

CFD APPLICATIONS IN CHEMICAL PROCESSES

Prof. Arnab Atta

Department of Chemical Engineering

Indian Institute of Technology Kharagpur

Week-04

Lecture 16: Finite Volume Method

Hello everyone, welcome back once again with another lecture on CFD applications in chemical processes. In the last week, we discussed numerical methods for CFD and specifically we had an overview of finite difference method and finite element method. Now prior to that in one lecture I briefly introduced finite volume method. So today onward we will discuss in the whole week on this finite volume method.

We will go into the details of the finite volume method that how discretization is done how pressure velocity coupling is done and how taking some examples how this method is basically implemented for say one dimensional, two dimensional or even how this method practically is implemented for a 3D problem which is of actual or the real interest. Because all industrial or practical problem involves the 3D geometry. So how those things can be extended, we will have an overlook on that as well.

But as I told you in the introduction of this course that we will look into the details of the method or how that is done. So what is happening inside the solver? not relying on the default values, how we can develop an intuition. So those things we will touch upon. So today we start this finite volume method and we see that how this technique is applied when we work on this or any problem taking the help of any problem. So the first step of this finite volume method or FVM that we call is that the first step

is the control volume integration of the governing equations. the first step in the finite volume method is integration of the governing equations like in the finite element method we approximated the governing equation with some variational methods or the methods that are suitable and approximated that and over each sub domain or over each element We had then the assembly of those and solved it. The key step here in the finite volume method, it similar to the finite difference or the finite element method that any domain is at first discretized in several nodes or several subdomains.

Here we call those subdomains as the control volume or the CV in short form. So at first we have to draw the grid. We have to understand what is the control volume, which we are considering here as the control volume. And then we integrate the control that governing

equation over the entire control volume. And this state is actually distinguishes this method from the other methods.

Now the resulting expression that we'll have is the exact conservation of all properties within that finite cell or finite size cell. So, what will happen whatever we get resulting expression would have would actually conserve of each finite size cell or mesh. So apparently it possibly is difficult for you to grasp that what is happening here

So let us take directly an example and try to understand that how this finite or what is the finite volume method and how it is implemented or can be implemented in your CFD code. So say we take an example. is that one dimensional for the sake of simplicity $\gamma \frac{d\phi}{dx}$ one dimensional expression of any say scalar variable ϕ . if you now can immediately relate that if we use this ϕ as temperature T it becomes a steady state one dimensional steady state conduction equation with the source S or there is if there is any source A stands for the source. So, let us say this generic expression for any variable ϕ

we will apply finite volume method in order to solve this expression. This expression is provided this S is given and the γ value is given the diffusive coefficient here. So, this γ value is given then it is easy to solve analytically as well. So, what we will do In this lecture as well as in the next lecture, whenever we pick up such expressions or this equation, we will look into their exact solution if it is available.

Finite Volume Method (FVM)

- Control volume integration of the governing Equation
- Resulting expression — conserves the relevant properties of each finite size cell/mesh.

$\frac{d}{dx} \left[\gamma \frac{d\phi}{dx} \right] + S = 0$

Grid/mesh generation

Control Volume (CV) boundaries: A, B

CV properties: $\phi_A = \text{constant}$, $\phi_B = \text{constant}$

Cell faces: W, P, E

Distances: Δx_{WP} , Δx_{PE}

Equi-spaced: Δx

Cell width: $\Delta x_{cv} = \Delta x$

Fluxes: $\frac{d\phi}{dx}|_e = \frac{\phi_E - \phi_P}{\Delta x_{PE}}$, $\frac{d\phi}{dx}|_w = \frac{\phi_P - \phi_W}{\Delta x_{WP}}$

Logos: IIT Bombay, NPTEL

And then we will try to understand that how accurate is this finite volume method in its prediction when compared with their exact solution. So, for this generic expression, the first step, although the first step that I mentioned is the control volume integration, but the point is

that to do that, you have to at first generate the control volumes. Okay. Which means, say, if I have a domain, since this is a one-dimensional, let us consider. Say consider we have a domain where these are the boundary points or the boundaries.

These are the boundary faces and we are supposed to get a steady state profile of the variable ϕ along the x direction. What would be the steady state profile of such by which governs by this expression or equation. So what we will do, so if we consider here this as A and this is B , where you have a boundary condition, say this is constant, ϕ at A , ϕ at B is also constant, which means you have Dirichlet boundary condition at both ends. These are supposed to be given.

You have a second order derivative with respect to ϕ , which means you require two boundary condition for ϕ in order to solve this problem, which are given. ϕ at A is constant and ϕ at B is also constant. So finite volume method, the first step is the grid generation. So at first we do the grid or mesh generation. So, what we will do here? We divide this domain into number of finite size cell or the meshes.

