CFD APPLICATIONS IN CHEMICAL PROCESSES

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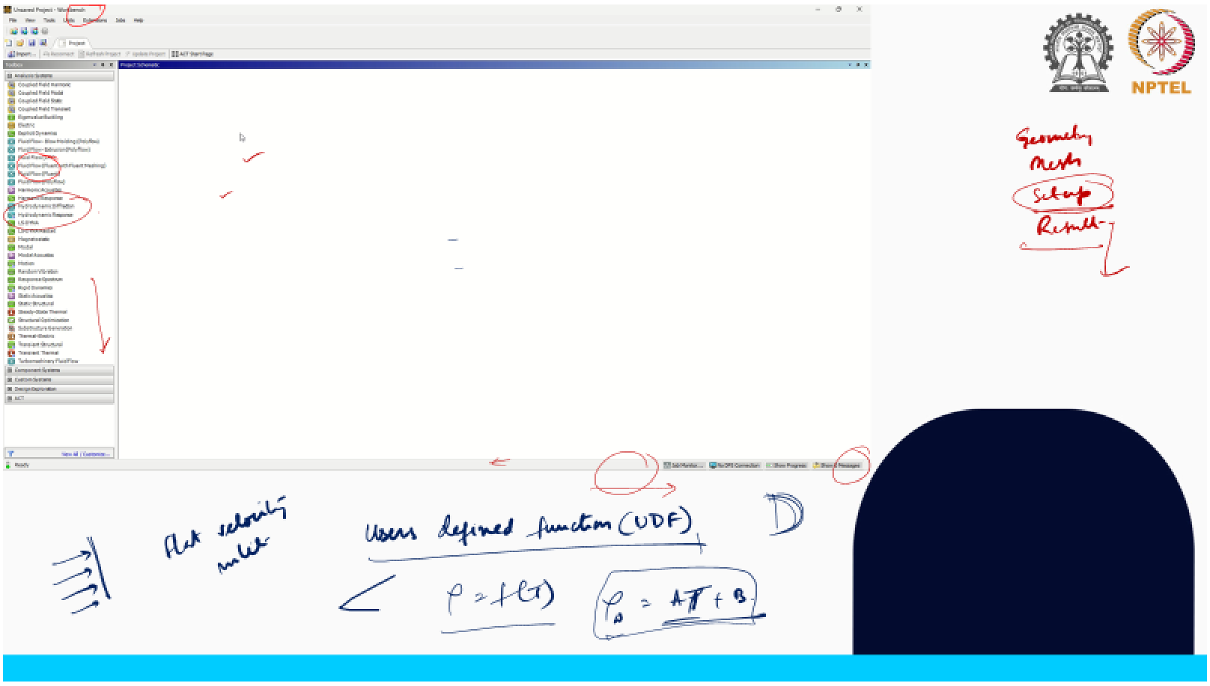
Lecture 35: CFD Tools & Modeling Single-phase System

Hello everyone, welcome back once again to the discussions on a particular CFD tool that we are demonstrating here, which is ANSYS Fluent, in the course CFD Applications in Chemical Processes. So, in the last lecture, we discussed the setting up of the problem, and we came to the point where we were discussing the velocity and pressure coupling. And different discretization or the differencing scheme I would not say the discretization schemes, but the differencing schemes that we should use or we have the option to use from these options that we see here. So, the point is, depending on the software that you are using or will use, these options may vary.

But the point is, you have the control of setting up those solvers, those differencing schemes, in nearly all commercial software. But the point is, when you develop your own code, then you use this or use or consider these options or this switch buttons as the subroutine for your problem, which would be triggered if you choose a certain kind of a differencing scheme or the velocity pressure coupling. So, here we see that we prefer to use the higher-order differencing scheme.

So, here you see there are different options in this case when comes to the momentum you see these are the higher order differencing scheme that we discussed we have not discussed in detail say this particular one third order MULES scheme MULES scheme. So, like this, there are several discretization schemes available, and it is difficult to cover all the details in this course. So, it is better if you use ANSYS Fluent and, typically, if you go for this third-order scheme, you understand that scheme first from their help or tutorial guide. Because we now have all the sufficient background to understand those derivations or those fundamentals.

