

Modeling of Tundish Steelmaking Process in Continuous Casting
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Lecture - 28
Finite Volume Method for Convection and Diffusion Problems

Welcome to the lecture on Finite Volume Method for Convection and Diffusion Problems. So, as we discussed in our last lecture, we talked about the different numerical methods and typically we will be talking about the finite volume method which is normally used for solving the problems, which take place you know which discusses about the cases in the steelmaking you know practices.

So, you will be talking about the finite volume method and its aspects you know different you know aspects which are to be taken into consideration, when we deal with the convection and diffusion problems. Because we have seen while dealing with these you know equations of the navier stokes equations or so, what we see that you have especially you have the convection term as well as the diffusion term.

So, apart from that you will have one term related to time and then you will have the terms related to pressure on the right hand side as well as the source term. So, that is how the you know overall you know shape of the you know equation is like. So, we will see that when you have the convection terms and also the diffusion terms, both you know into the governing equation then how this finite volume method will be working and what were those considerations which need to be taken to solve these problems.

So, going to the finite volume method for the diffusion you know problems, now we will be talking about the you know convection as well as the diffusion problems in the in that case.

(Refer Slide Time: 02:25)

Finite volume method for diffusion problems

Following equation is a simple transport equation for property Φ

$$\text{div}(\rho \mathbf{u} \phi) = \text{div}(\Gamma \text{ grad } \phi) + S_\phi$$

Formal integration over a control volume gives

$$\int_A \mathbf{n} \cdot (\rho \phi \mathbf{u}) dA = \int_A \mathbf{n} \cdot (\Gamma \text{ grad } \phi) dA + \int_{CV} S_\phi dV$$

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So, here its not about diffusion problems only, but it is about the convection as well as diffusion problems. So, you will have the one equation will be $\text{div}(\rho \mathbf{u} \phi) = \text{div}(\Gamma \text{ grad } \phi) + S_\phi$. So, this is the you know the convection term and this is talking about that terms related to convection and this is the about the diffusion you know and then you will have the source term. So, what you do is that, when you are integrating formally this equation over the control volume.

So, in that case, you will have once you integrate it. So, it will be n times $\int_A \mathbf{n} \cdot (\rho \phi \mathbf{u}) dA = \int_A \mathbf{n} \cdot (\Gamma \text{ grad } \phi) dA + \int S_\phi dV$. So, that is how you can you will have that is by the rule, you can write that once you do it over the control volume, that can be expressed in this form.

So, accordingly you will have the equation coming like $\int_A \mathbf{n} \cdot (\rho \phi \mathbf{u}) dA = \int_A \mathbf{n} \cdot (\Gamma \text{ grad } \phi) dA + \int S_\phi dV$. So, if you talk about the one-dimensional form you know one dimensional control volume that is what we have earlier.

(Refer Slide Time: 03:56)

Steady 1D convection and diffusion

In the absence of sources, steady convection and diffusion of a property ϕ in a given one-dimensional flow field u is governed by

$$\frac{d}{dx}(\rho u \phi) = \frac{d}{dx} \left(\Gamma \frac{d\phi}{dx} \right)$$

The flow must also satisfy continuity

$$\frac{d(\rho u)}{dx} = 0$$

Control volume around node P

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3

You know discuss this one dimensional control volume, you will have the node p here and you will have the west face as well as the east face and say accordingly you will have the distances δx small w capital P and capital P small e that is between the node p and the phase these are the distances. So, apart from that so, you will have the equation $\frac{d}{dx}(\rho u \phi) = \frac{d}{dx} \left(\Gamma \frac{d\phi}{dx} \right)$.

So, that will be normally when you do not have the source term in that case if you go for that equation. So, you will have the expression you can write $\frac{d}{dx}(\rho u \phi) = \frac{d}{dx} \left(\Gamma \frac{d\phi}{dx} \right)$ that will be coming from you know this, you know equation and also the flow has to satisfy the equation of continuity. So, in that case $\frac{d}{dx}(\rho u) = 0$. Now, what you see, what you have seen earlier where we have seen that you have found the control volume and again do you have once you have this equation. So, the equation must be rewritten further for the control volume.