So, for that we have to come up with the say the nodal points and for the time being let us say these are equispaced nodal points or the equispaced points by which I have divided this domain. So I have placed say four points in between the two boundary nodes to divide this domain. So which means I have divided this domain in one, two, three, four, five equal size cell. My control volume will be in this case is considering say a typical point P here for which I will calculate the property ϕ , the variable ϕ .

So if this is the point P , I have a right side node which say to avoid confusion right or left, let's say this is the east side. So this is the right side is the east side point of the point E and this is say west point which is west, W , okay? So around P , I have to draw a control volume because all the variables I will calculate at this nodal point. So what we will do, there are different strategies, two different strategies, we will discuss it later. But for the time being, since these are equispaced,

the distance between this east and west, say if I consider Δx capital W capital P , this distance is Δx capital P capital E . So, distance between the two nodal points. So, now for the Control volume what I will consider an imaginary midpoint or say the midpoint between the two nodal points. I consider this and this faces and I will close this considering that this as my one control volume around point P . So, this is my control volume or say the CV for the calculation. I have to integrate this governing equation over this control volume.

This imaginary control volume when point P is this. If I shift my attention or the point of calculation to east or west, then this east point becomes point P , accordingly point P becomes point W , and this point becomes point east. And so and so forth it will go for the each and every

nodal point. Now, just to clear the nomenclature or the notation that you are seeing, we have the nodal points are say designated by capital letters here, okay.

But at the same time, when I have this control volume, I have its east face as well as the west face. So this face is essentially a east face. So this point and this point on this line we designate that on the east side it is small e or the e in lowercase and say west point which is w in lowercase. So, which means we have another distance or the delta x between say the point P and the face east side face which is delta x capital P small e.

Similarly, this distance is delta X small w capital P. If you consider such nomenclature, then possibly it would be easier for you to understand that I have nodal points which are mentioned in capital letter. The faces, the control volume face, which actually, at the midpoint of the two consecutive nodal points, the intersection of that, the face and this midpoint of the two nodal points is the small letter I have mentioned. So accordingly, the distances are given. So this is essentially, so this distance between e, small e and, so delta x,

small e and small w is essentially the delta x that we are considering here. Because this distance, if these are equispaced, this is essentially the delta x point. The distance between two consecutive nodal points. So, eventually for such case, when these are equispaced, then this delta x becomes the size of one control volume.

So we have generated a grid for one dimensional case. Now we have to integrate it in the next step. So basically this step is similar to what we called earlier as the discretization ok. So, what we will do? So, called the discretization.

In discretization what we will do? We will integrate this over the entire control volume ok. So, what for that what we do is that say integration over the entire control volume d by dx . $d\phi$ by dx over the entire control volume. So, we consider the volume of this control volume as Δv plus integration of the source term over the entire control volume is equals to 0. Now, if you remember our last discussion about the Gauss divergence theorem, that tells us that divergence of, this is the expression I showed you last time, control volume plus control volume $S\phi$, which is, say, if it is the function of ϕ even,

That is essentially, that means the conversion of volume integral to surface integral by the Gauss divergence theorem. What we can write here is essentially the normal component of $\gamma \text{grad } \phi$ over the surface area on which it is acting plus the control volume. So we consider this as say a volumetric generation. Then we can have the constant value for the generation term. So based on this, this discussion we did in the last class that we are converting this integral to the area integral.

Once we understand this and you incorporate here what we can write or what we can approximate this integral is that after converting volume integral to area integral if you look at both the sides. this is the area on which it is acting on the east face because here is the node that you can see this is the east face small e and this control volume this is the so this is the east face this is the west face of the control volume. So, this is the west phase, this is the east phase. So, east minus west plus say uniform volumetric generation term which is as per multiplied by the dv is equals to 0. So with the help of Gauss divergence theorem what we did we convert this volume integral to area integral and then we integrate it over this area which we have

since here we have a one dimensional problem that is the east face minus west face whatever the flask that is going in and out. Now here, these are this γ cap in copper case, these are the diffusion coefficient or the diffusive values, diffusive flux associated with the diffusion coefficient. Now these actually will have their numerical values given or if this varies specially, Say this property is also varying spatially. Then we have to also approximate this value. That how, what is the value of say γ_E or γ_{west} phase that I will consider.

Now, usually when we initialize the solution or initialize because any solution programming that you have done, any code that you have done earlier, in the first couple of line of your code, you realize that you initialize those variables by setting the zero values or some known values. That is called the problem initialization. Now, once you do that, that means those values are stored on these nodal points or in this nodal points. for the finite volume method.