So, now we set here so pressure we have chosen as a second order here you can momentum as you can choose the first order, but since this is a simple problem or differencing scheme increases, the calculation becomes more involved or convoluted, and at the same time, there would be chances for the solution to diverge. Your initial guess or initializations, etc., are not proper with these higher-order schemes. So, it is recommended that the best practice is to initially start with the first-order scheme. Again, the point is that in those cases, numerical diffusion may happen, but you can still have an initial idea of whether it is approaching convergence or not.



For an accurate solution, it is desirable to use the higher-order schemes from the next iterations. So, once you choose these values, it is essentially desirable that you go for this monitor or the options. For setting up these residuals, as I have already discussed in the previous lecture. Now, here is the part that you should mix, and it is recommended that you follow the strategy from top to bottom of these menu options or the tree that you see. Then you would not forget any intermediate step.

So, for example, first you set this generic or general part, you look into it, you check the mesh quality, you set the units, you set the scale if required, and you report the mesh quality. And then you go to the model. Do not skip any of these and directly come to setting the residuals first, because some options may be grayed out here unless you choose the model options correctly. So, it is always recommended that you follow this tree from top to bottom. Do not just skip any of these intermediate parts.

If it is not necessary, you do not go in there, but if it is necessary, it has to be taken care of first before you come to the bottom of it. So, that is why the solution method has to be set first, and then you come to setting the residuals. And also there will be the simulation controls that also that you can set or you will have it when you run this simulations for other cases. But we have discussed this part.

So, I will quickly move on this part that we have set up this thing. Now, since we have set up all these solution methods as well as we have set up our monitor that what to monitor, which residuals we would monitor in order to check whether my convergence would happen or not within the steps or the iterative convergence, then I will come to the initialization of the problem. Because now you understand and also I gave this example earlier that when you write your code for any programming C, C++, Python, etc. The point is initially you define any variable and set its value.

If you do not set it usually it is taken as a 0. But usually it is the best practice that you set those values to a initial value. Now the same thing has to be done in this case. If you remember our discussion previously that these scalar variables depending on the choice of your solution strategy whether it is segregated or coupled. the staggered grid formation or the collocated grid formation.

So, based on these the point is you are storing the scalar quantities as well as the vector quantities in certain locations. Now, in these locations to start the simulation it has to as we assign with some value and those are done and that is done by this initialization method ok. So, in this initialization step what we do we assign those values. guess values or initial values to all in all the nodal points because in all the nodal points in the cell because remember again not mix these concepts.

Computational cells are essentially the control volumes that would exist, and those control volumes would be generated after you create this mesh. So, the point is, again, remember the concept of the P-cell, V-cell, U-cell, etc. For the staggered grid formations, then that would be clear for you—the control volume and all. So, with this initialization, now, how do we initialize the solution? Now, we can assign some random values, or we can take all the values from

say, the inlet, the outlet, or the wall—we can have those options. So, here, what you see is the initialization method: we have the standard option, and once you choose 'standard,' you can select the 'compute from' option. Because you are setting a certain velocity at the inlet, you can always choose to compute from the inlet value. So, initially that propagation would happen that whatever the velocity that you have set in the inlet by its standard algorithm or the standard initialization, all the nodal

surface or inlet plane would be assigned those values. Here, you have the initial values that you can provide for the x-velocity, y-velocity, or the pressure. So, here we can see as I told you that we can compute it from all zone from inlet, from outlet or wall because these three specifically assigned which is the inlet, which is the outlet, and what is the wall. Now, say we select 'computed from inlet,' and once you do that, you see automatically this inlet value appears at this point, which is

0.1 meters per second—that was initially assigned for this velocity inlet in our previous example, in our previous dialogue box that we have seen. So, at the inlet we had assigned certain value. And then we click this initialize button that you see here. Here we have the initial part. So we initialize and then this value is passed.

Now remember when we initialized it some y value with the extremely small quantity also appeared on the dialog box. Now that we have manually removed it. see once it is selected from the inlet the y velocity y component velocity to the very minimal point or minus 5 into 20 to the power minus 16 that appeared here. You can reset it to 0 value because there is no y component value that we are providing at the inlet. So, gauge pressure is 0 and this we can reset it to 0 and then what we did we can initialize the whole domain.

Because this initialization is important before we run calculation. And again you see the sequence since these are the commercial softwares. The sequence is after initialization this run command is there. So it means it is recommended that you use all the fields or whichever is needed and then you go towards the run calculation. So, after initialization, so initialization is happening.