(Refer Slide Time: 05:19)

Steady 1D convection and diffusion



- ❖ Integration of transport equation over the control volume gives

$$(\rho u A \phi)_e - (\rho u A \phi)_w = \left(\Gamma A \frac{d\phi}{dx} \right)_e - \left(\Gamma A \frac{d\phi}{dx} \right)_w$$
- ❖ And integration of continuity equation yields

$$(\rho u A)_e - (\rho u A)_w = 0$$
- ❖ The integrated convection–diffusion equation can now be written as

$$F_e \phi_e - F_w \phi_w = D_e (\phi_e - \phi_p) - D_w (\phi_p - \phi_w)$$
- ❖ and the integrated continuity equation as

$$F_e - F_w = 0$$

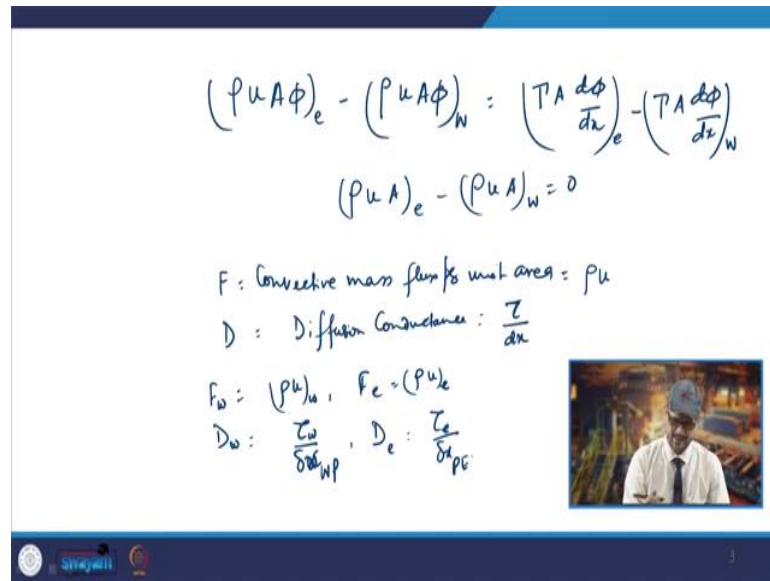
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4

So, if you try to write these do the integration over the control volume, in that case what will happen this $(\rho u A \phi)_e - (\rho u A \phi)_w = \left(\Gamma A \frac{d\phi}{dx} \right)_e - \left(\Gamma A \frac{d\phi}{dx} \right)_w$. So, that is what this equation needs to be solved.

So, that these values you are finding at this and these you know surfaces. So, you are finding at e and as well as w. Similarly for the continuity equation, that equation will yield to $(\rho u A)_e - (\rho u A)_w = 0$. So, what happens that once you have this these two equations, now what we do is that we take these you know you have the this is the convective term representation of the convective. In fact, and this is the representation of the diffusion effect and you take this ρu this ρu will be taken as the F.

(Refer Slide Time: 06:57)



$$(\rho u A \phi)_e - (\rho u A \phi)_w = \left(\Gamma A \frac{d\phi}{dx} \right)_e - \left(\Gamma A \frac{d\phi}{dx} \right)_w$$

$$(\rho u A)_e - (\rho u A)_w = 0$$

F : Convective mass flux per unit area = ρu
 D : Diffusion Conductance: $\frac{\Gamma}{dx}$
 $F_w = (\rho u)_w$, $F_e = (\rho u)_e$
 $D_w = \frac{\Gamma_w}{\delta x_{wp}}$, $D_e = \frac{\Gamma_e}{\delta x_{pe}}$

So, what we do is, we have we can write the equation. So, you will have the equation that is $(\rho u A \phi)_e - (\rho u A \phi)_w = (\Gamma A \frac{d\phi}{dx})_e - (\Gamma A \frac{d\phi}{dx})_w$. So, and then you got the you know $(\rho u A)_e - (\rho u A)_w = 0$ this is based on the continuity equation. Now what we do is you take you know these you have the convection as well as the diffusion terms.

So, what we do is we define two variables F and D . So, F will be the convective mass flux per unit area and we represent it you know. So, we are taking this value as ρu . So, So, we are taking this ρu and similarly the D , this is the you know diffusion conductance and that will be $\frac{\Gamma}{dx}$. So, this way you know you are taking these two terms. So, you know for the.