Now here, once these values are stored, which means all the scalar quantities values or the property values, the material properties and et cetera, all values are essentially known for these nodal points. If that is the case, then you think you can understand that this east and west face, which are at the middle of these two has to be approximated and better it is approximated by simple arithmetic average of the capital W and capital E divided by 2. Sorry, this is the east face. So, for the east face, we have capital P and capital E .

by two for the waste face capital W and capital P it is in between these two. So the arithmetic average of these is better approximated by two. So now again for the sake of simplicity consider that this area of the faces are uniform for all the grids or all the sides. That means the area of AE at this E point and area at the west side, both are same.

If that happens, then I have A is equals to AE is equals to AW . If that is not the case, in case of non-uniform grid, we will have different values of this. So, that means now if we further look at this expression, so this $\gamma_A d\phi$ by dx at the east face, so which means this I have A_E and then I have $d\phi$ by dx at the east face. Now, have a look at it.

② Discretization

$$\int_{CV} \frac{d}{dt} [\Gamma \frac{d\phi}{dx}] dV + \int_{CV} S dV = 0$$

$$\Rightarrow \left[\Gamma A \frac{d\phi}{dx} \right]_e - \left[\Gamma A \frac{d\phi}{dx} \right]_w + \bar{S} \Delta V = 0$$

$$A_e = A_w = A_0$$

$$\Gamma_e = \frac{\Gamma_E + \Gamma_P}{2}$$

$$\Gamma_w = \frac{\Gamma_P + \Gamma_W}{2}$$

$$\left(\Gamma A \frac{d\phi}{dx} \right)_e = \Gamma_e A_e \left(\frac{\phi_E - \phi_P}{\Delta x_{PE}} \right)$$

$$\left(\Gamma A \frac{d\phi}{dx} \right)_w = \Gamma_w A_w \left(\frac{\phi_P - \phi_W}{\Delta x_{PW}} \right)$$

$$\bar{S} \Delta V = S_u + S_p \phi_P$$

Gauss-Divergence Theorem

$$\int_{CV} \text{div}(\Gamma \text{grad} \phi) dV + \int_{CV} S_p dV$$

$$= \int_A n \cdot (\Gamma \text{grad} \phi) dA + \int_{CV} S_p dV$$

d phi by dx at the east face. So, here I have to estimate or approximate the value d phi by dx at the east face. And that is best done by if you now apply those concept of backward difference, forward difference or the central difference. So, in this case what happens that if we apply this the central difference that two neighbor points we consider here that phi E minus phi P divided by the distance between these two.

Similarly, d phi by dx on the waste phase we can estimate this as phi p minus phi capital W divided by delta x W p. So, this is the point here we are introducing approximation from the Taylor series expansion and here is the part that we discussed earlier that numerical errors are introduced based on the scheme that you use the discretization scheme either forward backward or the central differencing and accordingly the order of accuracy the prediction accuracy would improve or it may go in a different way So, here that means this part d phi by dx now I can write in terms of phi e minus phi p divided by delta x pe that we just discussed and d phi by dx small w this part

this part is further phi p minus phi w divided by delta x p w capital W. So, each and every we have to approximate in terms of the linear expansion or the linear terms. Once we do that and further similar to that, we have this term. So we consider S bar delta V is, say can be written in this way, not W, W is already there. say SU, it has two component, it can have two component.

One is independent of phi, that is not dependent on the term, but the other SP, the source term can be dependent on the phi P. So the overall generation in absence of any dependency of the phi, can be a constant value or it can be dependent on the phi p. So, in several problem, only this part remains that there is a constant volumetric source term. It may happen in some complex problem, there will be some additional source term. Now, source term in this finite

volume method will have another meaning that we will see later. The source term, when we try to segregate in this manner, the variables or the parameter or the coefficients that we can segregate, we will see that later,

that during segregation of variables, there will be several terms that are associated with ϕ_p . And we will call that also as source term, but not the actual source term, but a kind of a pseudo source term that appears during the solution of the problem. So now the final step is that we go back to the previous equation, or this equation, or this integration equation, and then we plug in all this simplified values. or the simplified expression. And then we find out that what is my ϕ_p . We write an expression for the ϕ_p . After replacing these terms here in this expression or this equation,

we will segregate the coefficient of ϕ_p and the other terms to find out what is the value of ϕ_p . Because that is our point of attention at p , what is the value of ϕ_p . And accordingly, we solve for the ϕ_p . So with this introduction, which we will take it to the next lecture also, because this is yet not has been completed, we will now put some numerical values on these parameters and we'll see that how it actually happens and how much it deviates when we compare this result with the analytical solution. So with this, I stop here today and thank you for your attention.