

CFD APPLICATIONS IN CHEMICAL PROCESSES

Prof. Arnab Atta

Department of Chemical Engineering

Indian Institute of Technology Kharagpur

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Lecture 31: CFD Tools & Modeling Single-phase System

Hello everyone, welcome back to another lecture on CFD applications in chemical processes. Today, we will see how a typical CFD solver looks by taking an example, because by now we have understood the fundamentals of the finite volume method. We have discussed how it works and several other things, and today I will try to show you where those ideas or concepts are actually implemented in a CFD tool. So, what I have thought of is that we will use a popular CFD solver called ANSYS Fluent, OK?

ANSYS is the company name, and they developed or, in fact, acquired a software called Fluent. Initially, it was known as Fluent. So, Fluent is a software or a CFD software name. It is based on the finite volume method (FVM) solver. The governing equations that you develop, if you solve them using the finite volume method that we have seen in previous classes,

you can develop your own code, but if that is not the case, you can try to do it through a software. One of the popular software that professionals use for CFD solutions or simulations is ANSYS Fluent. This is a typical example, and by no means are we endorsing ANSYS Fluent. You can solve it in OpenFOAM. There are other softwares star CCD and all these things are the star CCM and

of the most popular ones, I will try to show you how it looks and how a simple problem, such as a 2D pipe flow, and that too laminar, can be approached. If this is your first CFD simulation, you will see how step by step such things can be done. Because we are starting for the beginners as well and that is why we will initially start with the 2D pipe flow. That means a 2D representation of a 3D pipe considering it.

So the point is what we will try to see? We will try to see the velocity magnitude contours. That how the velocity variation is happening. How the pressure variations are happening. So velocity, pressure, the velocity profile, not only the magnitude, how the velocity profile also look like. So one thing can be the velocity magnitude along a line, along a plane, along a cross section or across a cross section. And similarly, when we try to plot it, those things how it looks like in a velocity profile.

The point is the reason of choosing this thing is that for such simple problem, go to any fluid mechanics book you find a standard analytical solution. You put the input values or this pipe dimension, you can in fact get this velocity profile, pressure profile, velocity magnitude at any

location. So, what it helps taking the simple problem is to understand that how it is implemented in a CFD tool. And when we compare, when we do the model validation,

we say that this is the model validation, that means whether this model is working correctly, whatever I have developed or whatever we will develop, whether it is giving me the correct result. that we establish by checking or comparing this prediction. So whenever we solve something in a CFD platform or a CFD solver or a code, we say this is the predicted value. Then this predicted value should be compared with the experimental value or the analytical result.

If those matches or at least closely matches, then we can say that we have some confidence on the developed model. And then that developed model can further be used for predicting some unknown vary or unknown means some the variables that are not easily quantifiable by experimental means. So, for example, in your laboratory, you have a pipe, a pipe flow experiment, you measured it.

