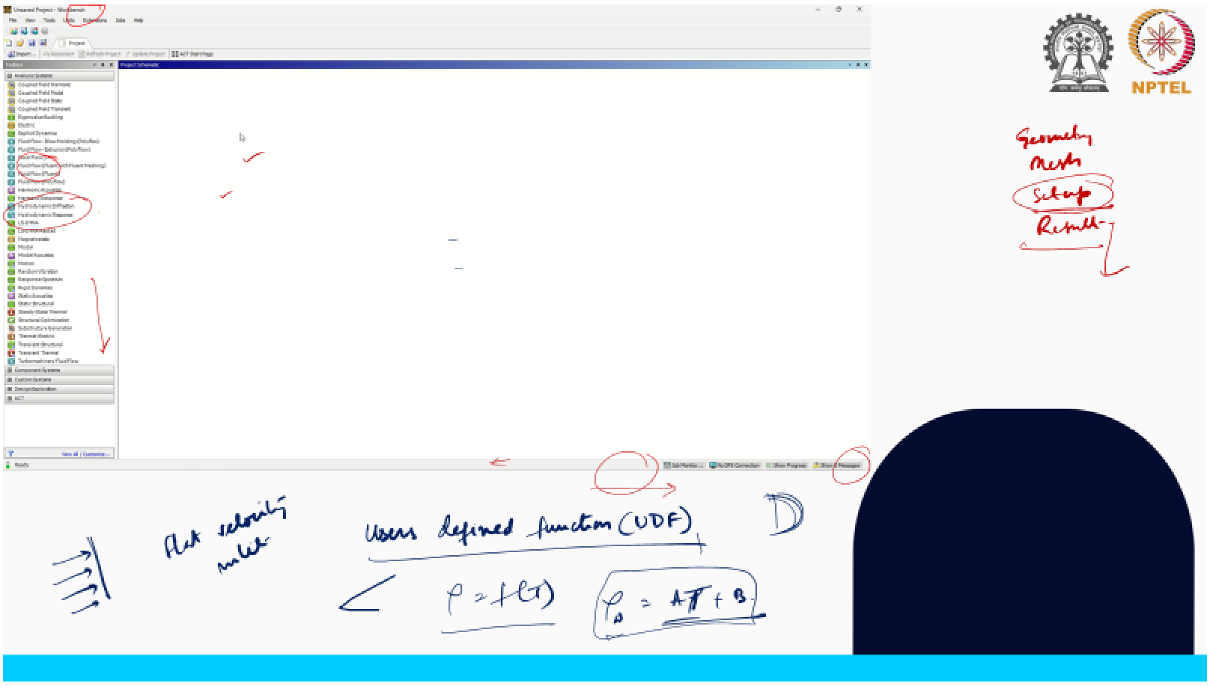
CFD APPLICATIONS IN CHEMICAL PROCESSES
Prof. Arnab Atta
Department of Chemical Engineering
Indian Institute of Technology Kharagpur
Week-07
Lecture 34: CFD Tools & Modeling Single-phase System

Hello everyone, welcome back with another lecture on CFD applications in chemical processes and we are discussing rather demonstrating a CFD tool namely ANSYS Fluent where we are modeling a single-phase system, which is a very simple system: a 2D pipe flow under laminar conditions. So, in the last couple of lectures, we have seen various components of this model setup. We started with the point called the ANSYS Workbench, and in ANSYS Workbench, we opened the Fluid Flow module, which is Fluent. Before we go into the actual simulation or solution of the problem, we had to create the geometry in the preprocessor.

So, with the help of Design Modeler, the geometry was created. We have seen the detailed steps and will not repeat them. If required, you can go back to the previous lecture and review them. So, the point is, we discussed generating the flow region, labeling the boundaries, and also the meshing part. So, we have seen how to control meshes because fluent does this ANSYS workbench does its default meshing, but if you have to have a control if you want to do it on is desirable—so that the user has control over the meshing type or scheme. We have also seen how to control that mesh and the mesh quality, how to check it, or the statistics.

