CFD APPLICATIONS IN CHEMICAL PROCESSES

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Week-06

Lecture 29: Pressure-velocity coupling

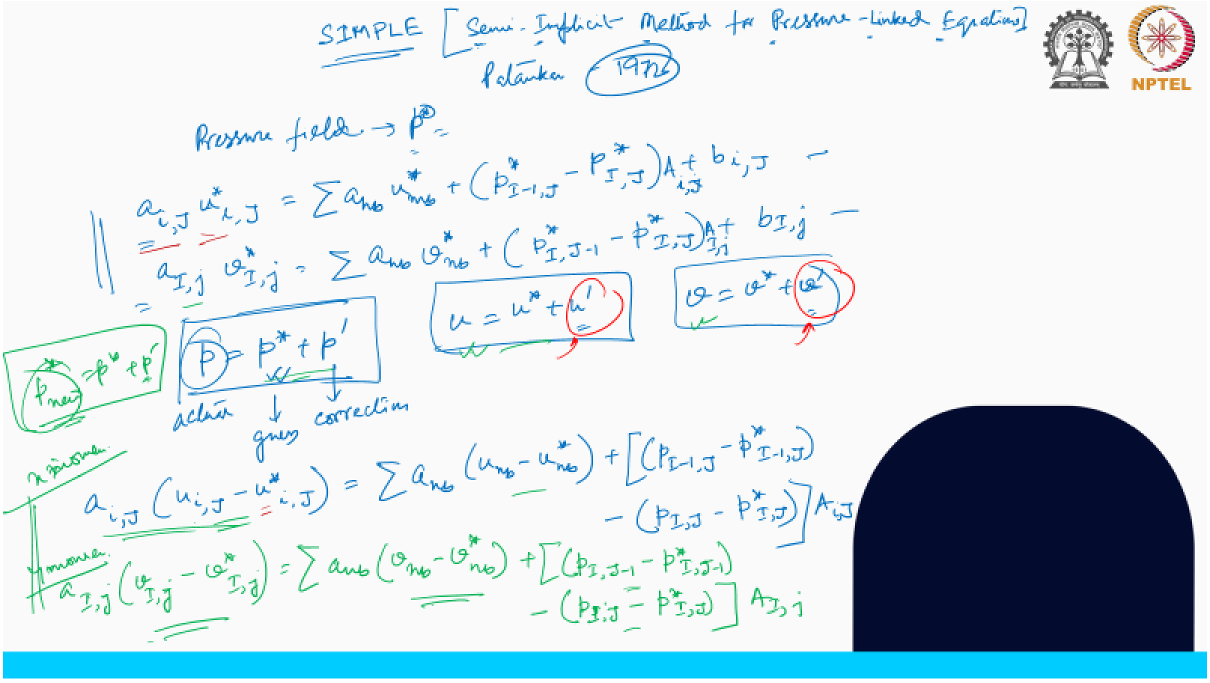
Welcome everyone to another lecture on CFD applications in chemical processes. We are discussing pressure-velocity coupling and specifically the SIMPLE algorithm. So, in the last lecture, we started discussing it, where SIMPLE is the semi-implicit method for pressure-linked equations. The first point in the SIMPLE algorithm is that we start with a guessed value of the pressure or the pressure field, and we pass the whole domain with that value. So, all p-cell values at the centroids are stored by that initial guess or the initial value, and then the iteration starts.

So, what happens is that with that known pressure field, we calculate or we estimate the velocity corrections. So, the point is, with that initial pressure field, we calculate the initial estimate of the pressure or the velocity field. Now, if those are actual, we would require no correction. That means our initial guess of the pressure field is absolutely correct because it matches the exact solution.

But, as I told you, that generally does not happen. So, the point is, we then try to estimate what correction is required for the velocity to satisfy the continuity equation. Because remember, the continuity equation does not contain the pressure variable or the pressures. So, there we have only the velocity; the flux has to be maintained. So, the point is, while calculating these velocity corrections,

we actually find out that we require the pressure corrections as well it is associated with this. Because if the pressure corrections are 0 we essentially reach that the estimated value of the velocity field is the actual velocity field. But the point is when we so and if this is the actual values then it must satisfy the continuity equation. and the discretized form of the continuity equation. So, if I draw a particular scalar control volume or the P cell again.

So, say I have this is my conventional grid and as you know if I consider this is my point P then I actually have the control volume faces like this. So, this is my P cell that is by this dashed line. So, this is my P cell or the scalar cell where all at this nodal point all the scalar quantities are stored or calculated. This is our usual convention that we have seen in several cases. So, this is the south, this is the capital not, this is small s, this is small n.

