same then mod of peclet number remains unaltered. If we know the result for a particular flow strength we can apply it or we can extrapolate it for different types of cases by using the information on the coefficient value based on mod of peclet number. So, that we will do next.

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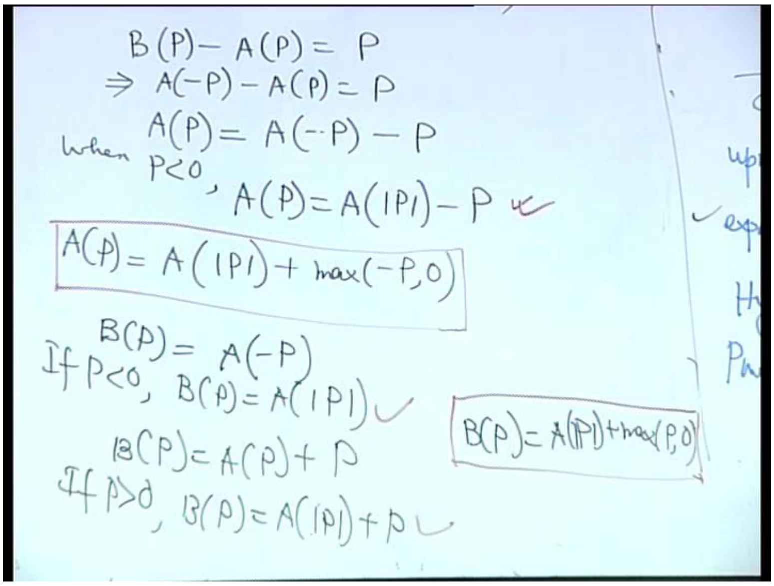

Our objective is to obtain relationships between A of p and a of mod p when p is greater than 0 A of p is equal to a of mod p right there is no difference because mod p equal to p now we can also write that B p minus A p is equal to p and b of p is a of minus p. So, a of minus p minus A of p equal to p; that means, A of p is equal A of minus p minus p. So, when p less than 0 you can write a of p is equal to a of mod p minus p because mod p is equal to minus p for p less than 0 now let us try to combine these 2 if you combine these 2 you can write a of p is equal to a of mod p plus max minus p 0 ok. Because, out of minus p and 0 you have 0 as max when p is greater than 0 and minus p as max when p is less than 0. So, it covers both of these cases. So, this is a very important relationship between a of p and a of mod p.

Similarly, let us try to obtain expressions for b. So, b of p is equal to a of minus p; that means, if p is less than 0 b of p is equal to a of mod p on the other hand you have b of p is equal a of p plus p that is also true. So, that means, you can say if p is greater than 0 b of p is equal to a of mod p plus p because mod p equal to p for p greater than 0. So, you can combine these 2 1 for p less than 0 another for p greater than 0 and say that b of p is equal to a of mod p plus max p 0.

It is possible to write a of p and b of p as a function of a of mod p alone. So, a of mod p is the sole important function because if you know a of mod p you can write A of p and B of p both without calculating them separately in a difficult way by straight forward use of that expression of A of mod p. So, that is a very important consideration and mod p a of mod p is important because it is something that you can calculate irrespective of the flow direction in the same way. So, it does not matter whether mod p is equal to minus 5 or plus 5 in either case a of mod p will remain the same.