So, you can see this your machine is busy in initializing depending on the values or the number of cells, number of grid points, etc. And the processor speed, it may take some time to initialize for all the points. If it is extremely fine meshes, this initialization can take time. Again, that depends on the computing processing power that you have. So, after this initialization is done you proceed towards this simulation part or the run calculation part ok.

So, this is the run calculation is highlighted once you click this the options that you see here are these and again it actually wants you of something which you should do is that this check case option because now that means what you have done you have a set a case file for ancestor. The rule again the recommended rule is that you again come from top to bottom looking at whatever options they have. If it is required you check that or you do that it is recommended you check this case Once you click on this check case, it automatically checks their intelligent compiler, automatically checks whether your meshing is fine, meshing is correct, you have

defined inlet, you have defined outlet, you have defined the values there, you have defined necessary solver setting, you have defined the modeling strategy, etc. It automatically checks and if there is any error, it would report on the console that some error is there. So, you need to go back to any of those options in order to modify that. And then here are the options of number of iterations that you want and the reporting interval on the console as well as the way you want the result to be retrieved ok. So, this is the profile update interval.

in the next option that you see. So, here what you see is the reporting interval and the profile update interval. So, say we set those values Say this number of iterations you can write as per your own requirement that you can give it 1 million, 1,500 etcetera any value of it. So, that your number of calculations will happen accordingly and then it is clicked on the calculate.

So, now this setup is completed. So, the setup has been completed and the calculations would start and for that you have selected or you have clicked on the calculate button. So, here if you look at it this process the progress bar that shows here. it is happening and here you have a stop button as well ok. So, the system is busy ok, now you see that 100 iterations have been completed and the solution is complete.

So, here is the number that you see is 100 is reported here. And that is why initially it was busy till the 99 percent and here you see the number of iterations on the console it is there as 100 and it shows that the solution is completed. So, it whatever the monitored we set those continuity x and y at different time with the different time interval it is showing those component values and subsequently the data has been written to this location that is the default location, but you can reset it in the control option here that where you would like to write that data file that it is has been done.

And before one thing I must tell you because this is the common error that or the common mistake that many people do is that after setting up all these parts sometimes what happens you forget to Go to file and save this case file whatever you have set up till this point. Because you have spent a lot of time on it and if you do not save it and say for any case if the solution is divergent or during simulation something awkward happens you lose actually all the data or all the setup. So, it is better that at a certain interval you start keeping this file in save mode, saving it regularly at regular intervals. So, once it is done—once the solution is complete, say for example—we consider this solution complete for the sake of demonstration, and then we go to

the result part again. You look at it; the result is located at the bottom of the solution part. So, which means you follow this tree. So, in the result again, you go to the graphics. You can now see that this is the post-processing part. So, now in the result, once you go to the result, it becomes part of the post-processing operation.

So, the geometry meshing, the pre-processing part, the model setup, setting of boundary conditions, your compiler setting or the model setting, et cetera, plus the simulation—I would call that the processing part. And the result, whatever it is obtained, if you try to analyze whether it is complete, whether it is converged, etcetera, and all, that comes as the post-processing part. So, what you see here is that this graphic option, different surface option, graphics option in under the graphics you can plot contour,

plot vectors, you can impose or superimpose these contours on the meshes. So, such options, such advanced options—all these things would be there. Here, as a typical window that you see, is for say, this—say the velocity contour you want to display. So, what you do here you go to this graphics options and in the graphics option you can see this contour is there separately, separately. And here, once you open that contour, you see that the contour options would be there—whether it is field, whether you want the contour lines only. If you want the contour lines, you switch off the field options—boundary values, node values, etcetera—whether you want to plot it on the same plot. The global range and auto range this color that you see from red to say the to the other extreme which is the black or say whatever that can be here. This you can change. This color combination or the color range that is here you can change by making your own color map option here that you have. Here is the color map option that you see.

