CFD APPLICATIONS IN CHEMICAL PROCESSES

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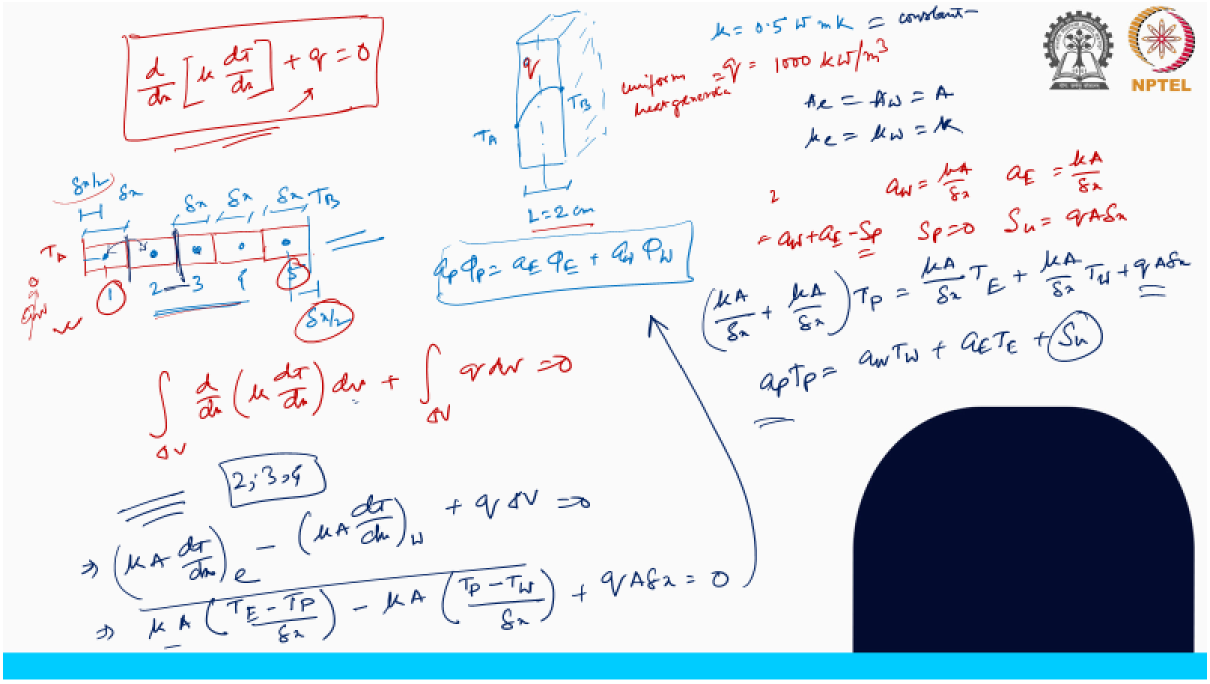
Lecture 19: Finite Volume Method

Hello everyone, welcome back once again with another lecture on CFD applications in chemical processes. We are on the topic of the finite volume method, where we have discussed its fundamentals, how it works, and its algorithm. In the last lecture, we described it with a simple one-dimensional steady-state ordinary differential equation. We have also seen its applications, such as ordinary differential equations for the one-dimensional conduction equation—a steady-state conduction equation. That was perhaps the simplest example through which the algorithm of the finite volume method can be described. We will further complicate or make that expression or equation more complex. Now, we will add its source term to it.

For example, this is also one of the very common examples that one can have: we have a slab. We consider this a kind of semi-infinite slab where our interest is that one side of this slab is kept at a temperature T_A, and the other side is kept at a higher temperature T_B. Or, say, a different temperature is maintained here. Now, we have a heat generation term—a uniform heat generation term or volumetric heat generation term. So, what would be my steady-state temperature profile between T_A and T_B?

This is another classical problem we see: steady-state heat conduction with a generation term. So, how do we discretize this? For this case, consider that we have a width of L = 2 centimeters. For this problem, we have a thermal conductivity of 0.05 watt per meter kelvin. And this uniform generation term, Q, is 1000 kilowatt per meter cubed. It has a constant thermal conductivity of 0.05 watt per meter kelvin.