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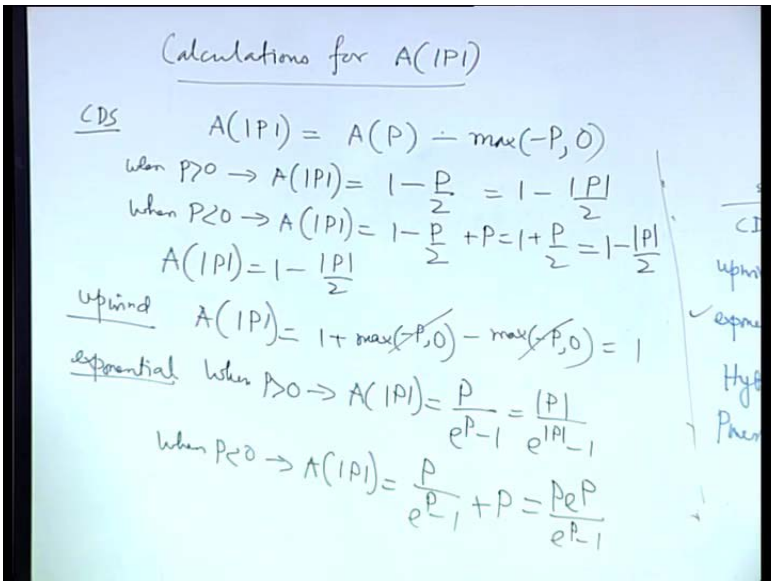

Let us try to calculate a of mod p for these different schemes and try to express those in terms of mod p calculations for a of mod p first let us consider the central difference scheme. So, A of mod p is equal to A of p minus max minus p 0 what was the formula A of p was a of mod p plus max minus p 0. So, that plus comes in this side ok. So, when p is greater than 0 A of mod p equal to 1 minus p by 2 right max of minus p and 0 is 0 when p is less than 0 A of mod p is equal to 1 minus p by 2 plus p. So, 1 plus p by 2 this can be written as 1 minus mod p by 2 this is also 1 minus mod p by 2.

So, you can see that in a interesting way what we see is that no matter whatever is the peclet number the general A of mod p is 1 minus mod p by 2 for the central difference scheme. Then upwind; this is perhaps the easiest. So, a of mod p is equal to 1 plus max minus p 0 minus max minus p 0. So, it is equal to 1 does not matter whatever is the range it is equal to 1.

Then exponential scheme when p greater than 0 a of mod p is equal to p by e to the power p minus 1. So, mod p by e to the power mod p minus 1 because mod p equal to p when p greater than 0 when p less than 0 a of mod p is equal to p by e to the power p minus 1 minus max of minus p 0. So, plus p - p plus p e to the power p minus p by e to the power p minus 1 divide both the numerator and denominator by e to the power p if you do that it will become p minus p by e to the power minus p minus 1. So, this is nothing, but equal to mod p by e to the power mod p minus 1 because mod p is minus p when p is less than 0. So, for the exponential scheme the general a of mod p is mod p by e to the mod p minus 1 ok.

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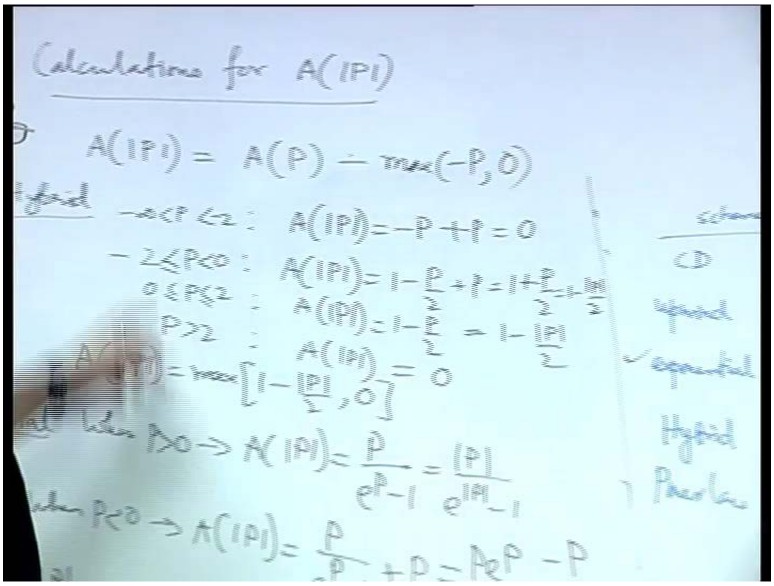