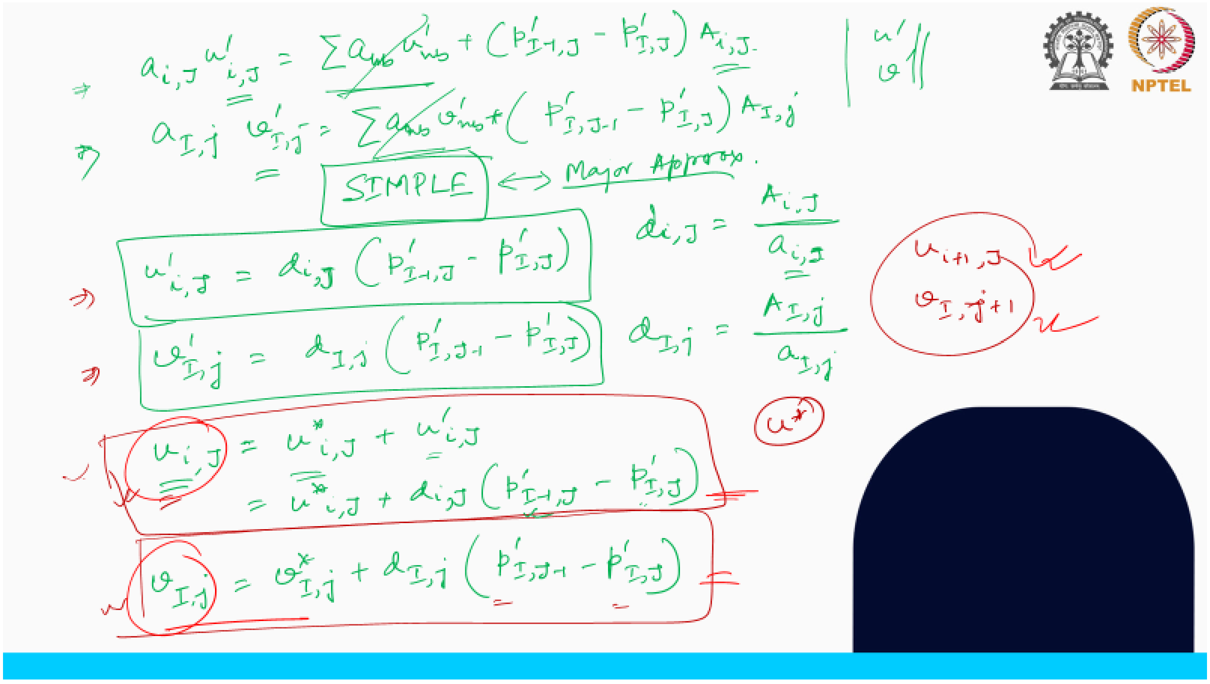


So, here the flux or the differences between this input and output has to be conserved, which means if I try to write now in terms of ij. So essentially, these hard lines, as I told you, are basically capital I and this is the capital J. Say my junction of capital I, capital J is the point P. So it is capital I plus 1, it is capital I minus 1. It is capital J minus 1, it is capital J plus 1. And these cell faces, these imaginary lines, dotted lines or the dashed lines, are essentially is say the small j this one and these are on the i cases say this is the small i. So, this is small i plus 1 and this is small j plus 1.

So, the continuity equation for this control volume. The thing that we can write is essentially rho u a that is i plus 1 capital J that is going out of the system minus which is coming from this west face which is small i and this is the capital J. Plus, similarly for the other face, rho v a that is going out from the north face is essentially I have capital I and small j plus 1 minus rho v a that is going in is capital I and a small j through the south face is equals to 0. So, this summation has to be 0.

