CFD APPLICATIONS IN CHEMICAL PROCESSES

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Lecture 33: CFD Tools & Modeling Single-phase System

Well, everyone, we are back with another lecture on the simulation setup in a course that is CFD applications in chemical processes. So, we are discussing the implementation of a 2D pipe flow problem, a laminar flow problem. We have discussed till now the geometry part—how to draw the geometry—and we have also discussed how to mesh. taking a simple example of this 0.2 meter diameter 0.2 meter height sorry this is the 0.2 meter wide pipe and say a 3 meter length so in that case so we have seen this meshes the grid generation the default setup how to modify it, and how to name the different edges in this domain.

And then we go for the setup option, where we need to set up the solver and the boundary conditions. So, we have seen this Fluent launcher option. In this Fluent launcher option, we can choose the double precision because this will help reduce the computational time and enhance accuracy. So, we will choose the double precision solver and the other necessary settings that are defined, particularly the choice of parallel processing units or the parallel processes that one can use. Depending on your workstation capability, you can use that, but also at the same time, Fluent has its limitation for this number depending on the licenses that you purchase.

So here, we choose this double precision, and then we look into these options—that is, the start—and then we came to this window, which is called the solver window. This is the part we covered in the last lecture. So once this mesh is successfully read by Fluent, which is the processing part, now we will discuss the processing part. So here, you can see the meshes, and you can see I can identify how this inlet and outlet have been identified.

So, here this blue line that you have seen identifies the inlet part. And here this red line that you see this identifies as the outlet part and the arrows accordingly it is automatically shows that thing. Now, here there are few options that I would like to tell you, but before that if you look at the console the details of whatever the means statistics that can be seen here. How many nodes are there? How many quadrilateral cells are there?

All the details that you can see or you can read from here as well. Here you can see that what are the inlet, how many edges you have defined, what are the surfaces that you have defined, all that information that you can see. And here in this part that you will see, The meshes again you can scale it if you had drawn earlier in a different dimension. So, you can using the scale option you can scale these dimensions.

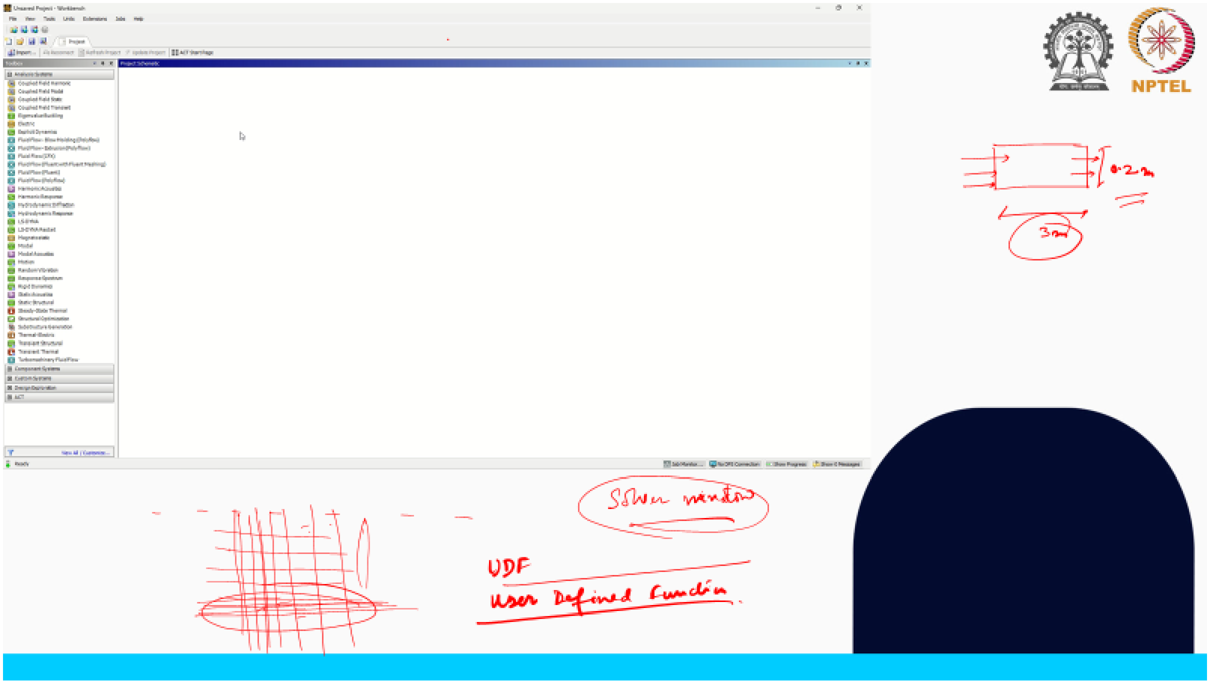
Here is the mesh check option that we discussed in the last lecture during discussing the skewness of the meshes. The point is the mesh quality can also be reported by clicking this option that is the report quality. Here you can look at the units and accordingly work with the proper units. These are the solver type that it uses that is the pressure based solver or the density based solver. Here is the velocity formulation which is absolute or the relative velocity.

