CFD APPLICATIONS IN CHEMICAL PROCESSES
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Lecture 08: Boundary condition

Hello everyone, welcome back with the another lecture on CFD applications in chemical processes. Today, we will discuss about the boundary conditions ah that are essential to solve any CFD modeling problem or in fact, this boundary condition in general if we speak are necessary to solve any set of any partial differential equations or even any ordinary differential equation. So, the utility of boundary conditions are well known. Today we will see couple of well known boundary conditions and how those are mathematically interpreted when we assign those in the solution domain.

So, in the last class I specifically told you that the utility of boundary conditions is that it demarcates the solution domain from the surroundings and also it tells that how the solution domain is influenced by the surrounding or how it is communicating with the surrounding. So, the so first of all the flow has to come into the solution domain ok. So, the most common boundary condition that we speak is the inlet boundary condition. So, any CFD package any CFD code that is set initially we have to let the flow come to the solution domain and that is your inlet. So, but inlet what does this mean mathematically speaking because this coding the CFD solver etcetera it understands.

that how these variables that we will work on or will work with, how those variables are set at that point. So if you have a solution domain, say for example this tank is filled with water, So one would be essentially the inlet. How the tank is filled. After fill you can take it out through an outlet. So the first thing is that inlet and this is we say that the outlet.

Now in this case our domain solution domain is simply this part. We usually consider this. which means a some part of the top surface, this top surface according to this diameter of the hose or the pipe through which the water is coming to the tank say for example. So, only this part is interacting with the surrounding where the flow is happening. fine or say for you can consider that the from whole top it is coming that means, this whole top surface is my inlet. Now, this inlet usually we know that what is the flow rate that how much flow is happening.

from that flow rate and the area of cross section of this pipe or the nozzle whatever you say that we can find out the superficial velocity of the fluid that is coming in and that is set at this point. that means, the Uin the inlet is the Uset or the known velocity. That is the mathematical impositions that you are putting in when you set that my this portion is the inlet with a given value. So, similarly for any other scalar variable all the parameter if you are that is known or that has a set is that the which means or we can say these are the known values. So, phi can represent any scalar quantity for example, temperature

species concentration, any physical property etcetera except pressure. So, when the normal component of the velocity is known at the boundary, the boundary condition for the pressure is then not required to be specified because the velocity field depends on the pressure gradient fine. So, when this So, that means, here specifically we can call this kind of the inlet as the velocity inlet. So, in inlet boundary condition when we impose or set this superficial velocity. Then we can call specifically this kind of boundary condition as the velocity inlet boundary condition, where the specification or the imposition of pressure is not required because as I told you that when the normal component of the velocity is known at the boundary, the pressure is not required there because the velocity field depends on the pressure gradient.

is related with the pressure not on the absolute pressure. it does not depend on the absolute pressure. So, sometimes also it can happen that we do not know what is the velocity. In that case we may have to set the pressure that it is this much above the atmospheric pressure or this much above or whatever the static pressure, but then I will also show you that how this information is converted to velocity or can be converted to velocity when we start the simulation. But before going into that inside this velocity inlet condition

there can be some complex situation. That velocity inlet I have told that for this much of specific part I have this information of the velocity that is known to me. But the point is that means, when you set this kind of a value it considers there at this much of this area it considers that you have a uniform velocity profile that there is uniform value of the velocity at each and every point, but is it true or is it ok. Because, in certain cases you do not know how this water is coming in there are several complex cases or industrial cases where say a vessel or a reactor or a tank is filled where this feed

is coming through a tortuous path or maybe through a long pipe which is not straight and having bends, valves etcetera. So, in those cases so, also we know what is fully developed flow ok. In those cases we have a parabolic profile of the velocity when the flow is fully developed Now, whether the flow is fully developed in those cases that we did not consider here. If we had a simple case that this vessel is getting filled with a long straight pipe, then considering a flat we call this as the flat inlet or the flat velocity boundary condition.

Now, in such cases when we have our known flow regime and we can calculate or we can understand whether the flow has been developed or not. In those cases considering flat velocity boundary condition may result inaccurate physics or may not capture the right physics that is there. In those cases it is appropriate to have a parabolic boundary condition.

That means, the parabolic profile of the velocity as the boundary conditions there. So, simply this u in is not simply a known value, there is a parabolic profile and you know that profile. So, that has to be set there. This is one way to do that ok. That means, you need here two different solution strategy. That means, you would definitely solve this your solution domain, but to know the actual boundary condition of the velocity inlet you have to solve this section separately.