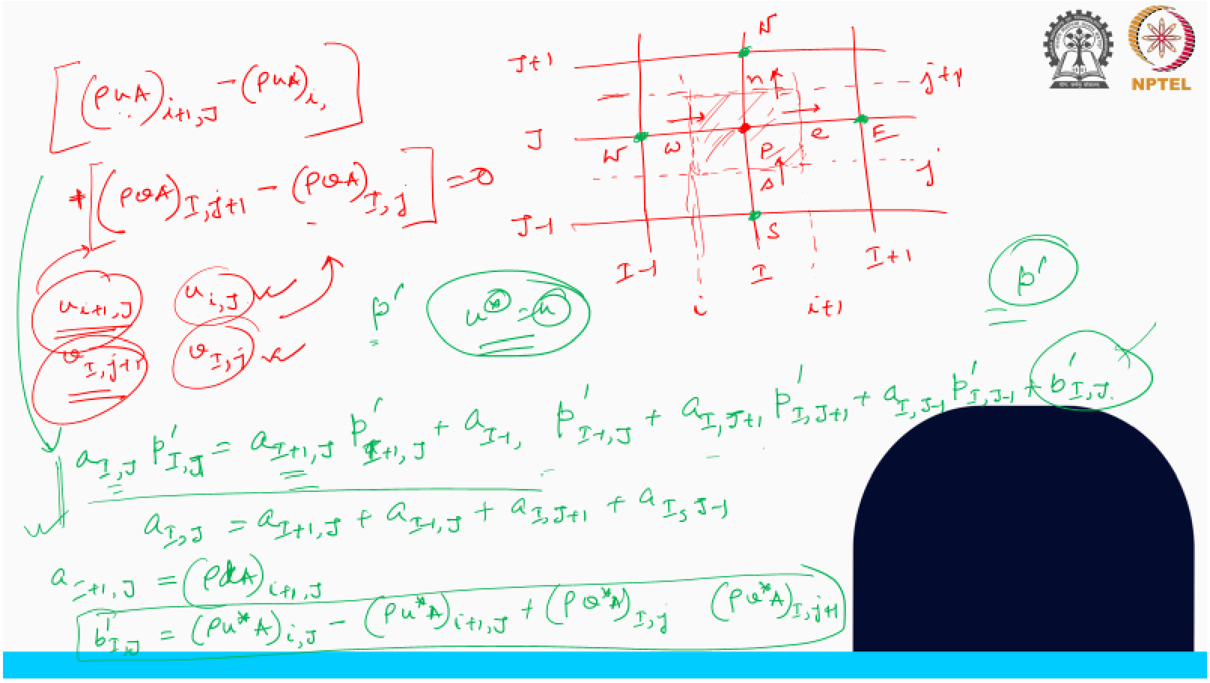
So, now what I see or what we see here, this requires the value of u i plus 1 j, we require u ij. We require v i small j plus 1 and v capital I small j. Now by this formulation, we see that we can calculate u small i capital J. We see that I can calculate or we can calculate v capital I small j By the same manner, we can also calculate u i plus 1 j and v i j j plus 1 analogous to this derivation or this understanding. So, once we calculate these expressions, what we do is we will replace it here. In the moment in the continuity equation, because we now consider that these are the correct expressions or the correct values of the velocity field, so it must satisfy

the continuity equation once we replace these expressions, that means these forms that are there, okay, along with these other expressions in terms of this guess and the correction, and we rearrange it So, what we will see—I am skipping several steps—it is for you to do this: that you write this expression of u ij here, v ij here, and the expression of u i plus small i plus 1j and v ij plus 1. And then you rearrange it to give a form that we have seen that a p phi p is equals to the summation of the neighbor coefficient and the points plus that any source term that appears due to this rearrangement. And if we do so, what we will see? For this particular case is that we will have an expression once we identify the coefficient of P prime because all these expressions will have C the P prime values, okay?



But in this continuity equation, you do not have any pressure term. But because you calculated this U with the initial guess of pressure Here, it comes with the pressure correction term. And it eventually, this equation would look like something like this, that A capital I capital J p prime capital I capital J is equals to a i plus 1 capital J p prime i plus 1 capital J plus a i minus 1

capital J p prime i minus 1 capital J plus a capital i J plus 1 p prime capital i J plus 1 plus a i J minus 1 p prime i j minus 1 remember here I am not saying repeatedly capital or small because this is the expression I am writing for the p prime and eventually it will happen an expression for the p prime and this p prime is nothing but a scalar quantities. So, this i and j would be at this conventional nodal locations which means or these nodal locations conventional points which means these are essentially all capital I capital J intersection either capital I plus 1 capital J plus 1 or capital I minus 1 capital J minus 1 so this is so these are actually all these points on the right hand side okay so this is essentially if you look at it I plus 1 J east point, this is i minus 1 j, this is the west point, this is i j plus 1, this is the north point and this is the south neighbor point.



Now, the point is once we rearrange it and because of this imbalances due to this guess and the corrections, we will have some term that is b prime ij kind of a pseudo source term due to this imbalance. And where we see that aij capital I like the ap expression if you remember is essentially j plus i minus 1 j plus i j plus 1 plus i capital j minus 1 and these coefficients are also again say for example a i plus 1 j is essentially equals to rho d a i plus 1 j. So, similarly all the other expressions can be written and particularly this imbalance B prime i capital J would eventually be consisting these known terms.