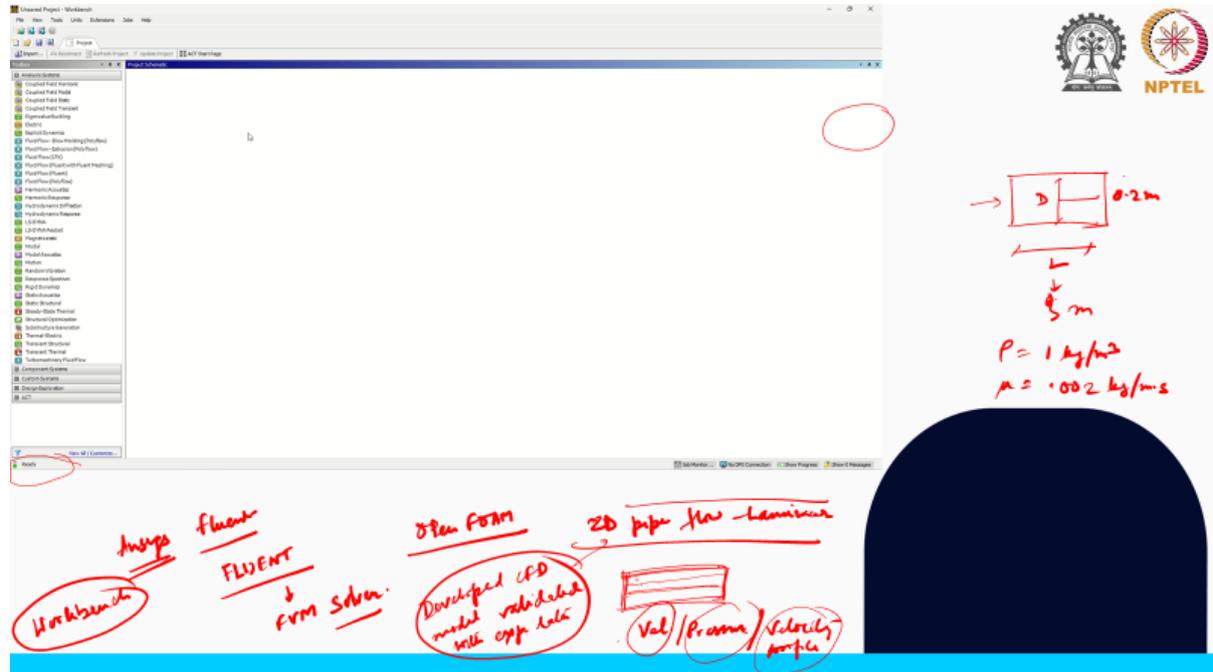
But in a laboratory scale by simply say open eye or in fact with the camera, can you capture that how the velocity profile along this axial line. or say what is the difference between the velocity profile along the center line and a line closer to the wall. That is difficult to collect such information from the simple experiment or in general the experimental say these are the cases. This is the pure example. Now, similar situations can happen with more complex geometry and more complex flows where the

experimental understanding of certain points or certain parameters are extremely difficult to quantify. Now, there comes this developed and validated CFD model handy which means that a model is developed in CFD. You have checked certain parameters with the experimental value that it is fine. The CFD model is giving me the accurate or more or less accurate result with certain degree of accuracy if it is not exactly matching. So, we say this is the developed and validated.

So, developed model CFD model that is validated against or with the experimental data. Now, this model can help us predict scenarios that were difficult to quantify by experimental methods. That is the utility of this CFD model, along with other things that we will discuss later. So, one point is that it gives us insight into the flow that is not easily comprehended by experimental analysis. So, the point is, for example, here we have a problem—say, a 2D pipe flow problem.

say the diameter is the D and this is the length L . We all know the values say the diameter is of say 0.2 meter, the length is say 3 meter, this length is 3 meter. say a fluid is flowing that has density of 1 kg per meter cube, the viscosity say 0.002 kg per meter second. So, the point is,

all the physicochemical properties or chemical properties of this fluid flowing through this pipe are known to us.



The diameter of the pipe and the length of the pipe—the dimensions of the pipe—are essentially known to us. Now, we have to check the velocity magnitude, the pressure magnitude, the velocity profile, and the pressure profiles also. And finally, we will see how this CFD model stands against the analytical result. Because such problems can easily be solved analytically, and we can get the result.

So, for that, if we open ANSYS Fluent—which is essentially called ANSYS Workbench, where ANSYS Fluent is one of the modules—ok. So, we say that we open ANSYS workbench that is the workbench. because it is not only the fluid flow problem ANSYS solved or it helps us solving there are several other things that are there and it is a combined package for several problems in which fluid flow can also be solved. Now it is not only fluent there are other modules also available with ANSYS Workbench.

