

CFD APPLICATIONS IN CHEMICAL PROCESSES

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Lecture 28: Pressure-velocity coupling

Hello everyone welcome back with another lecture on CFD application in chemical processes. We are discussing velocity and pressure coupling and how to resolve that in the finite volume by the process of finite volume method. So, in the last lecture we started discussing this that the utility of understanding this concept because the problems that we will have in hand is essentially where we will see that we have to simultaneously solve for the velocity field as well as the pressure field or at least the information of pressure has to be known from the given problem.

So, here in the last lecture we have shown that if we go by the conventional process that we have understood earlier for the finite volume method implementation that the velocity pressure everything would be calculated or would be stored at a particular fixed point which is the conventional nodal points what can be the issues in certain cases. with an example of say oscillatory pressure profile where the calculation of the velocity or the pressure gradient at the same location could result into some meaningless or not the actual pressure information that could provide. So, to avoid that we have seen what is staggered grid.

$$\frac{\partial}{\partial x}(p u) + \frac{\partial}{\partial y}(p v) = \frac{\partial}{\partial x}(\mu \frac{\partial u}{\partial x}) + \frac{\partial}{\partial y}(\mu \frac{\partial u}{\partial y}) - \frac{\partial p}{\partial x} + S_x$$

$$\frac{\partial}{\partial x}(p u) + \frac{\partial}{\partial y}(p v) = \frac{\partial}{\partial x}(\mu \frac{\partial u}{\partial x}) + \frac{\partial}{\partial y}(\mu \frac{\partial u}{\partial y}) - \frac{\partial p}{\partial x} + S_x$$

