

CFD APPLICATIONS IN CHEMICAL PROCESSES

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Week-06

Lecture 30: Pressure-velocity coupling

Hello everyone, welcome back to another lecture on pressure-velocity coupling in the course CFD Applications in Chemical Processes. In the last couple of lectures, we discussed pressure-velocity coupling. How it is implemented through the finite volume method in the solution of unknown velocity and pressure field calculations. In that context, we have seen what the SIMPLE algorithm is. So, in the SIMPLE algorithm, which we discussed last time, it is essentially the Semi-Implicit Method for Pressure-Linked Equations.

developed in 1972 where we started with a guess pressure value and then with that guess pressure value we calculated the velocity field which is further corrected those corrected velocities were used in the continuity equation because the corrected velocities are supposed to satisfy the continuity equation, and then what happens is the continuity equation becomes the pressure correction equation. If there is any imbalance it results in form of the pressure imbalance or the pressure correction term and that pressure correction was then further used to correct the velocities and show the loop continuity. So, that was the algorithm for the SIMPLE case that we discussed in the last lecture—in fact, the last two lectures.

SIMPLE [Semi-Implicit Method for Pressure-Linked Equations]
Patankar 1972




Pressure field $\rightarrow P^*$

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

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

$P = P^* + P'$
 actual guess correction

$u = u^* + u'$

$v = v^* + v'$

2. pressure

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

1. mass

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

So, in that context, we discussed another important parameter called the under-relaxation parameter, why it is useful, and how a typical algorithm for SIMPLE works. Now, as I told you, there have been further refinements and developments based on this SIMPLE algorithm. So, later Patankar again came up with a strategy which is based on simple, but it is called simple R which stands for the simple with revised. So it is the simple revised version which is the simple R you would find this algorithm you would find this option to demystify the pressure velocity coupling in the CFD solvers But what it does is essentially follow the same steps as we have seen in the SIMPLE algorithm. However, here, instead of calculating or correcting the pressure through the continuity equation, the continuity equation becomes a discretized

pressure equation. So, the continuity equation eventually becomes a discretized pressure equation instead of calculating the pressure correction. So, that means the pressure field is directly obtained. Without this pressure correction and velocities, but the velocities are still corrected through the velocity corrections that we have seen earlier. So, what it means is that earlier, if you remember, if you go back here, you would see that we had this form of the expression.

Handwritten mathematical derivations for the SIMPLE algorithm:

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

$$a_{I,j} \phi'_{I,j} = \sum a_{nb} \phi_{nb} + (P'_{I,j-1} - P'_{I,j}) A_{I,j}$$

These equations are labeled as **SIMPLE** Major Approx.

$$u'_{i,j} = d_{i,j} (P'_{I-1,j} - P'_{I,j}) \quad d_{i,j} = \frac{A_{i,j}}{a_{i,j}}$$

$$\phi'_{I,j} = d_{I,j} (P'_{I,j-1} - P'_{I,j}) \quad d_{I,j} = \frac{A_{I,j}}{a_{I,j}}$$

Final corrected velocity and velocity correction formulas:

$$u_{i,j} = u^*_{i,j} + u'_{i,j} = \bar{u}^*_{i,j} + d_{i,j} (P'_{I-1,j} - P'_{I,j})$$

$$\phi_{I,j} = \phi^*_{I,j} + d_{I,j} (P'_{I,j-1} - P'_{I,j})$$

Additional handwritten notes include $u_{i+1,j}$ and $\phi_{I,j+1}$ with arrows, and a circled u^* .

To calculate the velocity corrections or, specifically, the discretized momentum equation looks like this form. So, here again, if we look at the discretized momentum equation, one typical example if we look at it. Divided by K_{ij} plus, so this was the form for which we wrote in terms of D capital I and V capital I small j was. So, in a simpler algorithm, what happens is that instead of correcting the pressure through the continuity equation, the continuity itself becomes a discretized pressure equation or equation for the pressure, and here that means in this simpler algorithm, one pseudo velocity is calculated.

And that pseudo velocity is this part, say here in this case, it is. And V capital I small j, capital I small j. So, these are the pseudo velocities that are defined here. Now, instead of correction, So, what U_{ij} becomes then is this pseudo velocity plus D_{ij} , as we know this term is the $D_{ij} P_i$ minus 1 capital J minus P_{ij} , and V capital I small j becomes. Minus 1 p ij, and then this is used in the continuity equation, OK.