This if you are considering that much of accuracy this inlet section separately by prolonging it or by extending that part. So, one way of considering this scenario is that I do not care what is the situation upstream I have, I might consider my solution domain is like this that I extend my solution domain and I give flat velocity inlet there. that I do not want to calculate this parabolic profile or how much would be that beforehand and I extend my solution domain like this and there I give my flat velocity inlet profile. So, and let the float be developed and whatever the way it would happen it would come here accordingly. This is one way of doing that or the other way that I just told you that if you anticipate

what would happen at that point with a given physics you capture that and then impose that as your boundary condition only for this much of the solution domain here on this part here you impose it. So, sometimes the point is sometimes you have to extend your solution domain to capture this inlet information ok or you have to be careful because as I told you if you have bend like this and you are giving say parabolic profile here. or fully developed profile here. Then you are not considering that this fact that whether this much of length this much of the length or the distance of flow is sufficient to be again it fully developed because it just came across a bend where there is a flow mixing due to the secondary flow is happening. Because here suddenly the flow paths changed and whether again I got my fully developed profile here.

So, if you impose fully developed profile here you may get a different result or inaccurate result than what is happening actually in the real case. So, either you extend it or you anticipate the physics that is the point here. Now I told you that there can be situations where you do not have the information of the velocity. Say here this is the case of a boundary this is say the atmospheric point you have a known pressure here. and here you do not know how much velocity is there.

So, we consider that instead of velocity inlet as the pressure inlet. So, here we consider a pressure P0 and the velocity that we have to calculate based on this information based on this information the pressure from the pressure difference between this Ps and P0 across the boundary. and how it is done?

$$P_o = P_s + \frac{1}{2}\rho v^2$$

I mean that we consider by say Bernoulli's equations we can initially estimate that P_0 would be this value.

And accordingly the velocity that we can calculate or we would estimate at that point if we had to initially give this as velocity inlet is:

$$v = \left(\frac{2(P_o - P_s)}{\rho}\right)^{1/2}$$

This is my solution domain and say a closed location to this solution the boundary conditions where we are putting as a pressure inlet and P0 is my say the atmospheric value that we have. the total that this thing we can consider as the total pressure at the inlet that we are defining.

It is composed of the atmospheric pressure plus the static pressure that would be there. So, this absolute pressure is considered and accordingly your V can be calculated based on this that would be set to this boundary condition. but the point is that this is the simple case of incompressible flow. for the compressible flow more complex situations would be there will be several non normal flow associated with this. But the point is that when we have to use this boundary condition we have to be careful that whether we are giving only one value that is either pressure or the velocity.0

If we give this inlet as the pressure value we call that as the pressure inlet with a known pressure that is the one depending on the solver it takes the your gauge pressure mostly, because it is when it is added with the atmospheric pressure it gives the absolute pressure. And then based on that with the value and this simple approximation it calculates the velocity and this velocity is then propagated in the domain. Now, coming to the other boundary condition that I mentioned here which is the outlet. So, the flow goes in either by velocity value you are defining or the pressure and then there is the outlet condition that it has to go out from the system as well.

So, in those cases the surface through which the flow exists the flow that goes out of the system. So, this is the inlet and say from here it is going out of the system. So, this surface or the part of the surface we call that as the outlet. So, this outlet boundary conditions are normally applied or is meant when the gradients normal to this outlet boundary are 0 for all the say. So, normal those are the normal gradients

to this outlet to the outlet boundary is 0 for all variables except pressure. which means mathematically speaking. Now, again here we need not specify pressure at the outlet boundary condition, but the point is this outlet boundary condition would not be applied if you anticipate that the gradient at the outlet ok it influences back to the solution domain. that this gradient of this outlet boundary condition are you expecting to be non-zero and the condition at this downstream we call this is the upstream, this is the downstream conditions at this downstream influences or have a feedback to the system to the solution domain.

In those cases we cannot apply the outlet boundary condition. Say for example, the flow is happening through a smooth tube, this is the inlet and this is the outlet, but you suddenly place or there are some constrictions that are put there. So, flow is happening there is a constriction. So, what you expect that there will be recirculation of the flow.

Now, if you put here as your outlet boundary condition that would be or that would capture a wrong physics that would not give you the actual result. It has to be far away from this influence due to the constriction. So, had you just a smooth pipe or tube this is your inlet you can place outlet anywhere, but as you have kept or is there is some constriction you expect the fluid circulation to happen here. Therefore, placing the outlet boundary condition closer to this value would violate this expectation that the normal gradient at the boundary condition of these be 0.

that would not be the case or this outlet condition is eventually having a feedback mechanism or influencing again this flow till this position. So, here is completely no, but you have to be careful that whether you can place in this locations because of this velocity or the magnitude of the velocity. So, I would say that these also would be a poor choice of location. It has to be far away from this influence to place that as an outlet boundary condition. Okay.