If you look at it on the left hand side what you see different modules are shown in which here we have one thing which is ANSYS Fluent for solving the fluid flow problem. There are other different modules available and that relates to different subjects or different physics. here you see there is another software called the CFX that also solve the fluid flow problem, ok. But that is for a different kind of flow which will not will different type of solution process

we will not go into the details which we will follow that this ANSYS fluent we will select it, ok. So, once the ANSYS is loaded you will have a screen like this and this left hand side of

your screen you will see the series of simulation packages that are offered by ANSYS. Now here we will use ANSYS Fluent. So what we usually do is that we

if you look at it now this small video that here this is these are the different modules that are available there in which we will drag and place the ANSYS fluent here so let me show you once again so in which we choose the ANSYS fluent and drag it on the open space among this different module we choose ansys fluent and place it there and what it shows this kind of a screen again this kind of a window where it shows so this is basically a standalone kind of a module

that now is there in a workbench now there are series of operations that has to be done in this ansys fluent Here, if you look at it, this actually has loaded the ANSYS fluent that is evident and it has a series of operation that we have to perform. So, to complete any simulation, what do we have to do? We have to create the geometry starting from the beginning. The point is,

Since these are commercial software, they try to make our lives easier by showing the sequence of steps. The sequence of steps is like this: first, we define the geometry, and then we make it. So, define the geometry and then we mesh this create grid then we set up the problem that means, we define the boundary conditions material properties etcetera etcetera on that or say whether it is a steady state whether it is a unsteady state different relaxation parameter values and all this thing that we discussed.

Then it says to proceed with the solution. The solution starts—this is essentially what we call our processing part. So, this still setup you can consider this as the specifically this geometry and mesh you can consider that as the pre-processing part and in the setup and solution you essentially process the solution or this process this problem and finally, you have result.

Once you have the results, these results have to be analyzed. So, here are the sequence of steps that have to be done: in the setup, you define the boundary conditions, solution methods, and report the function, OK? In the setup, you also define what your accuracy tolerance limit is. Those criteria are essentially given there. So, now, the point is the first step is to define the geometry. Now, to do that, we will first determine whether it is a 2D or a 3D analysis, OK?

So, we click this geometry tab. And again if you look at it here this arrow or this blue button, blue small arrow shows that it has some other functions that means the advanced menu options are available. So, let me just show you how that happens. So, now when you click on the geometry.

You see there exist different advanced level suboptions or the menu. And here it gives options since it is a huge software this ANSYS workbench. It gives me or gives us several options to

create the geometry in different platform. That is, say the new discovery geometry, new space clamp geometry, new designer modular geometry and etcetera. So, here what we will do?

We will do go to this new design modular geometry. That means, this design modular is essentially my preprocessor where I will develop the geometry. I have to draw the geometry. What we do? We click that option and we see here the status. So here it shows all the status that if you just look at it, the previous screen, you will see this is the point where

the status of your work progress is would show now in this bottom corner you see the starting design modeler after you have clicked it and then this design and modeler would be launched and that would look like something this So it gives us a canvas and by the look at this point or this corner, you can see that which version of the software has been used or you are using. And here are the x, y, z axis levels are there, you can rotate it and accordingly your design will rotate inside this canvas. So, I will just erase this part so that it does not create any confusion.

So, what we see here is that the option in several softwares also exist not only and also it depends on version to version that means when this 2023 is used or maybe the recent versions when those are used you can find a different type of those advanced options, but the basic methodology remains same. In fact, in the beginning itself you may have an option to change or to choose the domain dimension or the analysis type where you can choose whether you are going to do 3D or 2D analysis.

So, the point is those different modeling the different geometry solvers that exist depending on that you have to choose your appropriate menu in order to come to this design modular area. And then in the design modular area what you have the default unit that it will have are there is in usually in centimeter. And this you can also set in the setup that what would be your default values are there, default domain dimensions.

So, when you see this geometry you would be able to look into the different properties and there. So, design modeler we have opened and here we have to change the default units that are there to centimeter because our problem is in the meter. So, accordingly we can choose that. So, when we select this x y plane ok, we have to select the x y plane and accordingly you see that it has been adjusted the view has been adjusted which were initially in the isometric view, but it has now been adjusted to the x y view.

