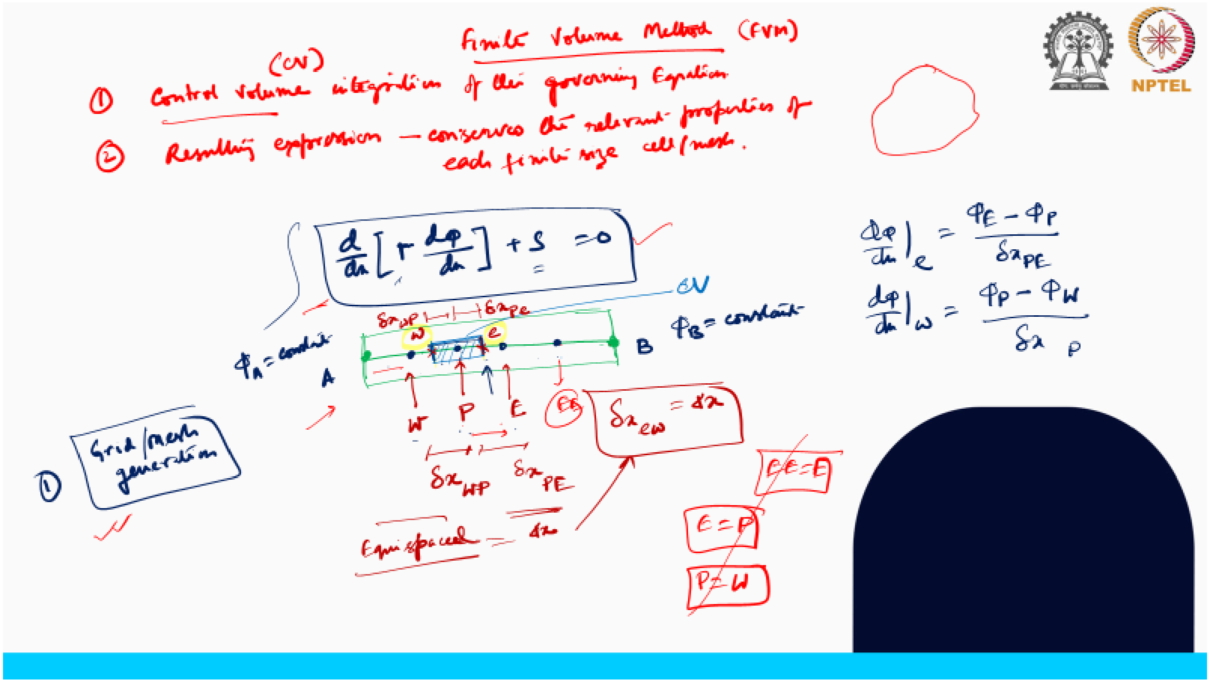
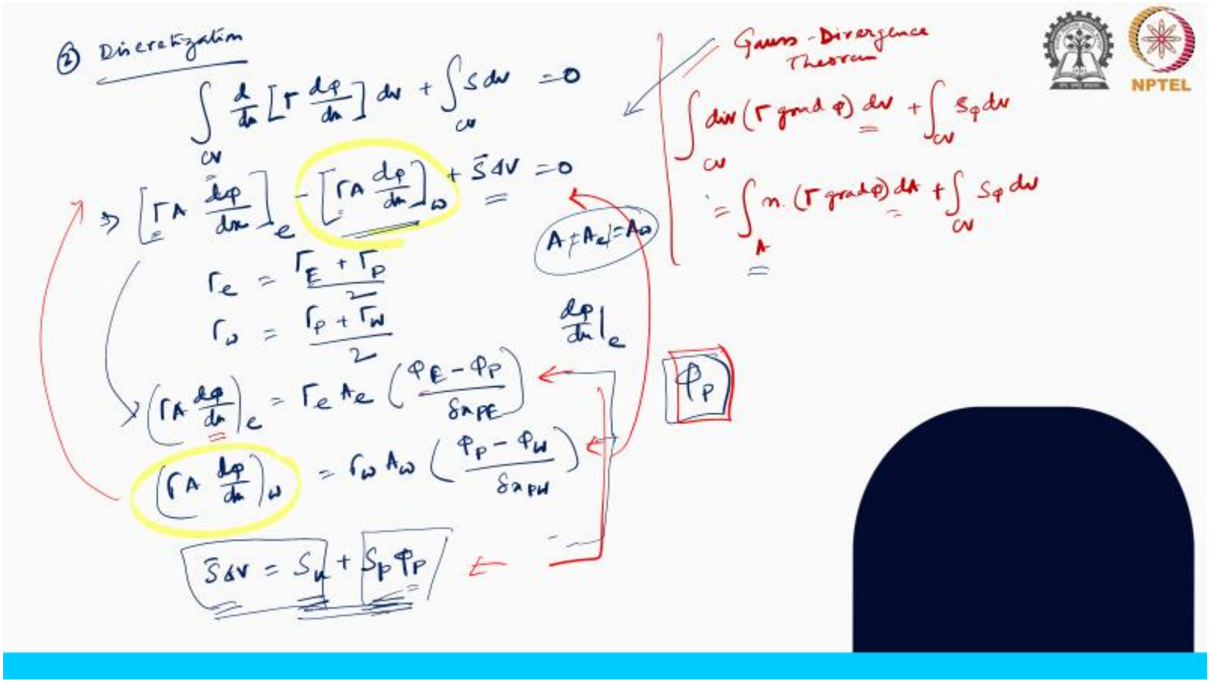
CFD APPLICATIONS IN CHEMICAL PROCESSES
Prof. Arnab Atta
Department of Chemical Engineering
Indian Institute of Technology Kharagpur
Week-04
Lecture 17: Finite Volume Method