Next let us consider the hybrid scheme in the hybrid scheme we have how many different ranges one is between minus infinity to minus 2 another minus 2 to 2 another is greater than 2 here the range of minus 2 to 2 also we have to divide into 2 parts one is minus 2 to 0 another is 0 to 2 because mod of peclet number is different in these 2 regimes because in one case peclet number is less than 0 and in another case number is greater than 0

So, let us consider first the range minus infinity to minus 2. So, in the range of minus infinity to minus 2 a is minus p max of these 3 is max of these 3 is minus p. So, minus p. So, a of mod p equal to minus p minus max minus p 0. So, minus p plus p that is equal to 0 between minus sorry between minus 2 to 0; A of mod p equal to 1 minus p by 2 that is a of p plus p that is 1 plus p by 2 that is 1 minus mod p by 2 between 0 to 2 a of mod p is equal to 1 minus p by 2 plus 0. So, 1 minus mod p by 2 and for p greater than 2 a of mod p. So, this is 0 and this max also written 0. So, this is equal to 0.

You can combine all these and write a of mod p is equal to max 1 minus mod p by 2 and 0 because if you reduce mod p if you increase mod p to say a value greater than 2. So, this will become negative and therefore, 0 will dominate over that. So, max will be 0. Similarly, here also max will be 0 similar expression you can derive for the power law this I leave on you as an exercise. So, just here what are the ranges in which you should divide minus infinity to minus 10 minus 10 to 0, 0 to 10 and greater than 10 instead of 2 it is just 10.

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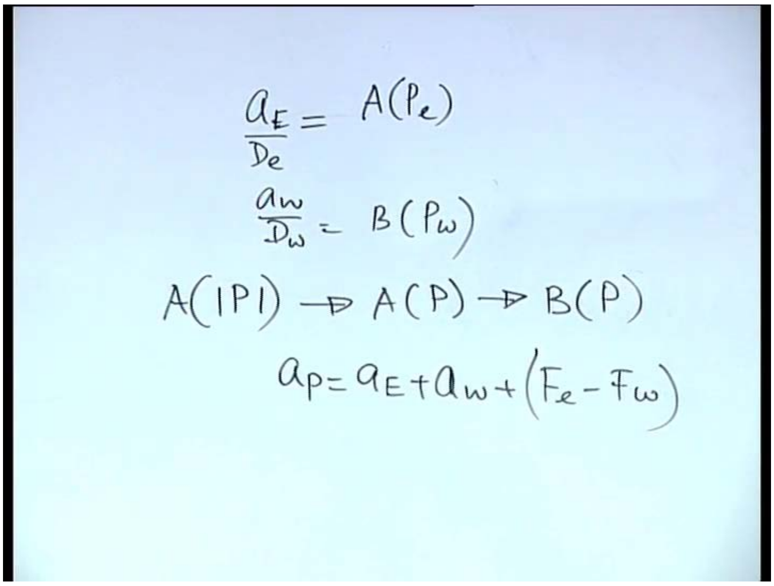

Till now we have seen how to write the generalized coefficients and how different schemes fit a special case of this generalized coefficients and we have seen that once you calculate the generalized coefficients you can calculate even the dimensional coefficients like a E a w. So, you can calculate a e from a of a E by d e is equal to a of p and a w by d w is equal to b of p w.

So, the scheme may be that you first know what is a of mod p from that you calculate a of p and from that you can calculate b of p by using the their respective relationships once you know that; that means, you know a e by d e and a w by d w and a p is a e plus a w plus f e minus f w this we have derived in one of our earlier lectures by giving the example of the central difference scheme.

So, this you can show to be valid even for other schemes. So, you can calculate first the generalized coefficient then the dimensional coefficients and a e a w and then a p as a function of a e and a w that is how you can create the discretized equations. So, this is a fairly straight forward consideration for a 1 dimensional problem.