And the continuity equation then acts as a discretized pressure curve, and then from there, once we have this pressure field. So, that is then used as the new pressure value and subsequently the discretized momentum equation is solved and the loop continues. So, essentially in simpler algorithm what happens that in simpler or simple R what happens that we start. with the initial P^* , U^* , V^* , and any other scalar quantities required for calculation. And in step 1, what is done is we calculate the pseudo velocities.

Handwritten notes and a grid diagram illustrating the derivation of the pressure equation in a finite difference method. The diagram shows a grid with nodes labeled $I-1, I, I+1$ and $J-1, J, J+1$. It includes equations for continuity and momentum, and defines coefficients a and b for the pressure equation.

Continuity equation (summed over faces):

$$\left[(P u A)_{i+1,j} - (P u A)_i \right] + \left[(P v A)_{i,j+1} - (P v A)_{i,j} \right] = 0$$

Momentum equation (x-direction):

$$a_{I,J} p'_{I,J} = a_{I+1,J} p'_{I+1,J} + a_{I-1,J} p'_{I-1,J} + a_{I,J+1} p'_{I,J+1} + a_{I,J-1} p'_{I,J-1} + b_{I,J}$$

Definition of coefficients:

$$a_{I+1,J} = (P u A)_{i+1,j}$$

$$b_{I,J} = (P u^* A)_{i,j} - (P u^* A)_{i+1,j} + (P v^* A)_{i,j} - (P v^* A)_{i,j+1}$$

The diagram also shows velocity profiles u and v at the faces, and a pressure correction p' at the center node.

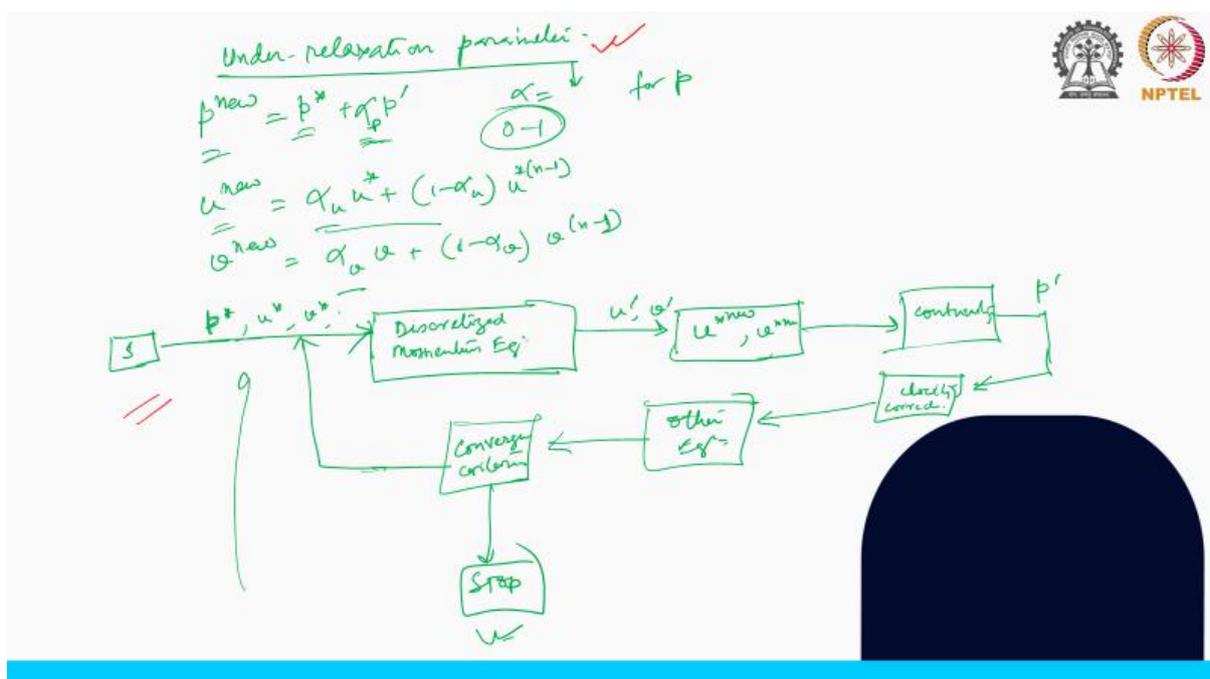
which means u hat, v hat, these terms, okay, based on the expressions we have seen. So with those values of ij , corresponding ij , we solve in step two the pressure equation. which means we calculate the pressure equation by going back to the continuity equation. Like exactly the point that I have shown that with these values we feed into the continuity equation and we come up with the format that is $A p$ phi p is equals to $A e$ phi e that kind of a thing that we discussed several times. Once we solve this, we get a pressure field, which is different from the initial pressure field.