It has a uniform heat generation term. So, this is the uniform heat generation this Q. We have to find out how this temperature what is the temperature profile at steady state from T A to T B. given that we know say the temperature T A and T B both are known we will fix those values later. But for this problem what we have is that the governing equation this is the part that we have solved already plus it has this heat generation term. So, this is the governing equation and this is the additional complexity compared to our previous illustration that we have seen that how finite volume works.



So, in this case again what we do? The first step is the control volume integration, but even before that the step is the dividing the domain into number of control volumes. We discussed in the last class how that can be that is either you can fix the grid points and then surrounding it you can draw the control volume or the other strategy can be that you draw the control volume matching with the boundary condition or the boundary surfaces faces and then at the centroid you place the nodal point. You demarcate the centroid as the grid point at the nodal point.

For uniform meshes or the for uniform grid both strategies result in same grid structure. There is no difference in between when we have uniform spacing of the grid points or say the uniform size of the control volume. So, here again for the sake of simplicity we will continue doing with the uniform or equispaced or equal volume of the control volumes. So, that means, now in the previous problem I mentioned that what you should do the previous problem you should have repeated with the 3 needle points. or 7 nodal points or 10 nodal points and see whether the result is more accurate or less accurate compared to what we did with 5 nodal points.

So, in this problem also we will continue to work with 5 control volume. So, this distance of 2 centimeters, we will divide it. It is a one-dimensional problem. So, we divide this distance or this domain into 5 equispaced grid points or, say, 5 equal-sized control volumes or equal-volume control volumes. So, I have my boundary condition here, which is T A, and the boundary condition here, T B. So, what do I do?

I will take 5 equispaced control volumes and say this is 5. So, I will consider that this is my This is my control volume, which is T B instead of this part. So, what do I have now? So, now if I have the centroids demarcated as the grid points, I have 5 nodes or grid points: this is 1, 2, 3, 4, and 5.

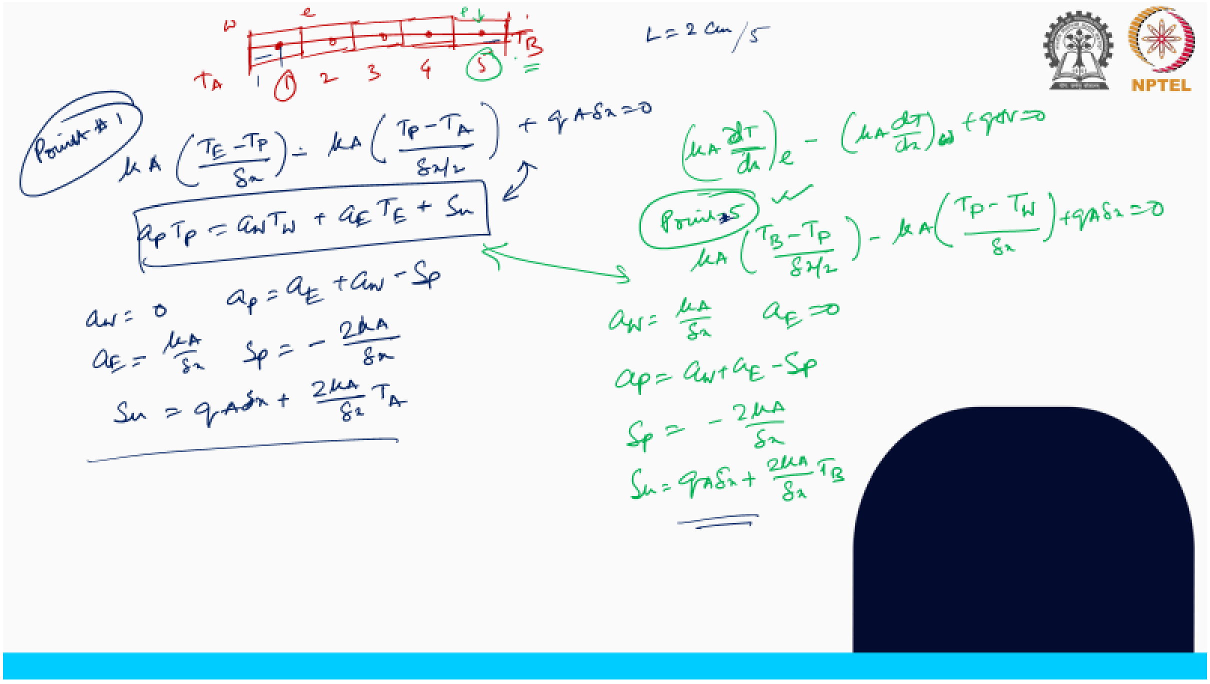
The distance between the first nodal point and the boundary is delta x by 2 because we consider this as delta x. So, all these are delta x. Similarly, from this nodal point 5 to its east face, the nearest east face, the distance is delta x by 2. So, this thing we understood in the last class: what we are going to do is try to develop a generic expression for a p phi p equals AE phi E plus AW phi W.