That means, this is the values that we have calculated based on the gas pressure field or gas pressure values. It is of small ij minus rho u star a for the point i plus 1j plus rho v star a capital i small j minus rho v star a capital i small j plus 1. This would be the expression for the B prime. So, what it looks like this equation if we consider point ij what it looks like is that this becomes this continuity equation eventually becomes an expression to find out what is the P prime ij or the pressure correction term. And as I told you that this is the imbalance that arises for the incorrect velocity field

That is the difference between the actual u minus u star or v star. So, once we solve this equation, okay. So, once we solve this equation or the set of equations considering all other points together, what we will have? We will essentially calculate or estimate the P prime. So, this p prime we will calculate from here again if this p prime is 0 which means you already reached the convergence point where whatever the you estimated value was calculated is essentially the actual value.

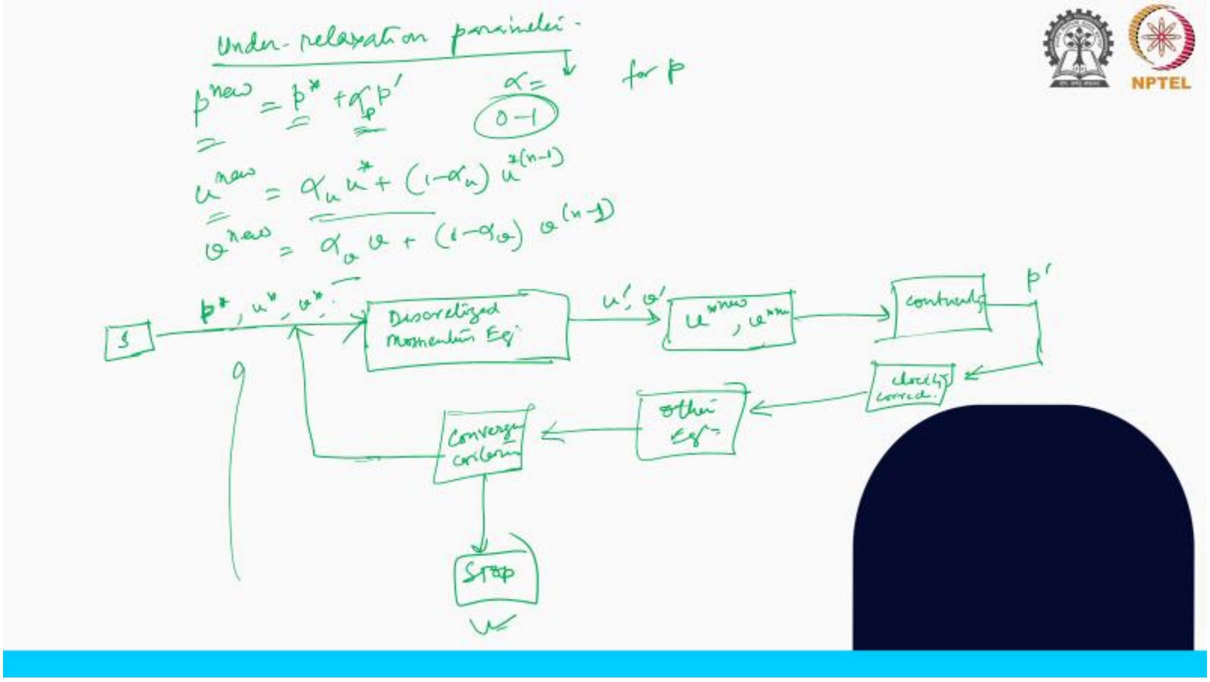
But if this returns a nonzero value of p prime that means with this p prime again we go back here and we calculate our nu p which is the initial guess plus p prime and we consider that this is the correct value of pressure. If this is the correct value of pressure then it is linked with with the calculation of u and v once again or the u star and v star for the next iteration once again that with that p nu or the p nu star specifically we again calculate this expression. We again go in this loop and again we calculate the nu values of the u star v star

From there, we estimate or we actually calculate the new values of u prime and v prime. Again, with the new values of u prime and v prime, we correct our velocities. Again, we recheck whether the second corrected or the corrected in the second iteration—these u and v values—are actually satisfying the continuity equation. Once again, this loop would continue—okay, this loop would continue until we reach a desirable value, that is, within an accepted convergence or tolerance limit for this pressure correction and, accordingly, the velocity corrections as well.

Now the point is when we go from one iteration to the next iteration we here as I showed you by simply writing that P new star is essentially the have calculated from the moment the continuity equation and the previous guess value or the first guess value. Now, the point is, there we introduce a parameter called the relaxation parameter. Usually, it is the under-relaxation parameter. That means my p new is essentially not p star plus p prime as a whole, but with a factor, say alpha p, where alpha is the under-relaxation parameter for pressure.