$$\frac{\partial}{\partial x}(p u) + \frac{\partial}{\partial y}(p v) = 0$$

$$\frac{\partial p}{\partial x} = \frac{P_E - P_W}{2 \Delta x}$$

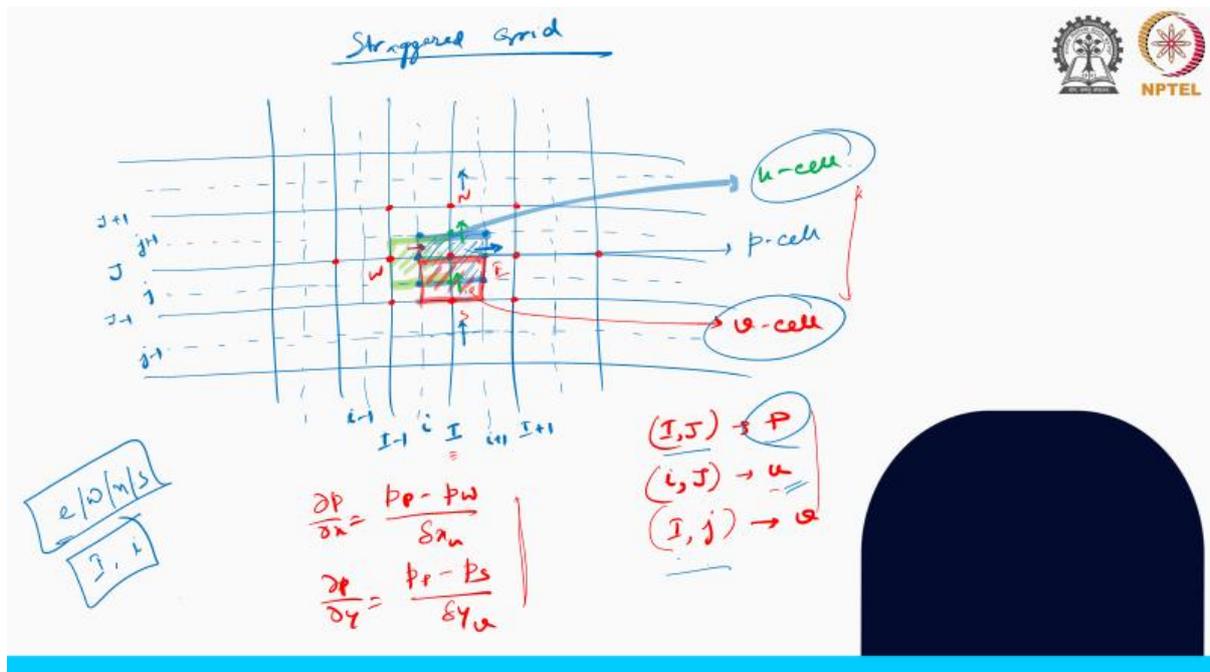
$$\frac{\partial p}{\partial x} = 0$$



how it is formed, what is the scalar cell or the P cell that we call here. So, if you this blue cell that we used here is essentially the scalar cell which is the conventional control volume that we had done so is the P cell. the green one was the U cell and the red one was the V cell and how it can be formulated. So, with that concept we have discretized the momentum equation. We have seen one example of it that how that the convention of east, west, north, south was replaced by the capital I and small i this sign convention.

So, that it does not it is not further complicated we understand how this process we can go iteratively. The conventional grid lines that you see are designated by capital I and J lines. And the control volume faces are enclosed by these small i and j points, j lines, small j, or the small i, the i and the j with the lowercase letters. So, that means the intersection of capital I and capital J is the conventional grid point where the scalar quantities are stored or calculated, and the intersection of small i capital J or capital I small j at this intersection accordingly we find the u component velocity or the v component velocity for this two-dimensional example.

Now, with that concept illustrated, I have shown you a bit of derivation on how we can write these terms f, which we earlier knew as f e, f w, or d e, d w. So, these quantities are then expressed in terms of i and j. And with that, we have seen the discretized form of, say here, the u and v momentum or the x or y momentum equation. So, on that note, we stopped at the last lecture. Because it is essential for you to understand that there can be several different conventions of writing this P cell, U cell, or V cell.



But essentially, the point is that with the help of that staggered formation, we can avoid this checkerboard formation or the checkerboard kind of scenario where the oscillatory pressure

profile exists. We can accurately capture the information that is happening in the domain. And the point is that with that, we can discretize. We have seen we can discretize this set of momentum equations, and then we have to solve those with the Now, today we will discuss different processes of the algorithm by which we can solve this set of equations. Because we have now discretized, but still those are coupled because not only do we have to solve this.

At the same time, we have to satisfy the continuity equation as well. So, we will start with one of the algorithms, very popular or, in fact, the most commonly used algorithm in several CFD solvers, or to start with, to understand the velocity-pressure coupling, how it is resolved, we would start with an algorithm called SIMPLE. Which is coming from the semi-implicit method for pressure-linked equations. So, simple is the acronym for semi implicit method for pressure linked equation.

Now, this algorithm was developed by Patankar whose one of the books I showed you as the reference book. So around in the 1972, he developed this algorithm to resolve this velocity and pressure coupling for the staggered grid formation or for the staggered grid formulation. Now, what is done here, we illustrate with a two-dimensional case. So, what is done that for this kind of governing equations or the discretized equations after it is discretized by the finite volume method, what is done is that at first a guess value we have to set for the solution domain. that what can be a say pressure field, a guess pressure field and that can be your say initial value throughout the domain.

So, that is the first case you are doing for the start of the algorithm and then with that pressure field we solve the discretized momentum equation. So, discretized momentum equations that the form that we have seen this are solved with the help of this guess value at each and every location. So, if this P in these equations are replaced by a guess value, then what would happen that a velocity field would be generated based on this guess value. and how it would look like the equation. So, this is the equation that we will write it once again with the gas pressure field which is ρ of u , ρ .