Such a generic expression for nodal points 2, 3, and 4 or the grid points 2, 3, and 4. For the first and the fifth, we have to pay more attention because this distance is delta x by 2, and this distance is delta x by 2 from pipe to east face. Similarly, from point 1 to the east-west face is delta x by 2. So, this governing equation we will now integrate over the control volumes of 2, 3, and 4. So, although this initial part is the same for all the nodal points, when we simplify it later, we will see that we can write

is equal to 0. We can write these simplified expressions for 2, 3, and 4 compactly or in a generic manner, but for points 1 and 5, we have to write a different equation. So, this we integrate, we apply Gauss's divergence theorem for converting the volume integral to an area integral and then writing in discretized form. What we can directly write here is that k t t by dx where, since we are converting the volume integral to an area integral, I will write

that K A d t by d x at the east face minus K A d t by d x at the west face plus Q delta V is equal to 0. For any nodal point 2, 3, or 4, if you see that this has come, this expression, then we can write its generic expression because that expression will, in the next step, be since we have a constant this is a constant value throughout the domain. So, we write K A directly, and since we have taken a uniform size of the control volume and this is of a uniform cross-sectional area. So, K A also remains.

So, instead of A E or writing A W we can write A. So, similarly instead of writing K E K W it is essentially thermal conductivity K. So, then T east face for all the nodal points 2, 3, 4 the east face which is say for nodal point 2 this face for that what we can write T e minus T p divided by the delta x. It is east point minus the point that we are considering here T p. divided by the delta x this distance between 2 and 3 which is delta x minus. Similarly, this part we can write that T p that this waste face the flask at the waste face that we are calculating is essentially the difference this 2 points divided by the distance between these 2 points.