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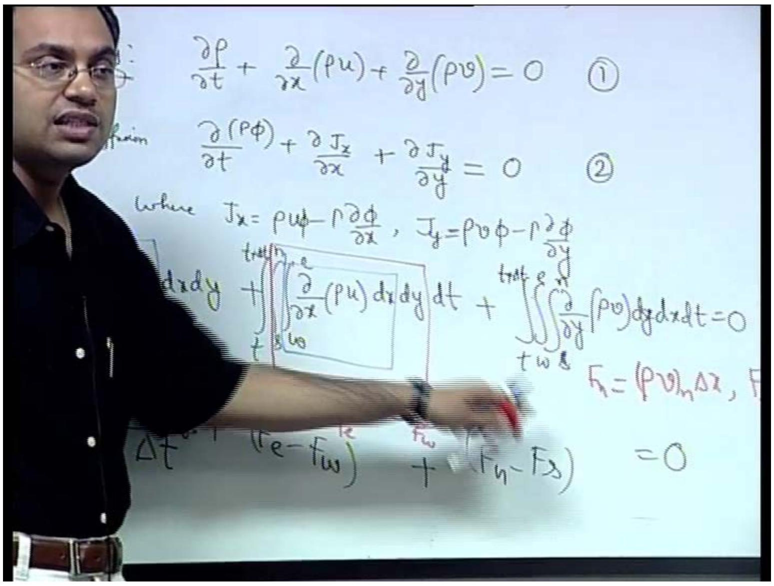

What happens if we consider a 2 dimensional problem in a one dimensional problem? Remember, the continuity equation was straight forward in a way that it it just indicates that f e equal to f w. now, for the steady state one dimensional problem that we have described in a 2 dimensional problem convection diffusion problem the same concept can be extended to extend it to a bit more general case.

Let us consider that the problem can also be unsteady. So, we are interested about the discretization of a 2 dimensional unsteady convection diffusion problem. So, what are the equations that we have first of all first we must have the flow field satisfying the continuity equation this is the continuity equation let us call it equation number 1.

The convection diffusion equation where j x is rho u minus rho u phi minus gamma del phi del x j y is rho v phi minus gamma del phi del y let us consider the grid layout let us say that this is the control volume. So, we have the grid point p its neighboring grid points are capital e capital w capital n capital s this is delta x e this is delta x w this is delta y s this is delta y n this is delta x and this is delta y. So, this is your control volume.

Now, we have to dicretized the convection diffusion equation along with the continuity equation to get the corresponding discretized equations in 2 dimension that is our objective. So, let us begin with the continuity equation. So, what will be the first step integrate the governing differential equation remember we are considering a finite volume discretization.

So, integrate the governing differential equation over the control volume and also with respect to time. So, you have del rho del t d t d x d y . So, the limits of integration are from time t to t plus delta t from x small w to small e y small s to small n as an example let us consider a fully time implicit scheme for the time integration. So, if we first integrate this expression. It will be rho at time t plus delta t minus rho at t we can make a profile assumption that rho is constant over a control volume piecewise constant at each time. So, it becomes rho p minus rho p 0 which is the rho p at the previous time into delta x into delta y.

Second term we can calculate; this integral it is rho u e minus rho u w and that the next term will come as that integral of that d y. So, we can say we can combine these terms together; this along with integral of d y to call this as integral of rho u d y for or integral of d y. you can simply write it as rho u e delta y minus rho u w delta y. So, this we give it a name f e and this we give a name f w. So, this plus this plus f e minus f w into delta t. similarly, what will be the last term if this is f e minus f w this is f n minus f s delta t where we can define f n and f s as follows what is f n rho v n delta x and f s is rho v s delta x. So, that is equal to 0.

We can divide both the sides by delta t so that, we can ultimately get rho p minus rho p 0 into delta x delta y by delta t plus f e minus f w plus f n minus f s is equal to 0 it is essentially an integral expression for mass conservation. So, f e plus f n is a flow, in flow f e f e plus f n minus f w minus f s is the difference of flow in and flow out and that accounts for the change in the mass within the control volume which is the first term with respect to time.

So, it is an expression for the conservation of mass we will stop here in this lecture and we will continue from this in the next lecture to calculate what will be the corresponding convection diffusion fluxes corresponding to the same problem; thank you.