So, all these things we have seen in our previous lectures, and then we came to a point where—We had to set up the boundary conditions: the inlet, outlet, and the wall. For this case, we set up this problem, and this is the Fluent launcher that you see. We discussed the different options available when we open this launcher and the several options it provides or gives us to model a specific system. So, till the last class— or the last lecture what we did we set up the model and again I will take it from there that what we have done is that we have from the fluent database we chose the water as the fluid that would flow through that space or through that pipe.

Through this green zone, for that, we selected water as the fluid from the Fluent database. By default, we have seen the water properties are taken into the calculation. The point I mentioned is that you have to be careful because this is a simple— So, in your specific case, if say the water temperature varies and for that if the density is changing, then here you essentially have the option that instead of taking a constant value for all the properties that you are seeing. So, those constant values can eventually be changed as per your preference. Requirement, which is usually defined by some function, and that we call the user-defined function in the case of Fluent, which is extremely popular and it gives the user defined function or in short called UDF you frequently hear this name UDF when someone does the simulation in ANSYS plane because you see here the several If those components vary, then you have to change this instead of a constant; you can change it to your user-defined function. That is how to write a user-defined function. It requires, again, a special—I mean additional—time to understand that, but we will not go into those details. For that, you can look into their help files and the tutorial guides on how to write a UDF.



Say, for example, if you have density that varies with temperature. So, you will definitely have a function that density of water has some density at a certain temperature, and it varies, say, linearly with temperature. If that is the function you want to implement here, you have to write a small code for that which would be compatible with the language that ANSYS Fluent understands, its compiler understands, and for that, you have to learn a bit about the syntaxes that are used in those user-defined functions. So, this user-defined function makes this solver, this particular software, user-friendly.

Although there are limitations, the point is that this gives you flexibility. It gives the users flexibility to incorporate their own ideas or their own equations in such places through the user-defined function. So, based on that, we chose water as the flowing fluid, but the point is that we also have to make this code understand where this flow is happening. So here, as you have seen in the last lecture that I elaborated, there are different setup options are available.

In the setup itself you see there are different models materials that we discussed in fact. And then here we chose this cell zone where we converted it to the fluid instead of solid. And then which fluid is flowing that we have set in the previous dialog box that we have done. So, by default it is air, fluent takes this as air, but then we have changed it to water in this case because that was our requirement.

And after that we went to the boundary condition. This is also I have shown in the last lecture that inlet outlet and all these boundary conditions how we solve. I also briefly told you about the different grout options that you see here and when those would be activated. Say for example, again that if you have temperature variations, heat transfer that are happening due to radiations, due to other cases, there you see that the thermal and the radiation buttons, these are grayed out at this moment, those would be activated in this case or in that particular case. The species says those would be activated if any reaction is involved.

The dispersed phase model DPM or the multiphase those accounts for the multiphase flows that we will learn later in this course. there if it involves this battery and all this kind of a simulation the potential or some other gradients that are there that can also be fed to the system or that information can be fed to the system when these options would be activated. Because accordingly the model has to be set and you have seen earlier that if you expand this model tab at first because the general options that are available here I told you what are the functions of scale check report quality display units etc. These are the default options that are there. You can choose the solver type, the velocity formulation when absolute and relative are required with an example of porous media.

I told you that about this formulation briefly, although we have not discussed in details because those are research specific. Then the point is if you expand this model you would see that you have seen in fact earlier that there are several model options available and in that case. So, I will just take you a bit in a So, these are the models different kind of models that ansys fluent give you flexibility to do that for a system, but since in this case as I told you that we have a laminar flow we went to the viscous option and then we chose the laminar option here. And then accordingly all the parameters that you see for this k omega option which we will discuss during the turbulent modeling part in this course.

So, this laminar options actually switch off all the unnecessary data that are shown here for which are necessary in fact for the k omega model. Now the point is again, so we have defined the boundary condition. So this is the velocity inlet dialog box that you see and you can clearly demark it by looking at the geometry because ansys fluent has its own color code that here you see we have the blue line or the blue plane that is for the inlet and the red for the outlet here. Now, these are the preset thing you can change, but the point is that these are the default color notations or the color combinations that it shows. So, here you give the velocity magnitude setting this as the velocity field.