$$a_{i,j} u_{i,j} = \sum a_{nb} u_{nb} - \frac{P_{i,j} - P_{i-1,j}}{\Delta x} \Delta V + S \Delta V$$

$$a_{i,j} u_{i,j} = \sum a_{nb} u_{nb} + (P_{i-1,j} - P_{i,j}) + b_{i,j}$$

$$D_w = \frac{\Gamma_{i-1,j}}{\alpha_i - \alpha_{i-1}} \quad D_e = \frac{\Gamma_{i,j}}{\alpha_{i+1} - \alpha_i}$$

$$D_s = \frac{\Gamma_{i-1,j} + \Gamma_{i,j} + \Gamma_{i-1,j+1} + \Gamma_{i,j+1}}{\rho(\gamma_i - \gamma_{i-1})}$$

$$D_n = \frac{\Gamma_{i-1,j+1} + \Gamma_{i,j+1} + \Gamma_{i-1,j} + \Gamma_{i,j}}{\rho(\gamma_{j+1} - \gamma_j)}$$

$$a_{i,j} u_{i,j} = \sum a_{nb} u_{nb} + (P_{i-1,j} - P_{i,j}) A_{i,j} + b_{i,j}$$

$$a_{i,j} u_{i,j}^* = \sum a_{nb} u_{nb} + (P_{i,j} - P_{i,j}^*) A_{i,j} + b_{i,j}$$

In the top right corner, there are logos for IIT Bombay and NPTEL. A blue circle contains the text $f_e - f_w$ and $D_e - D_w$. A blue vertical line is on the left side. A blue arrow points from the final equation to the right.

Now, this is the value that is being calculated based on this guess pressure field, which is the A neighbour point, U neighbour point again, all the neighbouring point velocity would be calculated based on this pressure field, because we have assumed So, this is the ij v_{ij} . So, similarly we will have the The y momentum, which is which would start with this capital I small j, is equal to summation. I_j minus 1 I_j plus B capital I small j. So, with the gas pressure field or the initial gas, we will have this set of momentum equations.

Now, say if we had this is the actual field or this is the actual answer. Then the difference between this equation or these equations with these essentially results in the correction that we require from this guess value, which means with the guess, it is not the actual solution. So, the difference between the guess and the actual is essentially the correction that we require. So, if we subtract this respective equation of the x momentum and the y momentum of this guess from the actual one and we define the correction as P prime, that means if I add or subtract depending on the value of P prime and its coefficient.

positive or negative. So, essentially this is my actual pressure; it should have been the actual result, and this is the guess value, and this is the correction. Actual and this is the guess. So, similarly, what will happen is that if I have the actual value u then it is essentially what we have calculated with the help of P star plus some correction. If the correction is 0, that means we have in the first iteration, we have assumed the actual value and it is solved correctly, but that does not happen.

$$D_u = \frac{\rho_{i,j-1} + \rho_{i,j} + \rho_{i,j+1} + \rho_{i,j}}{4(\alpha_{i,j} - \alpha_{i,j-1})}$$

$$D_v = \frac{\rho_{i,j-1}}{y_j - y_{j-1}}$$

$$D = \dots$$

$$f_u = (\rho u)_u$$

$$f_v = (\rho v)_v$$

$$f_u = (\rho u)_u = \frac{f_{i,j} + f_{i,j-1}}{2} = \frac{1}{2} \left[\left(\frac{\rho_{i,j} + \rho_{i,j-1}}{2} \right) u_{i,j} + \left(\frac{\rho_{i-1,j} + \rho_{i,j}}{2} \right) u_{i-1,j} \right]$$

So, the initial guess may be some wild guesses, but at least if it is in the near about region, the number of iterations are less, and the convergence would be much faster. So, similarly, we define u and v where these primes are the corrections for the u and the v. Now, as I mentioned, how do we estimate these corrections? How many corrections do we require? If we subtract this equation, these respective x and y momentum from the actual one, what would result is that a small capital J minus u i capital J minus u star small i capital J is equal to the summation of

u nb minus u nb star plus p i minus 1 j minus p star i minus 1 j minus of p ij minus p star ij multiplied by a ij. So, this is essentially a ij small j a capital I and sorry a capital I small j and this one is a small i capital J. So, similarly for the y momentum we will have A capital I small j. multiplied by V capital I small j minus V star capital I small j is equal to the summation of a neighbor point coefficients V neighbor point values in V plus in the pressure similar to this that P

i j minus 1 minus P star i j minus 1 minus P i j minus P star i j multiplied by a capital I small j. So, we have x momentum. and this is the Y momentum. And now if you look at this the definition of this, these are essentially these P primes V primes U prime. So, in short because this is the actual minus the guess is essentially the correction that we require.