So the point is Again in such case like the inlet boundary condition we have seen that in such case if my domain just say for this case due to some disturbances my domain ends here. I would extend this domain further and place here I would consider my domain as like this and would consider this as the outlet boundary condition if I have some constriction here. So, that means, here also you may require to extend the boundary condition the solution domain in order to capture the actual physics or what is happening inside or the actual accurate result or for the prediction of the accurate result.

And then the other important thing that comes is the wall that means, I have this is my inlet this position this is the outlet, but then rest of the position through which nothing is going out going coming in etcetera. So, these are called the walls wall boundary condition ok. So, these are impermeable So, specifically we can also say that these are the impermeable wall where no slip boundary condition are usually specified.

No slip means that the normal velocity on this wall on these surfaces are 0 and the transverse component of the velocity is the same as of this surface which means since this is impermeable it is the here in this case there is 0. In some cases there may be deformable wall and that is why we mentioned that the transverse component of the velocity on those surfaces are moving at the speed or at a velocity as that of the surface, but the normal component remains 0 and we call those as the wall. if we say those are the impermeable static wall then these velocities the transverse component velocities are also set to 0. So, apart from the velocity in case of temperature a specific temperature has to be set. ok. That means, T at these positions are as T set or T norm or the T known values.

Heat or mass flux that has to be specified ok. If there is any internal heat transfer that is happening then the heat transfer coefficient and external temperature at the surface etcetera has to be specified. from that the other say the gradients and all these things are calculated. The fourth point or the other interesting boundary condition that we use are called the symmetric boundary condition or the symmetry boundary condition. we also have periodic boundary condition or we further also call sometimes as the cyclic boundary condition.

Now, the symmetry boundary condition is very important to understand because it helps us in reducing the computational domain or the solution domain size. If we have flow symmetry remember this flow symmetry not only the geometry symmetry. So, a computational domain if I draw a picture like this, there is a step increase in the So, if I have a geometry like this where this is my inlet and this is my outlet. So, we can clearly see that we have a geometric symmetry along this line.

So, which means that I can possibly define this line as a line of symmetry in computational Now, there is a point here that we can only define this as the point of the line of symmetry if there also exist of flow symmetry along with the geometric symmetry. What does this mean? If we have say uniform temperature everywhere on the walls and a fluid is flowing. in that case a fluid is flowing inside that.

Now, in that case we will have a perfect symmetry across this line whatever we will see here we will see here as well. So, in that case if we only draw this part of the geometry or we consider as our solution domain by defining this plane as symmetry. our result would provide accurate result or accurate information. But you consider that here we have temperature difference that this surface is having a temperature which is say 10 degree centigrade. and this top surface have a temperature which is 110 degree centigrade or the other way round we have just for simplicity we consider that this is also a 10 degree centigrade.

So, we also consider this as the 10 degree centigrade, but the fluid that is coming in ok. So, this fluid that comes in is say 100 degree centigrade or 110 degree centigrade. So, what will happen to this fluid when it passes through this region ok. Now, in those cases what will happen if this is 110 degree and this is 10 degree centigrade, this is also 10 degree centigrade, then due to the buoyancy effect there will be a flow circulation or the flow that here the hotter the hot fluid would rise due to the buoyancy. or due to the natural convection.

So, there we will not have the flow symmetry although we have geometric symmetry ok. in such cases we cannot consider our domain to be simply like this. In such cases this consideration of the symmetry would not be fair or would not be accurate but you would ask that I have my geometric symmetry in this cases, but in the actual flow you do not anticipate or expect the flow symmetry to be there. And that is why consideration of symmetry boundary condition is extremely important that

what or where that has to be used. So, choice of symmetry plane not only depends on the geometric symmetry there has to be flow symmetry. Then you consider that as so, here what happens mathematically speaking your normal velocity are set to 0 and normal gradients of all the variables except normal velocity. are 0.

So, what it does it actually ensures that no convective or diffusive flux exist across the plane of symmetry ok. So, and in other cases what happens along with the symmetry this symmetry is repeated ok. So, not only in this case if there is this kind of scenario is there and then you have a two symmetry line and if you anticipate that the flow is symmetry in this case then your simulation domain can only be one fourth of the total domain.

So, the utility of this symmetry plane if you identify clearly this flow symmetry then it greatly reduces it can greatly reduces the domain size the solution domain size and solution domain size reduction means your computational sales or the number of grids etcetera are greatly reduced. So, here for example, in this case it is reduced by one fourth. That means, your computational time computational resources that you require to solve this problem is greatly reduced. For example, here if the flow symmetry exist in this case the number of computational cells or the grid or meshes are reduced by half and you get the accurate result. So, I will stop here today.

In the next class I will discuss the other two similar boundary conditions which is the periodic and cyclic and how it is in which situation we can think of periodic and the cyclic boundary conditions we will look into it. So, thank you for your attention and we will see you in the next one.