So, we are back with another lecture on CFD applications in chemical processes. We were discussing finite volume method in the last class, which will continue here again. And If you remember, in the last class, we just spoke about the steps involved in the finite volume method. So, it has to start with the control volume integration. And then, we discretize that. So, we took this example, this equation.



We integrate it for the first time, In the first case, we have to create the grids that the first step is the grid generation. Then we integrate it over the entire domain and discretized it. That means we have simplified, we have converted the partial differential expression or the differential expressions here, not the partial one, since it is the one-dimensional case, the differential expression to the algebraic expression.

And I told you that once it is done, we have to put back these expressions here to find out the value of or the expression of phi p. Now, this conversion of the control volume, this integration of the control volume that from volume integral to area integral was done through the Gauss divergence theorem. So, once we plug in all these expression to the main equation what will happen is that we find an expression which is equals to zero.

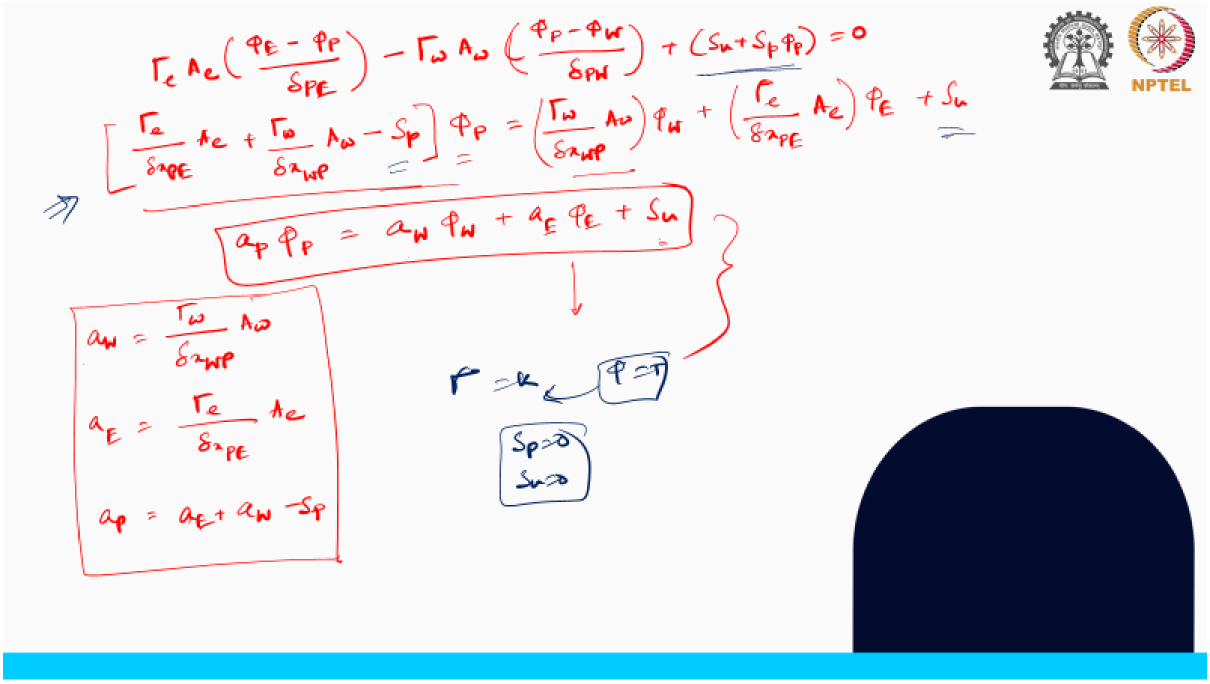


This all comes from this expression, this expression and this expression.

These two are put back in this equation. So now we have to, as I told you, we have to segregate the value or the coefficient to understand what is the expression for phi p. And that, once we rearrange these variables, what we find, if you do it carefully, you would find that I have this kind of expressions, a e term, this comes from here, plus delta x W p here I will have A w minus S p because I have phi p here is equals to a w this is multiplied by phi w plus capital e this is a e

phi E plus the independent source term. So, what is done in such cases or in this case is that the coefficient of phi P is identified and what we see here That in generic form, what we can write is that this term, if we consider this as AP, then what we have AP phi P, say this is in the west face. compact form of this equation where aw is essentially your divided by or say right AE PE AE and AP is essentially you see that AE plus AW minus SP.

So, what we get is that after discretizing that equation, what we get is a discretized form and that too we can separate the coefficients of the variables for each nodal point and we can compactly write that AP phi P is equals to AW phi W plus AE phi E Plus the independent source term. Where. This AW. Is all these. Point all these. Values. That are usually. Known to us. Say for example. As I told you. This is the gamma. Is the say diffusion coefficient. For if phi is. Temperature. It becomes a thermal diffusivity. Usually those values are known to us. So, gamma is known to us.