There are different default or inbuilt color combinations are available but you can make your own as well. The coloring this blend whether you want a banded or smooth that option is there. So several advanced options are available here. This auto range is automatically adjusted to the maximum and minimum. But if you say if you know that my minimum is this 0.

and I need not plot say this minus 5 into 20 power minus 6 kind of value, then you can reset that that from 0 I want wherever that maximum range is there. So, in that case you switch off the auto option and automatically this minimum and maximum that is grayed out here that would be activated. So, for a specific zone if you want to know that where my particular this kind of velocity is there you set up that as the minimum and the rest maximum from there that zone the coloring of the contours that would also happen. So, these are the very fine things or I would say advanced things that you can modify you can generate with this post processing tool.

Now, since these are the This requires the licenses and also here you see so the color combination is that from blue to red. Blue is the lowest value, and red is the highest value. So that you can also change. And you can zoom in on the particular part, the particular color.

And again here you see that the pressure contour, once you check the pressure in which there would be option whether it is a pressure, or other kinds of pressure, as per the definitions they have incorporated. So, accordingly, those values would be plotted here. See, this is the smooth pressure. It is not banded.

That is why there is a smooth transition of colors here. So Various options are available, but again, as I told you, this is not about looking at how good graphics you can make or come up with in your model. It is essentially about what the XY data is. Because XY data gives us further insight into it, and in the plot option, you have these XY plot options. In XY plot, again, the plot direction first has to be set. In the Y function axis. So, these are quite intuitive once you go into these dialog boxes.

I need not highlight all the options because these are quite intuitive, but the plot direction here is quite important. Depending on the plot direction, whether it is X is 1 or 0, this plot would happen in this case. So, here you choose say y function is pressure and x is the direction vector and if you then plot it, it will have an x y plot. So, now the setup is complete setup was already completed and this solution is also once you update it, it would show that the solution has also been updated or we have got the solution. See the solution would be updated and it would show a green tick button besides it and then the results have to be analyzed.

So in the results again if you specifically go to the result. So if you specifically now go to the result option. So it would show this window. This is now you see that here it has its own post processing part which is here called the CFD post. So, in the automatically CFD post processing part it would open here and there you have the flexibility to report several things.

And few things are shown here for example you want to insert the contour. So in this sub menu that you see here or the menu whatever you call it there. So there you can generate your desired contour by leveling it at first say the density, pressure, velocity etc. that is shown here. say for example, the velocity is set here.

So, once you create a contour for the velocity then you choose the domain part that for which part you want to have this contour. Now, since it is there it is for the entire domain and so again. So, once you choose it for the entire domain. location is the point that we are saying from here on the side bar in low from the side this three dot pattern we select all the faces or all the surfaces the variable we the pressure or the velocity because we have named this as the velocity. The range is, say, default global, and here we say apply. At this corner, we say apply.

And what we see is this: the velocity contour that we can generate. And then again, with the help of this view option, the zoom in, zoom out, or the fit to window, all these options you can adjust your view. And, it clearly shows that the blue option is the 0 velocity which is near the wall if you look at this closely which is that means no slip condition was retained and the there near the middle or at the core of the flow, which is the maximum velocity, which is a typical parabolic velocity. This is again for the pressure contour that we see. The point is again here, similar to our previous window. Here, this global range can be changed, and this color combination can also be changed.

Here, the contour parts that are shown are in number 11, which you can further reduce or increase for the smooth plot. So, all these options would be available, and then what you see. As per your requirement, you plot this data. But the point is again, once you update this, your result analysis is complete. So, beside the result, you would also get this stick option that the result has also now been analyzed.

So, the whole set has now been analyzed, and it is important that you save this whole project as, by your chosen file name, and you save that object. So, this brings the window of, or the demonstration of, a particular CFD tool, which is ANSYS Fluent, where we have taken a simple problem. Now, what I have not shown here is the verification and validation. The point is, once these results are obtained, it is up to you to show how accurate these results are. So, at the end of this course, we will discuss verification and validation in detail, but the point is that validation is where you ensure that your developed model is capturing the correct flow physics.

And verification is a process by which you get closer to that accurate value that you determine from the experiment or from the analytical solution. So on this note, I will stop here, and from next week, we will have a new topic or new sessions on other things that were mentioned. So with this, I hope you have an idea or overview of the particular CFD tool that we demonstrated here. Similarly, if you work with a different one or if you work with any open-source software, you have to go through these processes, but the point is these functions would be there as well. So these are universal functions that would be there whether you use any commercial software solver or any open-source software.

So on this note, I again thank you for your attention and will see you in the next session.