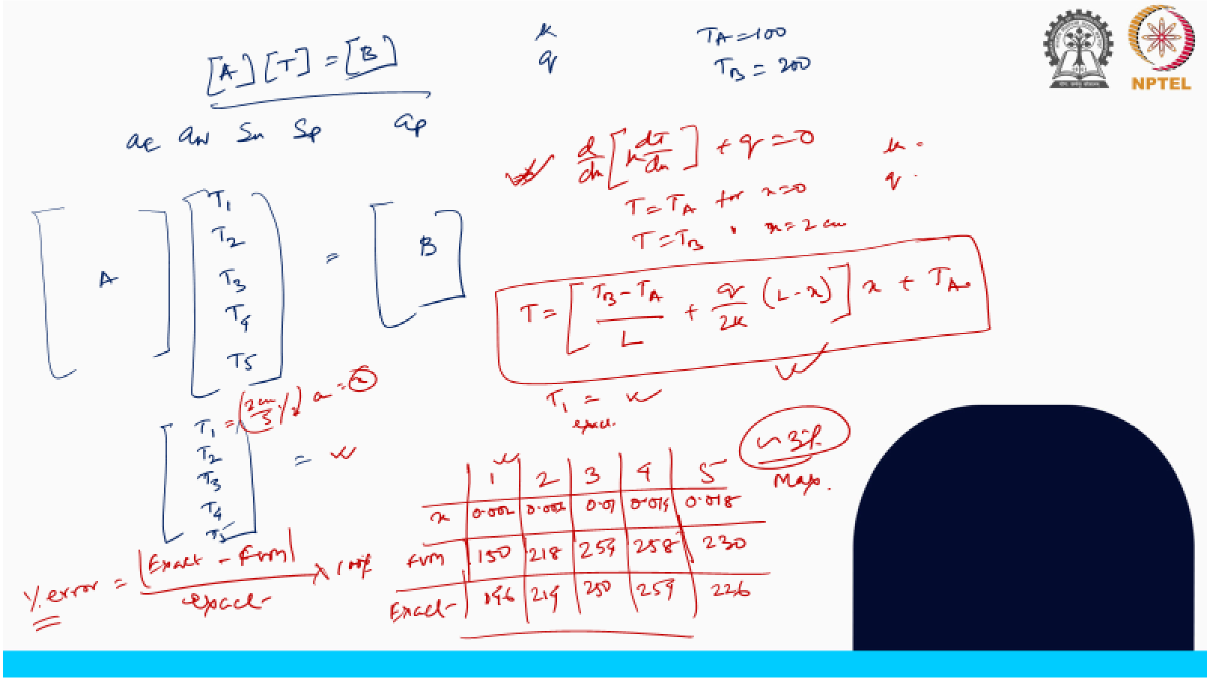


So, T p minus T w divided by the delta x plus Q A d x. So, delta V is A delta x is equals to 0. So, once we write it again we try to have this in this form and if we try to get that in form by separation of these coefficients what we can find is that k a divided by delta x plus again another k a divided by delta x. So, basically 2 times of this multiplied by T p it is just the separation from here. is equals to K a delta x T e plus K a divided by delta x T w plus Q a delta x which is in the form that A p T p is equals to A w T w plus A e T e plus a term that is arising due to this source term.

So, which means here what we have that A p is equals to k A by delta x sorry not that really what we can write is that a w is equals to it is basically 2 times this a w is equals to k a by delta x a e is equals to k a by delta x and a p is essentially 2 times of this which is a w plus a e minus s p where s p is 0 at this for this formulation. So, S p is equals to 0 and S u is equals to Q A delta x. So, this is for 2, 3 and 4 mesh points or the grid point 2, 3 and 4. Now, if we move on to say 0.5 or 0.1 say for example, we go for 0.1 the first point.

First point for the same case we have its east face, but we do not have the traditional west face. So, A w is essentially 0 for the nodal point 1 and there we incorporate the boundary condition as we discussed in the last lecture. So, for this point 1 again if I draw this considering 5. say if you have 5 nodal points.

So, this is your T B this is T A. So, for point A although we have the east face, but the west face coincides with the boundary face or with the boundary. So, in this case my formulation would be K east which is again simply the K because it is a constant value A T e minus T p divided by where T p point p is point 1 divided by delta x minus. So, T p minus now here instead of T w it will be T a because this is the nearest waste phase divided by delta x by 2 because that is the distance between these 2 plus U a delta x is equals to 0.



So, again if we try to find out such format because this helps us to form the matrix that we have to solve. If we try to find out if this format of this equation what we will have is that A w is equals to 0, A e is equals to k a by delta x. A p is the combination of these two that means, A e plus A w minus S p where S p in this particular formulation once you try to segregate this what you will find it is minus 2 k a divided by delta x. And S u in this form is q A delta x plus 2 k A delta x multiplied by T A. It is just the separation and rearrangement of this terms the coefficients. So, this is for 0.1 when you look at 0.5

So, for 0.5 similar to this what you have this time is essentially say if you forget basically d t by d x this is e minus k a d t by d x west small w plus q delta v is equals to 0. So, now, for 0.5 the east face for 0.5 east face coincides with the boundary having temperature T b. So, what will happen here is that we will write T b minus T p, T b minus now point P is this 5 divided by delta x by 2 minus K a T p minus T w divided by delta x plus Q A delta x is equals to 0.