The nodes we have divided that means how many numbers of nodes we want here for example 4. We have divided so we know that what is this delta x WP delta x PE WP all this delta x values we are usually aware of it. Because this is fixed by the user that how many grids points we are fixing accordingly delta x we calculate. And based on the size of the control volume area is also usually known for us. So, what happens is that the coefficients are known to us, which means here for point P, we get an expression where the coefficients and this is the source term.

If there is any source term that appears here, we know this value. So similarly, for all the nodal points, what we do? We find out this expression. So, this is for point P. Here, now I told you, if I now shift my attention from P to E, so E becomes my new P. And accordingly, the point P is my now waste point. And this next point, which we have not mentioned, say for example, double E, further east point.

This double E is my now new east point when this point P is shifted to the location of point E. So once this happens, you get another expression for point E. So, you basically get a set of expression, algebraic equation for each and every nodal point. that you have considered in the domain. Now you have to solve this set of equation for the phi p values. And that gives you the solution.

So how exactly it is, or say as I told you, now if we put some numbers in this equation, say we do not have any source term, we consider steady state conduction in a heat rod. In a rod that is having two different temperature at both their ends. This is a classical problem. So, let us consider that I have a domain or a heat rod. Where I have my both end at two different temperature.

So, say side A side B. I have TA as 100 degree centigrade. TB say we have at 500 degree centigrade. This rod let us say we have 0.5 meter of length. Fine, and this has a cross-sectional area A, say not A, I would say here it is the end that we have considered A. So, say small a, the cross-sectional area, and that value is given as say 10 into,

10 to the power minus three-meter square. The thermal conductivity of this rod is given as say 1000 watt per meter Kelvin. We have to find out what is the steady state temperature distribution in the rod. Extremely classical problem, very simple. The governing equation you can solve analytically.

And the governing equation is for this case is that the version that we have already seen but without any source term. So now you can relate the form of this this expression, we have replaced phi as temperature and without heat generation. So steady state heat conduction equation, governing equation is this, where the previous gamma is here the thermal conductivity. So, all the values are known to us. wherever it is needed.