So what do we do? We set this P^* as P , and then we go to step three. You can call it step three. And we solve the discretized momentum equations. So, this discretized momentum equation would result in u^* and v^* values because with these values, we then solve the pressure correction equation as we did in the simple case. So then again, we go back to

satisfying the continuity equation, and there we find out what is the—so in step four, we solve the pressure correction equation, which is the P prime. Once it is done, it returns p-prime values. With that p-prime, we correct our velocities with the help of an expression like the one we have seen earlier.

Because this involves u-prime, which includes the expression for p-prime. So, with this, we further correct our velocities. And we get rho again—the quantities we are looking for—while the different phi-star values still remain. So then, with these corrected values and this initial guess of phi (or any other scalar quantities), we solve any other equations that are required. Any other equations' solution.

So, solve any other equations. So, if this is step five, this is my step six. Then we check for the desired quantity's convergence criteria. If it is converged, then we stop. If converged, we stop. If not, we set all these P-star, U-star, V-star with the new calculated values that we have corrected. So, that means my initial guesses are then replaced by these corrected values, and again we follow this loop. Again, we calculate with these corrected or reset values of all the parameters to determine the pseudo-velocity.



And again, we solve the discretized pressure equation to calculate the pressure field. With that pressure field, we solve the discretized momentum equation to calculate the velocity field. That velocity is again supposed to satisfy the continuity equation. If it does not, then that continuity equation which is now in the form of pressure correction equation returns the pressure correction value with that pressure correction we go for velocity correction the velocity corrections and those with those corrected value and the pressure value and any other scalar

quantities we solve any other equations other equations that are required, such as temperature, species transport, concentrations, etc. Then, we look for the desired level of

convergence criteria for our set variable. If it is set or if it is converged, we stop our solution. If it is not, then again it goes back to the complete loop, and the loop starts again. So, this is the simple R algorithm. Okay, which again Patankar actually refined—his initial part—but it came into the range in the year of the 1980s. So, in 1972, he developed SIMPLE. In 1980, it was refined and revised, so SIMPLE-R—where R stands for the revised version—and further around 1984, this SIMPLE was further made more complicated or more robust with the concept called SIMPLEC. We say it together, although there is no space in between. But I wrote it here because this is the SIMPLE part, and then C—that C stands for consistent. So, SIMPLE-R was SIMPLE revised, and SIMPLEC is SIMPLE consistent. So, what is the difference between SIMPLE and SIMPLEC? Here, the point is, if you remember, in the SIMPLE algorithm, we mentioned that we actually dropped these parts, okay.

SIMPLER
SIMPLE-Revised

Continuity Eqⁿ → Discretized Pressure Eqⁿ

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

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

$a_p p_p = a_e p_e + \dots$

$$\hat{u}_{i,j} = \frac{\sum a_{nb} u_{nb} + b_{i,j}}{a_{i,j}}$$

$$\hat{\omega}_{I,j} = \frac{\sum a_{nb} + b_{I,j}}{a_{I,j}}$$

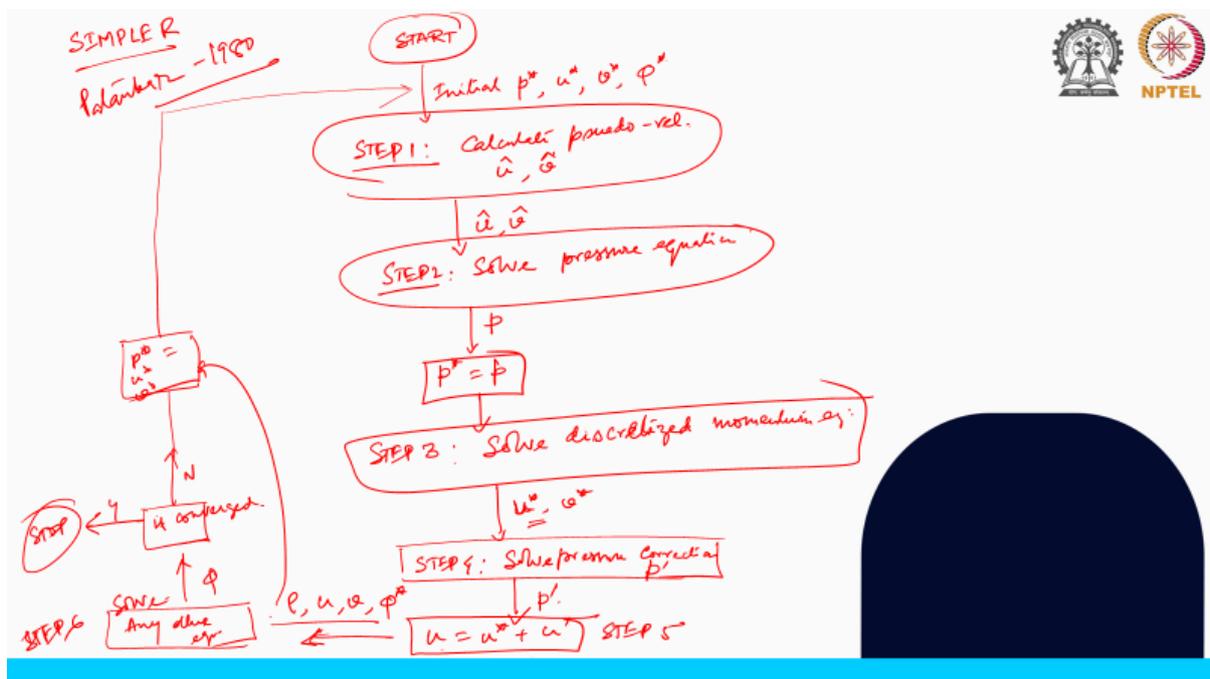
$$\left\| \begin{aligned} u_{i,j} &= \hat{u}_{i,j} + d_{i,j} (P_{I-1,j} - P_{I,j}) \\ \omega_{I,j} &= \hat{\omega}_{I,j} + d_{I,j} (P_{I,j-1} - P_{I,j}) \end{aligned} \right\|$$