So, now at these phases when you talk about the F_w . So, it will be ρu_w . similarly you have F_e , it will be ρu_e similarly you will have D_w . it will be $\frac{\Gamma_w}{\delta x_{wp}}$. So, for that you know west phase and similarly you will have D_e it will be $\frac{\Gamma_e}{\delta x_{pe}}$. So, this way you have you are taking that now A will be also A_w as well as A_e and if you take the A_w and A_e as the same one.

(Refer Slide Time: 09:32)

$$\begin{aligned}
 & A_w = A_e \\
 & a_p \phi_p + a_w \phi_w + a_e \phi_e = \frac{(F_e - F_w)}{2} \\
 & F_e - F_w = 0 \\
 & \phi_e = \frac{\phi_E + \phi_P}{2}, \quad \phi_w = \frac{\phi_W + \phi_P}{2} \\
 & a_e \phi_e = \frac{a_e}{2} (\phi_E + \phi_P) \\
 & \left(D_w - \frac{F_w}{2} \right) \phi_P + \left(D_e + \frac{F_e}{2} \right) \phi_P = \left(D_w + \frac{F_w}{2} \right) \phi_W + \left(D_e - \frac{F_e}{2} \right) \phi_E \\
 & a_p \phi_p = a_w \phi_w + a_e \phi_e
 \end{aligned}$$

So, and so, if you take the $A_w = A_e$ and you know we apply the central differencing formula which we have done earlier for the contribution of the diffusive you know diffusion terms. So, then you can see what you see we now you can see that. So, this A term will also vanish.

So, you will have the $F_e \phi_e - F_w \phi_w$. So, that is these two equations are there. So, this because we are taking the $A_w = A_e$ as same. So, you can write that on both the sides A ; A will cancel. So, then that will be equal to. So, that will be $D_e(\phi_E - \phi_P) - D_w(\phi_P - \phi_W)$. So, this is what you get you know once you go and see that you know equation.

Now if you have do you have another equation that is your continuity equation and the continuity equation becomes $F_e - F_w = 0$. So, you know that is how you get this you know these two equations which is found. Now, what we have to do is that you will have how you use because you have the ϕ_e and we need to have this ϕ you know expressed in terms of the you know the node nodal values. So, if you take the central differencing approximation. So, for that we will be talking this you know ϕ . So, we can have this $\phi_e = \frac{\phi_E + \phi_P}{2}$.

Similarly, you can have $\phi_w = \frac{\phi_W + \phi_P}{2}$. So, if you put these you know these values on in that equation. So, and you further do the rearrangement. So, in that case you will be getting the. So, you will be getting $\left\{ \left(D_w - \frac{F_w}{2} \right) + \left(D_e + \frac{F_e}{2} \right) \right\} \phi_P = \left\{ \left(D_w + \frac{F_w}{2} \right) \phi_W + \left(D_e - \frac{F_e}{2} \right) \phi_E \right\}$.

$\frac{F_e}{2}\}\varphi_E$. So, what you see now in this case what you are getting is that you are getting again the φ_P in terms of the φ_W and φ_E .

Now, this is coming because you know this we are getting after rearrangement because in this case F_e into a $\varphi_E + \varphi_P$ by 2. So, basically you are getting this expression from the expansion of this expression $F_e(\frac{\varphi_E + \varphi_P}{2}) - F_w(\frac{\varphi_W + \varphi_P}{2}) = D_e(\varphi_E - \varphi_P) + D_w(\varphi_P - \varphi_W)$

S. So, that is how now if you rearrange this equation. So, you are going to get you know this expression and that is what you see again φ_P will be in terms of φ_W and φ_e now you know if you identify if you did see the coefficient you know in this case where you can write that $a_P\varphi_P = a_w\varphi_W + a_E\varphi_E$.

So, what you see that again in this case a P will be you know this term D_w minus F_w by 2. So, a_P basically will be $a_w + a_F - F_e - F_w$. so, that is what we can write. So, what we see in these cases you get the value of a_P , you get the value of a_w and you get the value of a_E . So, what you get the value of $a_P = a_w + a_E + F_E - F_w$. Similarly in this case a_w we will be getting $D_w + \frac{F_w}{2}$. So,. Similarly this will be $a_E = D_e - \frac{F_e}{2}$. Now, this will be you know this will be a small one.

