

CFD APPLICATIONS IN CHEMICAL PROCESSES

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Lecture 02: Introduction

Hello everyone, welcome back to the second lecture on CFD applications in chemical processes. I am Arnab Atta. In the last lecture, I spoke about what is CFD why it is essential and its variations in terms of different software packages that are available in the market and why it is so. But as I told you that all the processes have a similar structure or the algorithm to solve it. So, basically what happens is that when you have a problem in hand while setting up a CFD simulation the first thing that is done is the geometry modeling. So, which means we at first draw the geometry or the domain for which this the process is happening or for the area that you are interested in to look into the flow dynamics.

So, the first thing that is important is the geometry modeling and for that sometimes you have may have to do certain simplification of the actual geometry. if required that you can do, if not you can use that complicated geometry as it is, if you can afford that computationally or your by your computational hardware. Now, the point is such complex geometry are usually drawn in the CAD softwares ok. So, those CAD geometry are sometimes imported in the software or in the CFD solver. But that is the tricky part because sometimes it works, sometimes it is not if the geometry is very critical or complex.

Say for example, your geometry is having several nuts and bolts and etcetera in terms of its structural stability. But the point is in the case of this flow dynamics understanding those are irrelevant because that is not necessary to have in the computational geometry for the CFD solver to have those nuts and bolts because flow is not happening there. it is the outer shell or some structure that you are having or giving it for stability. So those have to be removed before you import that in the CFD solver or some CFD solvers may have the ability to remove that after this import. So you can draw a very complex geometry in your favorite CAD software.

Several of these softwares the CFD solvers that I mentioned already those have the ability to import those CAD geometry. They have the compatibility but depending on their limitations as well they give a typical file structure that if this has to be imported it has to be imported in this kind of file nature with a particular file extension name. So once that import is done your geometry has to be set. The other way is to do that most of these or in

fact all of these CFD solvers have a unit called the pre-processing unit. So broadly classified what I can say that all CFD solver have a pre-processor

then actual solver and then they have the post processor. So, what is done? As I told you in the preprocessor those geometry can be drawn independently instead of your CAD software. You can draw the geometry there in the preprocessor There also the preprocessor unit contains defining or generating grids or meshes. I will come to that. In addition to that what is flowing? That material, that material property, that fluid property etcetera are usually set.

Those all happens in the preprocessor unit. including setting up of the boundary of the initial condition. Once it is done it is solved in the solver part. Once it is solved you basically get some x y z data. or with time if it is a time dependent sub simulation you get t x y z this data along with several other scalar quantities and the flow properties those are basically a table of data those has to be analyzed analyzed and has to be plotted So, plotting is basically one way of analyzing the data. Whatever way you want to analyze that can be done in this post processing unit either if you are fond of animation you can generate animated file from those data. if you want a 3D contour you can generate a 3D contour there if you want a x y plot you do that in the x y plot in this post processor unit.

So, this is the basically overall structure of any CFD solver. Now, as I told you if I go specifically in the preprocessor unit the first step the critical step is the geometric creation. And as I told you if there is any complexity in the geometry that you can simplify or approximate in this geometric creation. And then what happens is that as you are approximating or as you are anticipating certain geometry or certain simplified geometry. Remember that you are already have started incorporating certain percentage of uncertainty or maybe some error in the simulation.

If you do so, if you approximate the geometry, if you think, if you anticipate that this can be the simplified geometry. Because it is important to understand that what we are doing here is the simulation. the simulation of the actual process and that is why the benchmarking of the prediction is extremely important. And that is why in simplified cases as I told you in case of say single phase laminar flow this kind of cases the actual flow actual result and the simulated results merges. There is hardly any error in the predictions for the simplified cases.

But as the situation gets complex, this deviation increases. That is what is your actual or how do you understand what is actual? You basically experiment or you have the analytical

result available. You benchmark your simulated result against that analytical or the experimental result. because everybody says what you see is that you believe and that happens in experiment.

But then what is the utility of the simulation? I am just going a bit out of context here because there are these two views. One is that what you see that you believe is the experiment is the whole truth that is true, but then you do not get extreme details the minor details of all the phenomenon or all the species transport or all the minor details that you cannot experimentally measure. But with this simulated the validated and simulated result you can have those details. By experiment observation as I told you earlier you basically have some empirical result or empirical fitting of the data.

Sometimes it is difficult to state the physics just by the experimental result that what is happening inside the system. But once you validate the at this CFD model with those experimental result then you basically are capturing the physics the flow physics of the system of the process. Because this is a certain set of governing equations that you are solving in CFD and these set of equation tells the physics that what is happening. and if it is validated with the experimental result it matches with the experimental result which means the same thing is happening in your experiment. So, I would say both are complementary ok. So, you have experimental result you validate that

I mean you have your CFD result, your CFD result is validated with the experimental result, you get a robust CFD model and then you go on predicting for a certain or a different operating condition, different scenarios with that CFD model and that is the beauty and application of the CFD model. different scenarios with that CFD model and that is the beauty and application of the CFD model, Just simply validation is not that useful. until and unless you did not know the physics in the experiment what was happening that is told by the validated CFD model. So, coming back to this thing that once you have your geometry ready ok. So, you have to define boundaries that means from where the flow is coming from where it is going out of the system.

one is called the inlet the other one is called the outlet which are my impermeable wall that means, where across those the faces the flow is not happening. So, those have to be identified in your geometry and has to be marked in that preprocessor unit. Once you do that then because this is important because you have to always remember you have to make a small grids or meshes to solve the governing equations. Because, in finite difference method you have also seen which is the preliminary concept has been taught in all the

courses core courses starting from your fluid mechanics, fluid dynamics, transport phenomena even in conduction heat transfer this finite difference method. Where you had this I if this is the x directions that I say I and this is the j.