So, in the SIMPLE algorithm, in the momentum equation, we actually omitted these parts, considering them less significant. Here, those are retained in SIMPLEC, and then the whole derivations are made once again. So, since the velocity correction here in SIMPLEC becomes $d_{ij} P'_{i-1}$ capital J minus P' capital I capital J, where now here, look at this expression where D_{ij} is essentially A_{ij} and not only A_{ij} but also the coefficients that we dropped earlier. and then the rest process remains same for the simple case.

So, which means for the v prime case similar to this p prime i j minus 1 minus p prime i j this is there where d capital I small j is essentially a capital I small j by A capitalized small j minus summation of the neighbor points coefficients that we dropped in the case of simple algorithm.

So, discretized pressure equations accordingly would be the same except this the value of the d_i part is different. and the rest process the rest sequence is identical to simple algorithm. So, we discussed simple we have seen the details then it was further revised by simple R further there has been development

without omitting any term in simple called the simple C. So, simple R is revised once again and this is consistent C stands for the consistent. similar to this development or this chronological development of this algorithm, there has been several other schemes that actually resolve this velocity pressure or the pressure velocity coupling. Say for example, there is another scheme I will just briefly mention is called the PISO. So, this is called pressure implicit with splitting of operators. It came further later in 1986.



Now here it follows it actually the development of simple where a character step there are multiple character steps instead of only one time corrections by that we see we have seen in the case of simple algorithm. So, what it is done here is that all the steps of simple algorithm are initially followed and then what happens we go for a second round of pressure correction. So, there are multiple correction steps involved even in a single algorithm, even for the pressure. So, the pressure is corrected. So, P prime is further corrected.

We find P double prime, say, with that the velocities are further corrected, and the initial values are replaced by this second-time corrected values, and the rest remains similar to the pressure in the semi-implicit method that we have discussed. So, I hope now the idea is clear for you— how we can actually decouple, I would say, this pressure and velocity, or how, when one field is unknown, the other field is also estimated. So, basically, when both fields are unknown, how we can estimate or how we can predict or calculate this velocity and pressure, and how those

are coupled and how those are resolved. Now, the question may arise: which algorithm should I use?