So, that we can start on a x y plane because we would be working for the 2D problem. So, by doing this click on the Z and to make the sketch normals to the screen, what we have done? We have done here the switching of it. so let me once again show you so once it is open we click on the xy plane that is here if you look at it this xy plane once we select the view changes and then just to look at the xy plane we further

Rotate this so that it is aligned with our XY plane and now it has been aligned with that XY plane that we have seen there. So, we have attained a step where we can see the x y plane. Now, we have to select a rectangle at first because this is a 2D pipe flow problem that we are doing. So, at first we draw a rectangle and then we will define its domain. So, what we will do is that we will

draw a rectangle from the toolbox that are given there again that would be highlighted when we select it. When we do that our sketch would be complete and then we need to convert that sketch to the 2D geometry ok. And because that has to be defined as a region where the flow is happening because remember the fundamental of solving or making the grids or generating the grids are that the grids would be in these positions where the flow is happening okay so accordingly if you look at it

So, at first we try to do this if you look at it there is this rectangle option and then with that option we essentially draw a rectangle from the center. So, that this is the line that is aligned with the y axis and this line is aligned with the x axis. So, this actually completes this rectangle drawing and then we see here different options are there in order to modify dimension or putting the constant etcetera. So, once we define this. we go to this dimension because dimension is then important.

So, that is why we went into the dimension box and then if you look at it that this length has to be given a certain value, certain dimension as well as this diameter that is there. So, this is one dimension that we have to define and this is the other dimension that we will define. So this is the second dimension. Now here you see in this region in the dimension part we see H1 and V2 which means this is the H1 that we see here and this is the V2. So, here these are the dimensions currently and this has to be modified as per our requirement.

So, these values have to be now modified as per our requirement. So, these values are then modified as to 3 meter and the diameter is of 0.2 meter. Once we enter it, we see that it is from the dimensions initially it was in the order of 30 meter or so. it is basically this blue small width that has reduced to we cannot work in this domain. So, we have to fit to this dimension to the screen and for that if you look at it there are several buttons at the top ok.

So, here there are several buttons that actually adjust this view. These are the view adjusting buttons options are available. Once you hover the cursor on it, it will show you a small help that what it is to be done or you can click and check what is which function does what kind of action. So, once this is done we basically again on the screen if you hold and drag it you will see the our desired domain that has been drawn here ok.

So, now what we have to this is what we call where now we have to go is to the concept menu and the point is in the concept menu we can get the option of surface from this sketch because

this has to be defined as a surface. in which the flow would happen. So, this is the skeleton that we have drawn and then we go to the concept menu from there we create the surface of this sketch because currently it is just the outline. So, once you see this is done here the surface is created

So, initially if you look at it, if I go back to this, when we have drawn this, there was only x, y, z planes and all these things were there. But once we go to this concept menu after drawing this. the sketches surfaces from the sketch what you see along with the x y plane here we have the surface option available. So, here you see the surface option is appearing that means the surface has been created which is labeled by this. so what we see once we select it and click it on this domain we see that we have this option

that appears as a base object which has to be applied and according to that that one surface has been generated by clicking on this generate button here this generate button gives us this drawing of this sketch this is the generate button that is there and it helps us in drawing this sketch so now we have a surface body if we select it it shows that this is the surface that we have created okay so the point is here we have created a surface

and all the details of these are given here, but the surface it is showing here that this becomes a solid body, but here we will have to have a fluid that flows. So, we have to change this option from solid to fluid; we have to change it to the fluid option, okay? So, we select the fluid option there, and then again, we generate it. So, whenever we have to apply something, we have to click this generate button again and again to generate that surface, set that value, or patch that value to that domain. And then we go back to this geometry again to the workbench where we started with from where we started by

clicking the geometry and we see that a tick option has appeared on the geometry which was earlier or not there. This means we have completed the step of creating the geometry. That is why this tick mark has appeared. The next step would be to generate the mesh. But I will stop here today. In the next lecture, we will show how the meshing is done.

And the further setup of the problem can be done. Till this part, if you want, you can access the student versions of this ANSYS Fluent that may be available in your institution or can download from the ANSYS website for 30 days or so or so limited period. You can check for the trial period. You can look into it and give it a try. So, with this, I stop here today, and we will continue this discussion in the next lecture.

Thank you.