So, this will be $D_w + \frac{F_w}{2}$ and this is $D_e - \frac{F_e}{2}$ that is what you get and then you can solve them. However, we need to be you know concerned with certain aspects in the case of diffusion problems. Now, what we need to be aware when we deal with these convection and diffusion problems. So, we do the central differencing when we have done with the you know diffusion problems in earlier case, in that in that you can easily take the central differencing scheme.

Where you know you if you have to find the value at the phase you are taking the value at the two sites. So, you will have the east as well as towards the east as well as the west and then you can take the average of them. Now, this has not found to be going well when the numerical solution is done. So, in the case of diffusion problems or convection diffusion problems. So, it has been seen that when the convective effect is more, in that case you need to be careful how you are going, how you are using the discretization you know schemes that you have to know.

So, you know there you we should be you know the discretization scheme which we have to choose, that has to have certain you know properties and the common properties which the discretion schemes need to have are one is the you know conservativeness.

(Refer Slide Time: 17:33)

The image shows a whiteboard with handwritten notes under the heading "Discretization".

- Conservativeness:** This property is listed first.
- Boundedness:** Indicated by an arrow pointing to a mathematical expression:

$$\frac{\sum |a_{ni}|}{\sum a_p'} \begin{cases} \leq 1 & \text{at all nodes} \\ < 1 & \text{at one node at least} \end{cases}$$
- Transferviveness:** Indicated by an arrow pointing to the definition of Peclet number:

$$Pe = \frac{F}{D} = \frac{P \Delta x}{T/\Delta x}$$
- Δx:** Defined as "characteristic cell length (cell width)".
- Diagram:** A schematic showing two adjacent control volumes, each represented by a circle with a dot in the center. The left circle is labeled 'w' and the right circle is labeled 'p'.
- Inset Image:** A small photograph of a man in a white lab coat and a cap, standing in a laboratory setting.

So, you know conservativeness it tells that, because we are dealing with the you know the conserving property of the five when we talk about the control volume. So, what is desired in this case is that the flux you know balance has to be maintained. The flux which is entering from the adjacent phase so, that has to be represented in a consistent manner.

So, suppose you have two adjacent control volumes. So, for first control volume the the west phase will be same as the east phase of the or the east phase of the first control volume will be same as the west phase of the second control volume, and they should be represented by the same amount of flux which is suppose you know getting transferred. So, that needs to be you know that needs to be consistency in that case and there needs to be a conservation you know of the property.

So, that. So, you have to take the discretization scheme in in I mean properly which should so, this you know on this property. Similarly another you know property which a proper discretization scheme has to follow will be the boundedness value; boundedness property and what is seen is that you know there has to be the value has to be bounded by certain and the extreme values.

The suppose you are dealing with a problem of conduction as we discussed, now in that case the value which will be there in the intermediate nodes will be bounded by the you know extreme values. So, you know and that also you know it is seen that you are going to get the meaningful results, when you have the diagonally dominant condition. Because you are getting those you know as you have discussed we will see later, that the discretized equation which we get. Normally you get you know and the; so that you know equations you will have the three terms in one equation and then next on line also you will have the three equations but that points will be changing.

So, you will have a something like a third diagonal type of matrix will be coming up and then you will have a corresponding solver also. Now in that case what has been shown that depending upon the coefficients which is there of the neighboring node and which is there of the side nodes of the parent node that is p.

So, that basically shows you know the property that is also one of the desirable property you know for the that is a sufficient condition for the convergent iterative methods, which otherwise it will be diverging. So, for that the condition is that your summation of the these neighboring you know nodes $\frac{\sum a_{nb}}{\sum a'_p}$ we are taking because we are taking that contribution from the source term also.

Now if this has to be you know it has to be less than equal to 1 at all nodes and it will be less than 1 at one node at least. So, what happens that you know this a'_p this is the net coefficient of the central node that will be $a_p - S_p$. So, that is why it is a'_p , it is written as and this n v is the basically neighboring nodes. So, you are taking the summation of all the neighboring nodes. Now what you see that it will less than 1. So, it means you know what we see is that the if that differencing scheme which you are taking and if it is giving you the meaningful result.