I told you also the velocity specification method that are different kinds of velocity specification methods would be available to you. Here also you can fit in your user defined function because several times it happens that you consider for this problem that fully developed profile is already there at the inlet. So, in that case this fully developed profile as a user defined function you can set at the inlet instead of a magnitude and normal to boundary which we generally called as the flat velocity inlet. because it assumes that this kind of a flat velocity inlet or flat profile is there at the inlet which gradually develops and after a certain length it develops into a fully developed condition. So, here again, either velocity or pressure—you have to define one; you cannot or need not define both, okay?

So, you define the velocity here. And so, after this, you go to the outlet boundary condition after applying this. So, based on your requirement, you can set this velocity magnitude to anything, and that would be in meters per second. Also, you see here the dimensions and units are given. Again, for all the labeled parts, that is, the inlet zone. So, in this zone also, I discussed that there are several group options that you can see here, and when those would be activated—just a similar discussion to the inlet cases.

For the wall—again, since this is a stationary pipe, we had the stationary wall, and at the wall, we define the no-slip boundary condition, and that is taken here. Now the point is when you develop code you would not have such kind of nice GUI of course, but the point is that you would write the mathematical expression for no slip boundary condition that is would that would be the difference. that here by switching on no slip boundary condition you have seen or you now know what which mathematical expression it would eventually solve because this we discussed while setting up during the fundamentals of the problem of the finite volume method. So, similarly, here the problem involves a stationary pipe through which flow is happening. So, we chose the stationary wall.

If there is a deformable wall, we can have the moving wall option, where the wall also expands as the fluid progresses. Now, that also has different applications, or in certain cases, that is also necessary. So, it gives us flexibility in that case. Here the option we have is the wall roughness. Now, in practical cases we have the wall roughness in the real case.

So, those roughness factors the roughness constant, roughness heights etcetera those values can be given here. When we will discuss multiphase case or so, the granular flow. So, there particle-particle collision, particle wall collision or etcetera would be taken care or can be taken care by this point which is called the specularity coefficient. Since this is a single phase it is automatically grayed out ok, it is not active in this case in this window. Similarly, Marangani stress when if your problem involves that and you have interfacial tension activated flow in those cases this option would automatically be activated.

Now all these things would activate based on your choice of the model. For certain combination these things would be active when you see such window and as per the choice of the model. Because here we have single phase laminar flow that is why these are by default switched off. So, in real case the wall roughness can also be assigned. But, here we are considering smooth pipe.

So, after this we have set up this model as we see and now we will go to the monitor section. So, this is the part this is the part till this point we have set up the problem. So, if you remember that the options that we had is geometry, mesh, then we have the setup, then we have the result option. So, we came here on this setup part, but It is not only the problem or the boundary condition set up, but because you now remember based on our previous discussion that your model whether it is correct or not that has to be checked against a benchmark.

Now, that benchmark can be the experimental data or the analytical result. Now, how do you check that for that? As desired, or it is logical that we plot some residual. We check whether the simulation is converging or not. For that, we have to set up—so before we validate the model, at first, we have to have a converged model. Converged means there is hardly any difference between the successive time step in case of the transient simulation or successive steps in case of steady-state simulation.

We set a desired tolerance limit. Now, that setup is also a part of this overall setup option that is here in ANSYS loop. So, the point is that we have to set up some monitor in order to look into whether the simulation is approaching convergence or not. So now, here are other options that you see. The dynamic mesh option.

So here that you see there are different other options are also available for other kinds of problem where one of the important thing is the dynamic mesh where you have a moving interface or say the moving wall. So, the mesh would also move. So in such cases these options are used. For these specific cases, you can look into the solver specific help or tutorial guide in order to understand those function and how to implement those. So in the solution part, although it is showing inside the solution part, but the point is, these monitors that we set, Essentially, those are the monitored value when the solution is there or while solving we are looking at some residual in order to monitor the approach of the solution.

So, here what you see is that when we expand this monitor option we have several parameters one is the residual report file report plots etcetera these options are available. So, in those cases in this solution method also before trying to doing that in this case So, in the solution method if you click it you will see there also we have several options that we have to set up at for some problems. But let us look at this residual monitor at first that what are the options we have. So, here you see that the equations that this problem will solve is the continuity equation and the momentum equation x and y momentum equation. So, here by default these are the checkbox options which are switched on and these are the absolute criteria for the convergence. Now, these limits you can change or you can tune as per your requirement ok. So, here There are also some additional or advanced options would be available if you tick on this thing. There will be some more additional information which you can monitor or which you can set up.