So, respectively you can look at this V and also the P terms. So, what I can write in further compact form is that a small i capital J is the with u prime which is the correction we require is essentially a nb u prime nb plus p prime i minus 1j minus p prime ij multiplied by the area a small i capital And similarly, for this p prime ij minus 1 minus p prime ij multiplied by capital

I. So, this is the form we get for the correction values for the u prime and b prime. We understand how much correction we require.

SIMPLE [Semi-Implicit Method for Pressure-Linked Equations]
Patankar (1976)




Pressure field $\rightarrow P^D$

$$a_{i,j} u_{i,j}^* = \sum a_{nb} u_{nb}^* + (P_{I-1,J}^* - P_{I,J}^*) A_{i,j}^+ - b_{i,j}^-$$

$$\equiv a_{I,j} u_{I,j}^* = \sum a_{nb} u_{nb}^* + (P_{I,J-1}^* - P_{I,J}^*) A_{I,j}^+ - b_{I,j}^-$$

$$P = P^* + P'$$

actual \downarrow guess \downarrow correction

$$u = u^* + u'$$

$$\varphi = \varphi^* + \varphi'$$

u prime

$$a_{i,j} (u_{i,j} - u_{i,j}^*) = \sum a_{nb} (u_{nb} - u_{nb}^*) + [(P_{I-1,J} - P_{I-1,J}^*) - (P_{I,J} - P_{I,J}^*)] A_{i,j}$$

u prime

$$a_{I,j} (u_{I,j} - u_{I,j}^*) = \sum a_{nb} (u_{nb} - u_{nb}^*) + [(P_{I,J-1} - P_{I,J-1}^*) - (P_{I,J} - P_{I,J}^*)] A_{I,j}$$

Now, the point here is simple. We consider these terms, or say, before we do that. So, what do we do? We go into now if we look at how this is solved. The assumption we make here is that we simplify these equations further. We simplify these equations further and consider that these parts of the momentum equations—this summation of the neighbor coefficients—are negligible, or we omit this, OK?

So, what we end up with is not considering these terms further for the SIMPLE algorithm and by doing what we have. If we now look at this u prime to find out how much is the u prime i small j, by looking at this expression, what I get is d. I will define this term. But essentially, this is p prime capitalized mol j. What I get is an expression of this where d small i capital J is essentially a small i capital J divided by a small i capital J. So, this coefficient of U prime is the denominator, and the numerator you have this area of this shape.

The V prime capital I small j is again, say, d capital I small j times P prime capital I j minus 1 minus P prime I j. This is the expression where d capital I small j equals a capital I small j divided by small a capital I small j. So, dropping these terms—the neighbor coefficient, the summation of the neighbor coefficient—its influence Omitting this is the major assumption or approximation for applying this simple algorithm. So, once I have this correction term, which means my actual u

is essentially $u_{i,j}^*$ that I assumed or have the guessed value or the value that has been calculated based on the guessed pressure. This $u_{i,j}^*$ was calculated based on the guessed pressure field. So, this guess plus my $u_{i,j}^*$ is essentially the actual for this node. So, it means now if I replace that, it is $d_{i,j} (p_{i-1,j}^* - p_{i,j}^*)$, ok. So, similarly, my actual $v_{i,j}$

should be $v_{i,j}^*$ which is equal to $v_{i,j}^*$, which is the value that has been calculated by the guessed pressure, plus $d_{i,j}$ multiplied by $p_{i,j+1}^* - p_{i,j}^*$. So, what do I have here? What should have been the actual value or after iteration where I have calculated the corrections? I have corrected my guessed value by the correction, which I consider the actual value, ok. So, I started with p^* , a guessed value. With the p^* and from the discretized equation, I get the $u_{i,j}^*$ or $v_{i,j}^*$ or the first estimated velocity field in both directions for a 2D problem.