These are the options for some problem specific because say for example in the porous media that we will discuss in the multiphase system. So, we had two different kind of velocity one is the interstitial velocity the other one is the superficial velocity. So, the velocity formulation is equally important and that comes part that comes here. Here is the whether we would like to do the steady state simulation or the transient simulation and here whether I have a plane I have a this geometry whether I wanted to convert it to axis symmetry or the planar cases. So different options that you can see.

So accordingly, once this solution interface would be there, there are also here we see a series of options that are available. If you look at it, different kinds of models would exist. Now, each of these plus buttons that you see besides, say, for example, models, materials, sales zones, so all these can further be expanded. And once you expand, what you will see that this model, there are options where you can go for the, say, multi-phase options. So once you expand this models you would see that there are different other models that are available that I was talking about say for example multi-phase option that exists

but since this is a single phase problem we will not switch it on whether energy is involved in this calculation whether heat exchanger radiation different species etc all these things are by default off now whether your problem is inclusive of these multiphysics problems whether it is a heat transfer problem. Now, these different solver these different models would actually then has to be activated. The other vital part that the beginners usually miss is that this is the gravity option in several flows gravity have to be taken into account and if that has to be then you have to switch on the

gravity and accordingly once it is activated there will be options for the direction of gravity now the point is even say you have a downward pipe flow ok instead of this horizontal flow. Now, then the downward pipe flow what will happen the gravity would act on it in the direction of the flow. Now, you can consider say here this geometry is also a downward flow. Now, how to make that the solver understand such scenario. Now, in that case if you switch it on the gravity and since this is our positive x direction as per the design modular that we have designed and this is the positive y direction, then you have to define the gravity in the positive x direction. ok in the direction of the positive x the gravity is working and then automatically it is actually the real case where the pipe is vertical. So, accordingly you can adjust the setting of the problem although you have drawn the geometry horizontally, but if you define the gravity in a appropriate directions the orientation of the flow directions can be changed. So here these are the different options that you can see.



I would just read those options if it is it would be clear for you. So there are multi-phase option, energy, viscous which is the SSTK omega. This is relevant for the turbulent modeling, radiation. Heat transfer, species, these species are relevant for the chemical reactions. When we will discuss, we will see the species options.

This is the dispersed phase. Again, dispersed phase is one of the modeling strategy in the multi-phase flow modeling. Solidification and melting problem, acoustics, optics, structure, potential or lithium ion battery. So, battery case and all configurations can also be included or the solver would be adjusted according to that if we switch on to this options. The next option are the materials where you have to choose the material.