Here you make sure that while monitoring this you plot those as well. So, this plot tick has to be there. the tick mark beside the plot has to be there. Because then once you start the simulation the pop up window would appear or say it would be there in the plot results where these plots would automatically go on as the iterations goes on. Here the iterations to plot that after how many iterations those plot would be updated with the new data those frequency that frequency you can set it here.

At the same time it becomes important that at certain time step or at regular interval you store the data also. So, that option is here that by which you can store the data and in which frequency in how much frequency you want to store that transient data that you can set it there. And this print to console is that here in the console that this continuity and this x and y this absolute criteria all at each and every time step there will be some scrolling information that would also happen if the stick is on there. So, then we set this values or this absolute criteria which you can change you can see these are the editable field. So, here we edit that value to whichever the value that you require.

So, here it is you can write like 10 to 10 to the power minus 6 that is 1 e minus 6. So, it is set to a very low value we require highly accurate converge solution. So, that is why as low values that you set here it would require more time for the convergence to happen. So, again there are different activities or different things are there, but now the point is since we are ready to start the simulation What we do here is that we have to initialize the solution.

And that is done from this initialization button. So, this initialization once again is that the point. Now before initialization I forgot to mention this point that here in the solution method that I told you that there will have several options and those options you can look at it if you click this method the solution methods and there So, there once you click on the solution method what you will see this velocity pressure coupling options that are there which we have to select judiciously that which one we would like to use. So these are the options that are available that how do you plan to take into account the velocity pressure coupling that we have discussed in our previous lectures.

We have seen the velocity pressure coupling of various kind starting from simple, simple R, simple C, Pso, etc. Now those options are available here. You have seen the default option was they are coupled. But we have to specify for the better accuracy the kind of model that we choose here. And that is why we chose to understand the background or the theory before we came to this stage.

Because some of you are may be a few of you that who are doing this ansys fluent simulation without knowing that why what is simple simple C and simple R and all these options they may lead to inaccurate solution or simulation of a certain problem. But now the point is since we are starting or doing our first simulation let us start The first approach which is the simple algorithm, because we already know the difference between simple R, simple C and simple algorithm. Simple has widespread use, it can be used in several situations or many situations, but this is a very simple problem, so we start with simple.

Now, the point is here you have these options to redo your simulations if those are not accurate. Now there comes in the future we will discuss two points that along with the validation of your model you also require verification of the model. That means how much numerically correct these are to the experimental or the analytical solution. Now changing this scheme would lead you to go towards more accurate estimation or more accurate predictions by the CFD model. So, in this solution method you have these controls that what is the pressure velocity coupling that we learned earlier and which scheme we should use.

So, we choose here the simple scheme. And then we see that there are other type of spatial discretization schemes that are available which is the Green-Gauss cell based which is Green-Gauss node based and pressure or say the velocity or the momentum specifically how those are discretized or say which kind of differencing scheme that we will use. Now, here are those control that we have to set up and comes as a part of the problem setup those comes as a part of the problem setup ok. So, now you can possibly relate that why we learnt those basic thing or the fundamentals earlier before coming to this part of this course.

And what are these spatial discretization schemes? So, this means that how the gradient would be resolved. In future, we will have some recommendation in the final classes, we will have some recommendation that which kind of gradient should be used, the node based or the cell based. So, all these how we should discretize or what kind of differencing scheme we use. Now, usually in the first run or in the first simulation, you can go ahead with the first-order discretization scheme, okay.

To have more accurate results, it is desirable that you use higher-order schemes. Now, there are several higher-order schemes available. We have not discussed all these in detail, but we have understood what is second-order. And there are, in fact, third-order or higher-order discretization schemes, but that also depends on the solver or the software that you are using. They have their own schemes. Again, those are based on the research findings, and they have implemented them in their code.

So, before choosing those options, you must explore them in detail from their theory or the help guide. So, the point is, we will continue discussing this in the next lecture of this part, where we will see how the solution is finally obtained after setting all these parts that we are seeing here. So, with this, on this note, I thank you for your attention, and we will see you in the next lecture on this part. Thank you.