Handwritten notes on a whiteboard showing the derivation of velocity corrections in the SIMPLE method. The notes include equations for $u'_{i,j}$ and $v'_{i,j}$, the definition of coefficients $d_{i,j}$ and $d_{i,j+1}$, and the final corrected velocity fields $u_{i,j}$ and $v_{i,j}$. The notes are written in green and red ink. Logos for IIT Bombay and NPTEL are visible in the top right corner.

$$a_{i,j} u'_{i,j} = \sum a_{nb} u_{nb} + (p'_{i-1,j} - p'_{i,j}) A_{i,j}$$

$$a_{i,j} v'_{i,j} = \sum a_{nb} v_{nb} + (p'_{i,j+1} - p'_{i,j}) A_{i,j}$$

SIMPLE \leftrightarrow Major Approx.

$$d_{i,j} = \frac{A_{i,j}}{a_{i,j}}$$

$$d_{i,j+1} = \frac{A_{i,j+1}}{a_{i,j+1}}$$

$$u'_{i,j} = d_{i,j} (p'_{i-1,j} - p'_{i,j})$$

$$v'_{i,j} = d_{i,j+1} (p'_{i,j+1} - p'_{i,j})$$

$$u_{i,j} = u_{i,j}^* + u'_{i,j} = u_{i,j}^* + d_{i,j} (p'_{i-1,j} - p'_{i,j})$$

$$v_{i,j} = v_{i,j}^* + v'_{i,j} = v_{i,j}^* + d_{i,j+1} (p'_{i,j+1} - p'_{i,j})$$

Annotations: $u'_{i,j}$, $v'_{i,j+1}$, u^*

Now, I have also calculated the corrections, ok. So, which means the correction plus the guess, the first iteration value should be my actual result. Okay. The point is, we have received or estimated a velocity field which we think is correct. But now, how to ensure that? For that, remember that these equations cannot be solved in a standalone manner.

This velocity field also has to satisfy the continuity equation, okay. So, the continuity expression has to be satisfied by this example or by this calculation of $u_{i,j}^*$, the actual velocity field that we have calculated, fine. If that is satisfied, then what we can say is that these are the actual values. So, the point is, once we have calculated $u_{i,j}$ $v_{i,j}$, similarly for all other nodal points for which, I mean, when we look into this expression that is similar

to this. Considering the point that we are considering P , if we shift our attention to the other points, what we will get is the consideration for.

So, similarly, we can calculate say u_{j+1} or, in fact, v_{i+1} , etcetera. So, all the values we can calculate. And with those values, when we replace them in the continuity equation or the discretized continuity equation, what it would result in is an equation where P' has to be calculated. That would be the unknown value. So, which means the continuity equation will then act as a pressure correction equation.

Because if that is satisfied, that has to be zero. The east minus west face is equal to zero. So east minus west plus north minus south for the 3D problem, along with top and bottom. All these, the flux has to be zero, has to be conserved. So if that is conserved and we write for all these nodal points these expressions, what we will find is that we can find these P' values for a particular nodal point.

If that is also zero, that means these values are accurately calculated. But if it is not, it will return a P' value. So that means the initial pressure guess has to be corrected in the next iteration, and again with that corrected P' , we have to calculate U^* , V^* , and the process will continue until we reach a convergence limit for those corrections. So we will continue this to the final step in the next lecture, and we'll show you exactly the algorithm in a tabular form, how it is done.

So for today, thank you for your attention.