So, again if you find a link or the form of this equation in this form which would be the compact one and it would help us to write the set of matrix that in the form of A x is equals to B. what we find here that a w is equals to k a by delta x. a e is essentially 0 here and a p is equals to a w plus a e minus s p where s p would be minus 2 k a by delta x. and S u in this form the S u would be the similar to what we have seen earlier is 2 k A divided by delta x T b. So, this is for 0.5 and this is for 0.1. point number 1 and this is for point number 5. So, once we have this development.

So, this is for one boundary the nodal point nearest to the boundary on the one side which is say the west side point and this is the east side extreme point formulation. For all other points intermediate points this is our formulation. So, once you have it the previous case we form the matrix to solve this A x is equals to B or here A t is equals to B ok. So, in this case what will happen? We know the value of k, and we know the value of Q.

The t_a and t_b values are given to you. So, if t_a and t_b are given to you, then you can find a matrix that will have AE, AW, SU, SP, all these things, and eventually AP—all the things would be known to you. So, now here, if we consider that T_A is 100 degrees centigrade (or 100), and this is T_B is So, if T_A is 100 and T_B is, say, 200, then you can find this whole matrix in this form: A T equals B, and you can find the temperature profile in between. So, again, what you would find for points T1, T2, T3, T4, and T5—you will have, for this, a matrix which will be in the form of B equals A, and this is on the right-hand side; you will have the matrix B.

For which you have to solve for T1, T2, T3, T4, and T5. Remember, T5 is essentially just before this boundary value, which is if we have L equals 2 centimeters, which is divided by 5. Accordingly, you find out this delta_x by 2 value. So, at that location, you basically have this temperature where it is T5. Now, what you will see is that this equation, which is

this equation—if we solve it for T equals T_A, T equals T_B, for x equals 0, for x equals 2 centimeters. If we solve this analytically with the values that are given, which is T_n, we have k is a known value, and Q is a known value. So, this expression has an analytical solution that looks like T_b minus T_a divided by L plus q divided by 2k multiplied by L minus x, multiplied by x, plus T_a. So, this is the analytical or exact solution of this equation.

So, which means once you find out your finite volume estimation by this method for that. So, where T_1 is essentially at 2 centimeters divided by 5 divided by 2, at this position you have T_1. So, exactly at that same x, you find out from here what your exact value of the temperature profile is. So, here this will be T_1 exact. So, from here What you will have?

You can write such kind of points that for x = 0.1, 0.2, 0.3, 0.4, and 0.5, at these nodal points you calculate the value of your x. So, say, which is presently if I do this in the present case, 0.1 is essentially at 0.002. 0.2 is 0.006, this is at 0.01, this is at 0.014, and this is at 0.018. In this location, you have your FVM solution. As well as you have the exact solution. The exact solution comes from this by putting the value of x, and here for nodal points 1, 2, 3, you have the finite volume method. What you will see if you solve this,

The values are something like this: this is 150, the exact solution should have been 146. This finite volume would give you for the 5 nodal points 218, but it should have been 214. This is 254, and this is 250. This is 258, this is 254, and this is 230 as per finite volume prediction, and here you have 226. So, if you calculate the percentage error, which is exact minus FVM prediction, modulus of this divided by the exact value multiplied by 100 percent, you will find the percentage error. In this case, you will see the maximum error is in the order of 3 percent maximum.

This is very negligible, and we can say that this is a quite accurate prediction for the finite volume method by the way that we predicted. So, with this example, we have made the previous example that we discussed in the last class a bit more complicated or complex with the help of a source term in the one-dimensional case. So, we will continue this discussion in the next lecture, where we will further make this formulation complex to see what happens if we have, say, the convection term now, because these are only the diffusive terms that are present. So, what will happen for the convective term?

How do we discretize those terms? So, with this, I will stop here today, and we will be back on the same similar discussion on this topic in the next lecture. Thank you for your attention.