That a fluid is flowing, it is fine, but which kind of fluid is flowing, the solver can only understand by understanding its density, viscosity and the related physicochemical properties. Those can be defined in the material section. Now most softwares or the solvers are preloaded are preloaded with this database of material. So, you need not define the water properties if you are using it as a standard fluid that is flowing or at a standard temperature pressure condition. So, if you want say simple water is flowing at an atmospheric temperature and pressures its property are already loaded.

If you want that to be operated at different temperature and pressure where the values are not as such the default values you can change that in the material option as well. Then, we have the sales zone conditions or the different zones where you can define different conditions or I would say the different flow conditions, different regime conditions. Here in the next step you can define the or in the options here you can define the boundary conditions specifically. So, similarly there are several methods are there and then there is a solution. where you have to set the monitoring part that before setting up the problem.

So, let us go into this setting up whatever we have now discussed. So, these are the options that are available and as I told you that we will choose the laminar option because here what you can see in the model we choose the go to the viscous because this we would be considering a laminar flow. So, when we click on the viscous. And then we see there are a lot of options available, whether it is laminar or inviscid. And again, for the turbulent modeling part, when we discuss it, you will hear these names: the Splart, Almaraz, Keefe, Ceylon, Komega, and all, etc.

SST model, Reynolds stress model. So, different kinds of turbulent models are also available. Here, different variations of the K omega model, different options for the K omega model, etc., are available, but these would be switched on if we choose any of those options. For example, here K omega is switched on by default, and accordingly, the SST K omega model is chosen. So, its corresponding default values of the different parameters—this you would realize—are the values of the model constants in the turbulence modeling part.

But here, we choose the laminar option. So, here we choose the laminar option. Now, see, once we choose the laminar option, all the additional information that was not necessary for the laminar case is automatically switched off. Then we click OK for this. So, the laminar model is now set for us, and then we go for the materials, as I told you that there is a fluid flowing, and here it is showing air by default, OK, but here we have our own fluid.

So, here, as this window shows, So here, as this window shows, you have the create or edit material section. So here, what you see is the tab to create material. Once you double-click this air option, this window appears, and you can see there is a create or edit material option. So here, the material name is air, the material type is fluid, and the material that reads from the database is air.

Now, here is a database that Fluent has. So, in the Fluent database, once air is selected, you can see the default density and viscosity values it reads from its database. If you have a different value that is experimentally determined or if you plan to use something else then you have to change those values here and then you have create option, and then you can close this window. But here, what we will do We will go to the Fluent database, and here you see there are 568, at least in this case, different preloaded materials.

Once you select it, its properties will be shown, and accordingly, you can choose it. So, starting from carbon dioxide, hydrogen, nitrogen, different things are there, and here we will choose the water liquid option. Okay, because the water vapor option is there. Once you click it, then you see here that its properties—density, specific heat, thermal conductivity, etc. All values are already taken from the database.

If you have to change anything—say, for example, the thermal conductivity, the specific heat, or viscosity—if it is changing instead of constant, you have to change it to your user-defined value. You can change it to variable, and you can plug in here one thing called the user-defined function. In Fluent, there is a common terminology called the UDF, which is the user-defined function. So, this user defined function or as a user defined function you can plug in your variable density, variable viscosity that changes as per your empirical relation that can be plugged in. So now you see here on this right hand side water liquid is also added here.

And so there are several properties are there and also for which temperature it is there that is also mentioned in the reference temperature. So those things automatically appears here. Now if your material is not listed out of this 568 material in the database that is apparently there in this version of the ANSYS Fluent, you can always create your new material. You can always feed in the data that you have experimentally determined for your unique material and you can generate or you can contribute to this database that is locally stored. Then you close this window and what it makes that it appears here that the water also appears in the material section.

But it has yet not been defined. So in the fluid section you see along with air the liquid water also appears here. But it has not been defined that this water is flowing here. So that also we have to do. So, now if we see that this cell zone conditions through which it would flow the cell body the surface body that we defined in the mesh generation section.