This is the under-relaxation parameter for pressure—that is, the subscript p. See, this under-relaxation factor, what it does: if it is 0, that means whatever correction you have calculated from this step, you are taking that correction solely, as if this is the complete correction that I require. But remember, you started with a guess value—a guess pressure field—and that guess pressure field may or may not be somewhere nearer to the actual solution. And in this next step, whatever correction you are calculating, if you consider that correction to be completely true,

then there may be chances of oscillatory or non-convergence of the simulation. You may go far away from the actual solution because you started with some wild guess which is far away from the solution. So, that is why this under relaxation parameter is generally constrained with a range of 0 to 1. So, if you consider alpha to be 0 then you are not taking any correction at all into consideration. You are always iterating with the your initial guess value and naturally the convergence would not happen.



If you consider alpha to be 1 that is the scenario I just explained that you are taking complete correction from the previous iteration whatever has been calculated and you are considering that this is the complete correction and I am considering that to the and we are correcting my guess value with that complete correction. But anything in between 0 to 1 would take some lesser correction from the previous step and you would calculate your nu p value with which you will again calculate the v prime u prime and again nu u and v which will further satisfy has to satisfy the continuity equation and a nu pressure correction would be calculated.

So, the point is This is the experience that you require when you go into the actual simulation that there are certain set default values by the commercial CFD solver or the other processes. And this is where you can tune your simulation in order to make it faster if you had a initial guess value correct. by increasing this alpha value towards 1 ok. But again remember the chances would be oscillatory divergence from the actual solutions also be higher if you take a larger value of alpha

when the guess values are not close enough to the actual solution or they are not nearer to the actual solution. but again considering very low value of alpha would require more time towards going to the convergent solution. So, this is the practice that you would require, this is the experience that you require in order to understand how much value of the under relaxation parameter you would consider ok. Now, similarly for the velocities also there are the factors that see the solvers consider is something like this 1 minus alpha u to the power n minus 1.

So, v nu is essentially say alpha v plus 1 minus alpha v to the power v n minus 1. So, this alpha u and alpha v are then the under relaxation factors for u and v component velocity. So, the point is this formulation actually is further complicated by introducing not only this part that u ij is equals to u star u prime j, but by that expression that now my u nu is essentially this the initial guess part and this under relaxation parameter alpha part that includes there. If it is included this formulation becomes more complicated.

And this is what happens in actual CFD solver that with the incorporation of the under relaxation parameter to give you more flexibility or to give you more control over the simulation. This is essentially is implemented in the CFD solver and that is why you will find several spaces to insert this values of the under relaxation parameter. So, what it does in a nutshell? for this simple algorithm we start the simulation by guessing the p value of known p value ok. So, with the known p value also we have the u star immediately v star all these calculations are done immediately.

So, which means that is the first part that either you give this initial condition which is essentially your first guess and that initial condition can be propagated from the boundary conditions or from certain critical points that you may consider. And that is why you will see in the CFD solvers there are options to initialize the solution by the boundary values or some other points. So, with that with this once you start it with this initial values you essentially solve you essentially solve the discretized momentum equation. These are solved, and that results in u prime and v primes, by that I find my nu values of the u star.

So, u star nu and v star nu, and that has to satisfy my continuity equation. And by doing so, what I will get is the P prime, the pressure correction. This pressure correction results in the further velocity correction, the further velocity correction. And with that corrected velocity, we solve any other equations that are there. Say, we will see later that there will be species transport equations and other equations that we can see.

And we check whether we reached a desired tolerance limit or not, or the convergence criteria. And these are the other equations. If we reach this, then we stop the solution; if we do not, then again this goes on, this loop continues, and here I should mention this. So, either you stop by checking the convergence limit, or you continue with the same loop. Again, you go for the discretized momentum equation.

You solve it to get the further corrected value of the u prime and v prime. So, this is the whole idea of the SIMPLE algorithm. We have discussed in detail because the other algorithms that I will briefly mention are essentially mostly the development of this SIMPLE algorithm. And there are some new cases that, based on your interest, you can explore, but what I will cover here is mostly based on this simple algorithm. In fact, all are based on the advancement of the simple algorithm because it was developed first if you consider the chronology.

It had some limitations, but it is extremely popular for certain cases. It may not be sufficient for accurate results very quickly, but again, that is why there are developments, which we will discuss in the next lecture. So, with this, again, I thank you for your attention and hope to see you in the next lecture.