So, in that case the criterion will has to be satisfied and for that the resulting matrix of the coefficient will be the diagonally dominant one and for that you have to have the larger value of this a'_p . So, a'_p is $a_p - S_p$ and that is why many a times what we do is that, we take the S_p in such a manner that S_p has the negative value. So, that $a_p - S_p$ so, that will be adding. So, you will have the diagonal dominance and the diagonal dominance is desirable for the boundedness you know property boundedness criteria. And this property

tells you know this boundedness property tells that the value of the property ϕ , it should be you know bounded by its boundary values.

So, you know in the. So, in the case of study state you know as we discussed in those cases if its not so, it will be you know changing, it will be going above the boundaries that will be unrealistic in fact. So, this is you know the one of the other property which is there also you know the sign of the coefficients also you know matters. So, it should have all the coefficients would have the same sign. So, that is another you know property.

Then the next property which is also very important property when we talk about the convective type of problems. So, it is the transportiveness. Now, it is the you know transportingness is the property of the fluid and for that you know what is done is that you know when there is a fluid flow. So, it will be moving from supposed from the west towards the east or maybe from east towards the west.

So, you will have the effect you know when there is a you know largely convection oriented flow, then diffusion or it may be you know what is the order. So, it may be diffusion dominated flow or it may be convection dominated flow. So, you know for you know to understand or to properly you know model you know the such kind of flow, you define one dimensionless you know numbers dimensionless cell peclet number and that is defined by Pe and it is the ratio of $\frac{F}{D} = \frac{\rho u}{\Gamma/\delta x}$.

So, this peclet number is basically. So, δx is the characteristic you know cell width characteristic length. So, that is cell width. So, you will have you know the. So, you have one note towards the w and I mean towards the west and one note towards the you know east. Now, what happens what we mean to know in these cases that when you have a convection dominated flow, in that case you if you take this central differencing rule if you try to have the property at the point, as the average of the property at these two extreme streams.

So, in that case it will not give you the realistic result. Now you know when you have now when you have these this situation will be there. So, when the peclet number is 0 it means that it is purely diffusion type of you know situation, in that case if you take the you know contours of you know constant variable. So, in that case you can have this p as the effect of both the on this side w and p comes into picture.

Now, if you have a you know you know purely convective type of flow, when the peclet number is very high or outward tending towards the infinity, in that case you know the flow will be. So, the if you find these what you see is that if you this is the w. So, it has more effect on p and rather this e has less effect on p because it will be governed by these you know upstream values.

So, it will its value will not be governed by here, but it has bearing of this value. So, so what is they are. So, based on that so, if you take the central differencing you know schemes in these cases these central differencing schemes are not going to give you the proper results in these you know convection dominated cases.

So, what has been seen that if you look at the terms of the a_w and a_e and a_p in the case of the study is this convection diffusion problem, what you have seen that you know at a_e is $D_e + \frac{F_e}{2}$. Now, what is happening that if you see the ratio of f e $\frac{F}{D}$ is the you know it is the peclet number. Now if $\frac{F}{D}$ is more than 2. Now if you look at the $\frac{F}{D}$ value which is more than two in that case that term that coefficient becomes negative.

And then that will be affecting these boundedness property of the you know. So, the condition which we have discussed your constant this coefficient becomes negative whereas, in normal case what we discussed that it should be positive you know. So, because that also affects because it will be positive. So, one since increase will also affect the increasing on the 2 or less than 2, it has you know its bearing and that is why many a times we need to be carefully. Now depending upon these peclet numbers you will have to have the selection of the proper difference in schemes.

So, in our coming lectures we will be talking about the different schemes discretization schemes which are used you know to take into account this effect like the convection effect or so, ah. So, that the numerical results which you are getting it does not so, unrealistic results. So, that is why you have because when we talk about the convection dominated flow, in that case there are schemes like upwind scheme. So, in that case the if you have to define the value at the west cell phase, the value of at the western node has to be taken at as the value at the west cell phase.

Whereas in normal case we take the average of the west cell phase $\frac{\phi_P}{2}$. So, that is in the central differencing scheme. So, that is why you have the upwind scheme, then we have

also other type of schemes like quick scheme or habited scheme. So, these schemes are taken to take care of this transportiveness property in the case of convection diffusion type of problems so, that we will see in our coming lectures.

Thank you very much.