We select it and when once we select it we see that the material name is was by default is air. And before you can change it you had to add that material in the material section. So now here you will have an option to choose from that which material is flowing based on the material that you have added there. So it may happen that different fluids are flowing through different inlets. So, accordingly, those fluids, those regions, those zones would appear here as sub-zones, and then in those zones, you have to define your flowing fluid.

So, here we choose that the liquid water is flowing, we apply it, and then we close this window. Now, here I will highlight another feature because, as you see, This window appears, and you have to select the water. You would select water. There are several other things that exist here.

If you look at it, one of the things is the porous zone. So here, the things are the porous zones. In future lectures, we will discuss multiphase modeling or, if not multiphase modeling, if there is a porous zone through which some fluid is flowing. So, instead of a completely empty pipe, if this is a porous material through which a single phase is flowing, If that is the case you are trying to model, then

you have to switch on this porous zone option here. You have the option here that this is the green zone, this is the cell zone, which for this problem we are considering empty. But if that is a different problem having a porous zone through which fluid is flowing, then we can set this zone as a porous zone. And then this option here which is grayed out because the porous zone option is switched off here. Once you switch it on this porous zone option will be activated.

Here the porous zone. There the relevant properties has to be given. That means the permeability option, the direction of flow etc. that has to be set there. Also, there are few things which are you see grayed out here.

One of the other term is the source term. Now, say consider there is reaction happening. So, a component is going into this single phase although it is single phase system. So, say two reactants in liquid phase are moving or going into the system is reacting and producing again the product in liquid form. So, in a simple way this can also be considered as a single phase flow flowing together of different components and product is coming out.

Or say if I define the porous zone which means I have say catalyst stacked in the bed that creates the porous zone. So catalyst surfaces that can be coated with some reactive material and when a fluid is flowing the reaction can happen on the surface and the product is coming out at the outlet. So such complex scenario in a single phase system can also occur. We will discuss how to model such scenario in the multiphase section stating the fact that multiple thermodynamic phase can be considered as single phase while CFD modeling. This may sound a bit awkward to you those are the beginners, but the point is.

Multiphase in computational fluid dynamics does not mean that it has to be essentially three or multiple say thermodynamic phases or thermodynamic state ok. Even a single say liquid phase of two components I can consider that those as the multiple phase of two liquid phases of two liquids. So these things we will discuss in details in the multiphase modeling section. But the point here is that when you switch on the source term because say component is getting generated or by some other mean there is a source term of that component. So once the source term is switched on here the source term tab there will be this one would be active.

activated and there you will see the relevant properties that has to be set or given to the model before it can solve the problem. Similarly, here is the reaction option ok. So, this once the source term is there this reaction would also be generated or be activated because the reaction can also act as a source term for this component. So, this again the reaction how it acts as a source term we will discuss when we will discuss the reactive flow system.

But the point is these grayed out options you have to also look at very carefully because the last option here or in this case is there the multi phase option. This multiphase option would also be activated or eventually will be activated if we consider the model to be multiphase one instead of the single phase laminar flow. If we consider that there the multiphase single or say laminar flow exists then this multiphase option would be activated here. Similarly, depending on the problem statement there are several things are there. please look into the help file or the details of those solvers that you will be working with and accordingly get the clarity on what are the properties you have to feed in.

Now, once we apply this material we define that through this zone the water would flow then we have to now define the boundary conditions ok. So, the point that sequence that I have we have gone through is that we have specified the laminar flow model, we have specified the material or we actually selected the material that which is which material is flowing and we have set the through which or through this zone which fluid is will flow ok. By default air is there for this solver, but we have said that as the water and then we have to set the boundary conditions.