1989

SIMPLEC → Consistent

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

where $d_{i,j} = \frac{A_{i,j}}{a_{i,j} - \sum a_{nb}}$

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

where $d_{i,j} = \frac{A_{i,j}}{a_{i,j} - \sum a_{nb}}$

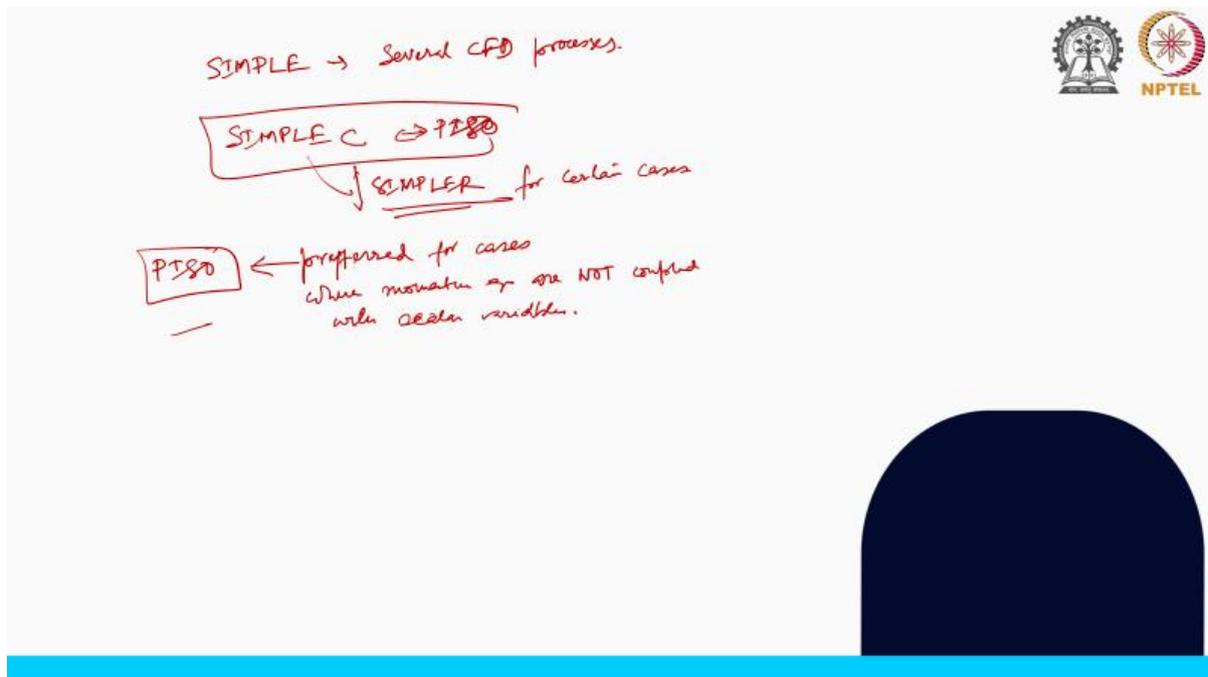
1986 PIISO → Pressure Implicit with Splitting of Operators
 p' is further corrected p''

SIMPLE	
SIMPLER	- Revised
<u>SIMPLEC</u>	- Consistent

NPTEL

Now, this comes with practice. A part of the best practice is that the SIMPLE algorithm is straightforward. It is very commonly used, relatively straightforward, and has been successfully used for several CFD processes. So, if you are unsure of which kind of pressure-velocity coupling algorithm you should start with, start with the SIMPLE algorithm. Now, since no terms are omitted to derive SIMPLER and SIMPLEC, those are supposedly better or more accurate than the SIMPLE algorithm. But again, since the number of calculation steps involved is more than in the SIMPLE algorithm, it naturally requires more time

to solve the same problem than the SIMPLE algorithm—between SIMPLER and SIMPLEC. But the point is, which one is better compared to SIMPLEC or SIMPLER? That is not very clear. And now, here, the point we must remember is that the CFD problem that we solve or try to Most of the time, in fact, all the time, those are actually unique. That has not been done earlier, and that is why you are doing it. But the class of problems may have been solved earlier.



So the point is that you get a recommendation from previous researchers about their experience and accordingly choose these schemes. But typically it has been seen that the simple C. So, based on that experience in fact or the that literature review or literature survey it shows that the simple C and PISO are efficient than simple R for certain cases, not for all cases, but for certain cases, okay. So, for typical some problems it has been seen that simple C or PISO are efficient than the simple R, but it is not generic statement. I mean, categorically, you can say that simple R is always less efficient than simple C and simple PSO algorithm.

The problem is that when momentum equations are not coupled to scalar variable, PISO algorithm have shown better convergence or robust convergence and requires lesser computational effort than the simple R and simple C. So that means PISO is preferred if I can say in other words that PSO is preferred for cases where momentum equation are not coupled with the scalar variables. It shows in those cases, it has been seen from the research that it shows better convergence criteria or better robust convergence than simple C and simple R, okay. So, the point is that we have gotten an overview of different schemes in how to resolve this velocity-pressure So, if you remember the finite volume method, we started understanding it from a one-dimensional steady-state simple diffusion problem, then we augmented it with a source

term, further we added a convection term, then we added an advection term, then further we have seen that now, okay, I do not know also what the velocity field is. So, what would be and how to resolve this velocity and pressure coupling. So, with this understanding, I will stop here today and, in fact, conclude this finite volume chapter that we have been continuing for the last couple of weeks. And in the next lecture, I will move on to another topic, which we will discuss

in the next lecture. So, with this, I thank you for your attention. And we will see you in another lecture.