So, two boundary condition, one is 100 Kelvin or centigrade whatever you consider and accordingly, correspondingly consider this as 500 Kelvin or 500 degree centigrade. The length is 0.5 meter and the cross-sectional area, it is uniform, uniform rod. or uniform cross section rod, having a uniform cross section. And where the cross-sectional area is this. So, this equation, you can solve it analytically. You do not require for this simple problem, the finite volume method.

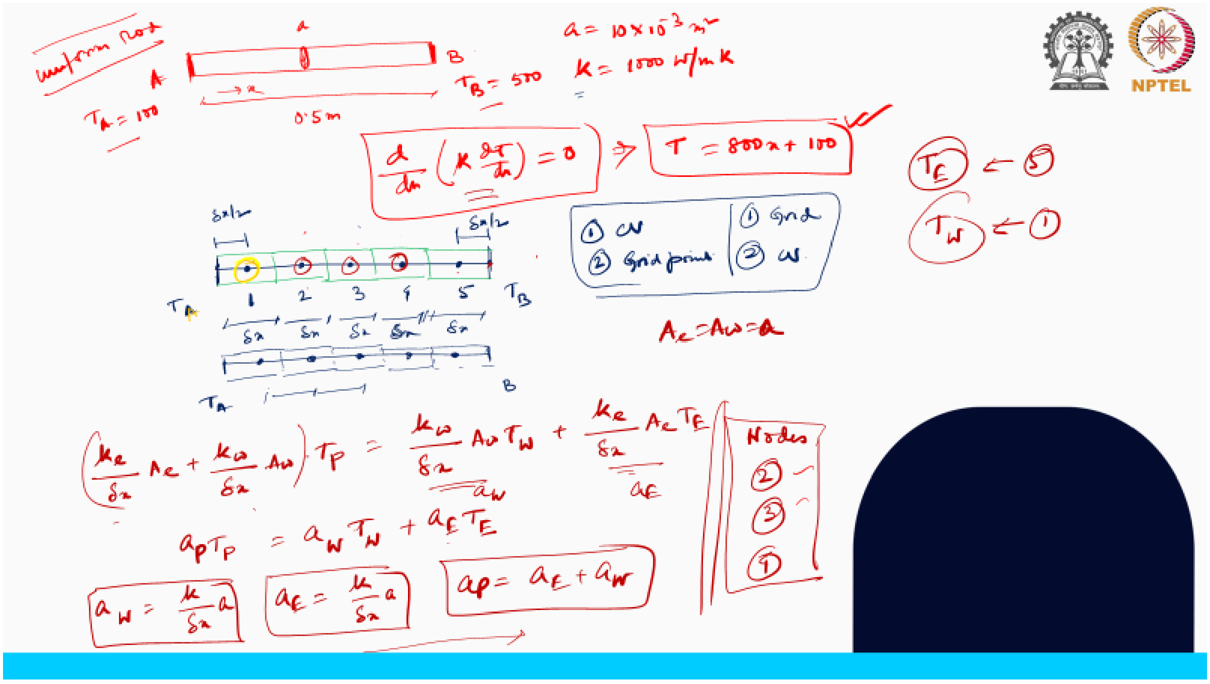
But since we are understanding how it works, let's apply finite volume method here. and see that how accurate finite volume method and what are the criteria of its accuracy that goes closer to the exact solution. What is the dependent parameter? Because here, for this case, you can always solve this for the analytical solution that I told you. And with this, so for this exact problem,

the solution that you will have is this profile, a linear profile that you will have. You put the value of x, you get the value of the temperature as you go in the x direction. So, this is the exact solution. Later, we will cross-check our result or the prediction of finite volume method with this exact solution. But for doing this, what we require is that we take the domain at first.

So, say these are my boundary condition, which is T A and T B. I divide this domain into say five equal division, okay? So, I consider that I have five. So, I consider that I divided this domain into 5 by giving 5 nodal points that 5 grid points. So, this is my grid point 1, grid point 2, 3, 4 and grid point 5 ok.