So, now, once we expand this boundary condition button. this boundary condition here, when we expand it we see the names that we defined in the meshing section or the meshing part. You remember in the meshing part we defined those as the inlet outlet wall because once we select this or once we choose one of those accordingly we have to set the boundary condition for that. So, again if we select that this inlet option, this would again once you click it this inlet option, it would window would appear like this, where it is showing the name that you given that you gave that time as the inlet and this different criteria. where you have to input your value or the properties.

Now, here you see this is initially the momentum. The next which are grayed out are essentially thermal, radiation, species, DPM, dispersed phase modeling, multiphase, potential structure, UDS. We will not go into the details, but few names you are now acquainted with. Say, for example, the multiphase options. If the multiphase model is selected, then it will be activated.

Species, the reactive species, dispersed phase modeling—again, a different type of multiphase modeling, etc. But the point is, Here, since only one option is available—that is, for momentum—we have to define the values or the flow rate at the inlet, but it only accepts velocity magnitude. So, that means here we are defining this as the velocity inlet, and the specification method is magnitude and normal to boundary. From the dropdown option, there will be other options—for example, you can provide a user input function. That means if you are already considering a fully developed flow, you can define a fully developed flow profile at the inlet.

Flat velocity, which we are considering here—the magnitude and normal to boundary—or any other flow profile your problem requires. But here, we will proceed with the magnitude and normal to boundary options. The reference frame is absolute. The velocity magnitude must be defined, and So, here, the initial or gauge pressures will not be specified because we will only define the velocity magnitude here. Specifying both these two would jeopardize your simulation.

So, here we will define a velocity profile or the velocity magnitude because that will automatically convert to a profile based on the magnitude and normal to boundary values. So, anything you define here is in meters per second. So, here, say it is defined as 0.1 meters per second. We apply this. So, this is what we have given as the velocity value. And then the next option is the internal, where the liquid is flowing. We will not define anything there; we leave it as it is. Then we select the outlet, and here we see again the reference is

the absolute or relative to the cell gradient. There is a gauge pressure, and there are other options, such as whether there is a backflow, etcetera. Those are there or not. We leave it as it is because this is open to the atmosphere. So, we consider this as the gauge pressure at 0 at the outlet, and accordingly, we leave the other options as they are. So, we leave the other options we do not consider for the reverse flow and we also not considering a targeted mass flow because what we expect is to reach a conserved flow that is whatever the inlet that in the outlet that mass has to be conserved.

So, once it is done we then go for this wall boundary condition where if we look at it in the wall boundary conditions there are the two walls that we defined we click that and what we see is that these are the stationary walls. So, again there are the different values or different criteria that we can see. that stationary wall moving wall and the shear condition we can specify whether it is no slip shear specified slip specified shear, but since here it is stationary wall and we consider no slip boundary conditions we just apply these things and close this. So, if we change anything, then only we have to apply it; otherwise, we can close it. So, what we have done is that we have now set the boundary conditions.

The inner boundary thing—that is, the inner surface boundary—has been created by the solver. When we do not need to, we do not change anything in that interior. We keep the default values. And since the pipe is stationary, we keep the default pipe wall boundary conditions also as stationary. So, that means we reached a stage where again if we look back we have set if we go back to this workbench point we drew the geometry, we had the mesh, we had the mesh done and then we came to the setup where we have now set up all the parameters.

That is required. And how did we do it? We have done the choice of model, the addition of material, then defining The cell zone condition—since here it is empty, we need not change anything. But if it is a porous media, if a reaction is happening, if some source terms are there, then we have to change the cell zone condition. In the boundary condition, we have defined our required boundaries and boundary properties.

So, this actually sets the problem. Now, we have to do the solution of it or the methodology and before that we have to initialize the problem or initialize the solution and then go for the solution that we will continue in our next lecture. So, today, whatever we have done, I have just summarized it—we have come to a point where we have now set up the problem with the required boundary conditions. And in the next lecture, we will see its initialization, the solution initialization, and the solution of this problem. Till then, I thank you for your attention.