So, once it is done fine. So, then what we have to do we have to draw the control volume. Now there are two ways it works. You have seen while I was drawing it, I drew the control volume at first. So, there are two ways one can draw, the first you can draw the control volume and then at the centroid of the control volume, you can place the grid point. The other way can be that you place the grid point, like for example here, between TA and TB, I place my grid point,

and then I draw the control volume by placing the midpoint as the face of the control volume. And then I draw the control volume. When we have equispaced points or the uniform grid both the strategy are or will give you identical result. When these are not equispaced points, so for example here the distance between one and two and two and three are basically identical. So here also these two are identical. the same value.



When this is the case, then both the strategy would give you the same result. But when it is not, we will discuss it separately for the non-uniform grid. But for the time being, consider that we have uniform grid. So, what I have done, I have drawn five control volume and, in the centroid, we have placed the 5 nodal points.

I know the total distance. So, I know each and every delta x value. Because it is equally divided by 5. We will come to the numbers later. But let us formulate that in a generic way. At the same time, you realize that from this nodal point to the boundary, we have delta x by two value, this distance. Similarly, the last nodal point, the fifth nodal point and the boundary, it has a distance of delta x by two.

Rest all distances are the delta x. Is it clear to you? I hope so. Because if you have to draw this on your own, then you can realize that what is happening. So now the point is we had this previous expression, the generic expressions that we had. Here the only difference is that we do not have the source term. So we do not have this source term.

So sp and su would be absent from here and here gamma is replaced by thermal conductivity k. Rest all remains same, the formulation. So what we do? We pick this equation, we replace gamma as k because here pi is T for this gamma is K and there is no source term. If you do that, what you will find from here, it is essentially Ke , Ke by delta X here, I would put it as delta X directly, the AE surface plus again delta E AW, this whole thing multiplied by the temperature at point capital P is equals to

delta x this multiplied by T capital W plus E delta x AE T capital E. So, it is this expression up to this because we do not have SP and do not have SU in this particular example. So again what we see here or we can write is that AP TP is essentially AW TW which is the waste point plus A capital E and T capital E. where a w capital w is essentially k by delta x multiplied by a because here we have uniform cross section so a e is equals to a w is equals to a or here small a the area so what i can write here instead of Is this A because this is known to us.

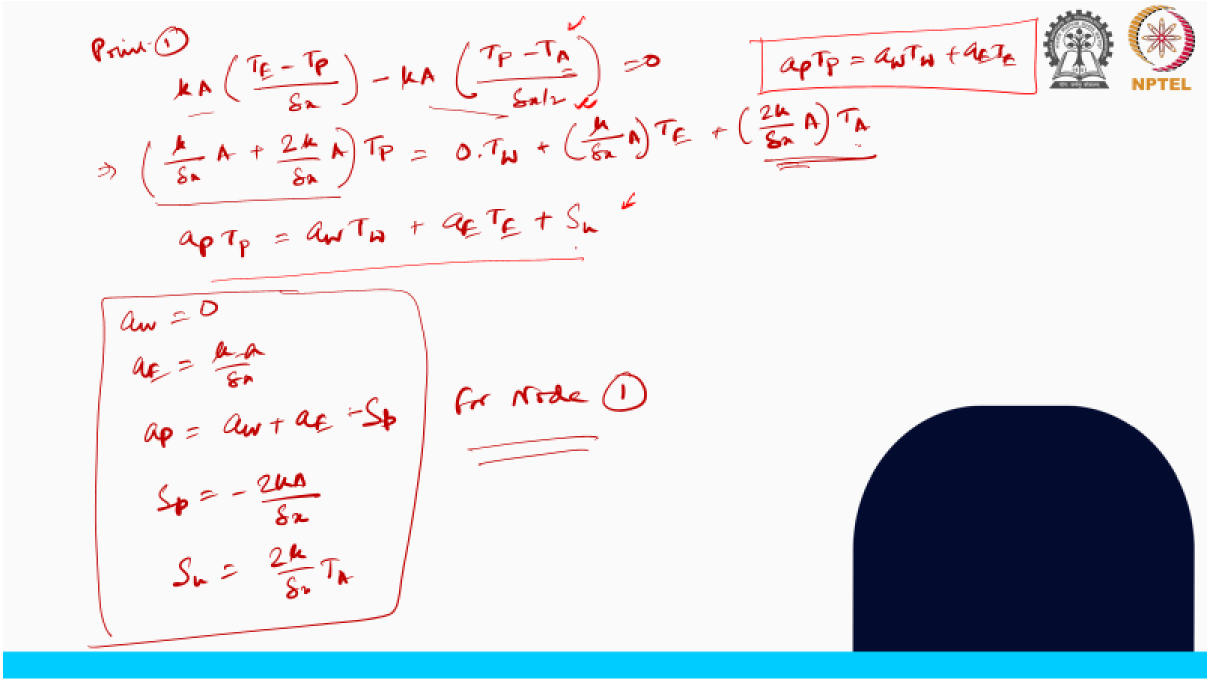
So thermal conductivity value is known to us and A is known to us. Delta X we have divided the domain. So, delta X is also known to us. A capital E here which is this term is also the same as this. and AP is equals to essentially AE plus AW. This term per this term which are AE and AW.

This is AE, this is AW. This is true for all the nodal points which are two, three and four. So, this is true for nodes 0.2. So, this two point and the fourth nodal point. Because I have clearly told you and you already understand that for 0.1 and 0.5, The distance between the next nodal point, which is coinciding with the boundary for fifth, it is the east point.

For this, it is the half of the west and it is the half of the east on the other side. So, this is delta x by 2. So, this last two nodal points on both the sides require some specific attention, a slight deviation from this. The formulation remains same. It is only the point where when we consider this approximation here that east to approximate this flask d phi by dx here dt by dx at the east face for the boundary condition.

There is no particularly phi E point or the temperature east point there. It is the boundary condition for the fifth nodal point. So for point five, what would be the T E? That is the question for point five. For point one, what is the point west? There is no waste point further to have such derivation. In this case, what will happen then? We have to consider, say for the point 1, again look at point 1. We are now focusing on point 1, this point.

this point one, the waste point, it's nearer waste point which is known to us based on which we approximate this gradient is basically the boundary condition TA. Okay, so for point one, the way we will write is the KA that happens there, east point we have, delta X, but for the west point, we have TP minus TA, but at delta X by two location, which is zero. If you consider this, on the east side, we have point two from which we can take the value, but for the west side, there is no west point, but the boundary condition is there.



So now, if you basically rearrange it, what will happen is that K by delta X A plus what you have here two times when you simplify it, K by delta X A. This is A of TP. 2K by delta X comes from this term. 1 comes from here. Is equals to there is no waste side coefficient or the term. So, we say 0 multiplied by TW. Just to have the parity or the analogy that we have done that AP phi P of this expressions if you remember.

AP TP is equals to AW TW plus AE TE. So, here there is no AW which is 0 plus what we have here K by delta XA multiplied by TE and then the other terms that has been segregated and that remaining term is 2K by delta XA multiplied by the boundary condition or the boundary temperature TA. Which means now this has a form that this is APTP is equals to AWTW where AW is 0 plus AETE. Plus, as you can see, there is some source term appear due to segregation of variables, although the problem didn't have any source term.

The classical meaning of source term that there is some heat generations, heat sink, that kind of a thing. But this appears for the particular node that propagates from the boundary. And that is how in the simulation, the boundary condition starts the value propagation or the calculation propagation. So now here, due to the boundary condition, the boundary temperature, the temperature gets propagated and is propagated. calculated in the respective other points, the consecutive points.

So, here we have an independent source term that does not depend on the further temperature. All the values are known here. So, here what we have? KW is 0. AE is basically KA by delta X, where again I am writing it in small a So this is basically capital A here is the small a because that value is known to us. AP is basically AW plus AE plus say or here we can say the minus SP where SP is basically minus 2KA

divided by delta x and SU here is the 2k delta x multiplied by dA for node 1. So, for node we have these coefficients. For all other nodes of two, three, four, we have these coefficients. Similarly, I want you to give it a try to develop or have the coefficients for 0.5 because that node, you will not have the east side coefficient. You will have the west side coefficient and the east side coefficient, you will incorporate another boundary condition.

So, we will take it in the next class but before that I want you to give it a try. Anyhow we are taking it for the next class where I will show you the rest of the derivation and the solution and I will stop here today. Thank you for your patience.