you had this calculated at this i j junction, this points. These are called in computational fluid dynamics as the grid or mesh or even cell. Different terminology you may find in different textbook but popularly we call these are the grids ok. So, we have to divide the geometry into small computational cells where this scalar or the vector quantities are calculated and stored. How that happens we will discuss in due course, but once your geometry say for any arbitrary

is drawn in the pre-processing unit you have to divide this in small number of parts that is called the meshing ok. Once that is done Now these are the cells that I told in the previous lecture that for the laminar case liquid phase if I try to have the mass diffusivity understood I told you that in general it requires a 3 micron grid size for the gaseous phase it requires 300 micron. So this is the size that we were talking about that time. that the size that the length if I consider this as a square one then this size or the one size one side length scale is in the order of 3 micron. Now consider this is to be of a industrial scale application process where you have the dimension in meter in the order of meter.

So now you understand that there would be the millions of sales or even sometimes it goes order in the much more higher than the millions of sales. So that is why it becomes computationally expensive when there is a complex geometry at the industrial scale length and also for the complex flow processes where multiple physics are involved that not only the fluid flow is happening there is also temperature change that means the energy equations to be solved there is mixing happening there is reaction happening when all those are augmented it becomes a Herculean task So, coming back here so, once the geometry is drawn then we draw the grid, the grid is drawn and then we set the solver that means, by which process we try to solve it. That means, if the flow is laminar we use the laminar flow model, if the flow is turbulent we have to use the turbulence model, if there is reactions happening we have to add some module for the reactions.

So those sub models or the models are then here added to the system that these are the things I have to solve. At the same time we also set the properties of fluids. or the things that are flowing as well as through which it is flowing say for example definitely if it is water or air flowing through a certain channel we put the properties of air or water along with the surfaces through which it is flowing if it has any specific surface properties ok

because whether there will be slip there will be no slip those are the boundary conditions that we have to set in the next step. But whether the surface has any specific property, whether the surface is hot or not because based on that we have to set the boundary condition.

So, that means, naturally after this the things that comes is setting the boundary conditions. Boundary as well as say we can say the initial conditions that at t is equals to 0 what is the scenario. and as well as what are my boundary conditions which means if I know the flow velocity the superficial velocity by with which it is entering a system that means we know its velocity at the inlet we have to calculate pressure at that point. if we know that this is coming with this much of pressure then that means, we do not know initially what is my velocity at the inlet. So, accordingly the inlet outlet and any other phases have to be set as appropriate boundary condition.

We will see in this context of boundary conditions there are several other boundary conditions called symmetry, periodicity and etcetera. We will discuss those in detail when we come to this specific topic, but the point is that where it is coming where from where it is going out those are the faces or the areas we have to designate as the inlet and outlet of the system as well as the walls of the system through which the flow is not happening because remember always that the grids or meshing are done in those places where flow is happening not on the walls or other places where flow is not happening it is mandatory to understand or it is let be very clear that the meshes are the computational cells where the flow is happening So, in those cases or those places the grid should be there in other places it is not.

And once it is done then we solve it. We solve here again I would say this is I would say solver setting. and I would say the solver process. In solver process what is then set is the say iteration method. If it is a time dependent process steady state unsteady state process. whether you want explicit solution or implicit solution or implicit methods the solution by the implicit method or the explicit method. So, these softwares have this capability that allows you to have or to go for the iterative processes, time dependent processes, implicit and explicit processes, your Setting up of the convergence criteria. Because convergence criteria you understand that you set when you compare two consecutive iterative steps.

That whether I reached my desired level of tolerance. That is set in these solver processes. that difference between the two values of the two consecutive iterative processes are set in for minus 5 which is I consider is negligible and I consider that these are identical or fine

I am ok with this differences. So, if that happens I stop my simulation that is where the this is where you set such criteria ok and then finally, you solve it and then you get the data where you start your post processing which means you analyze your result. So, these are the steps in CFD simulation irrespective of any CFD solver.

We go for this step by step processes and it is very I would say appealing. for any commercial software where you have this nice graphical user interface the GUI they have all these buttons readily available and you may be attracted to click those buttons as many as possible and you may think that you are trying to solve the problem complicated way but easily but that is not the case the rule is that keep it as simple as possible anticipate what you are trying to get because, but this anticipation comes after a lot of trial and error research that this is how I think the result would come. because in several cases you have because when you first set up this problem you have your experimental data or the analytical data available because against which you will validate your CFD model.

Remember here one key point that I always say is that the CFD model or the CFD simulations these are validated by your experimental or analytical result not the other way round. that means CFD simulations are benchmark or validated against these experimental or analytical results. Do not say that I have validated the experimental result by my CFD model that is a completely wrong sentence because as I told you the analytical solution if you get that is the whole truth or the experimental result that you are seeing that you are believing is considered to be the truth.

So, you are validating your CFD model or the CFD simulations against this truth not the other way round that you are having the whatever you have considered in your CFD simulations that you are then benchmarking this CFD results with the experimental results and you are saying that my experimental results are then ok that is not the case this is completely wrong. So, now considering this in the post processing unit the first objective is to analytically check the quality of the result here one of the vital thing or the most important thing in CFD simulation for any process this first step that you must do is called the grid independency test okay it is called the grid test or grid sensitivity test which means you started with a certain number of grids in the first or the second step.

Your results whether those are dependent on these number of grids or not. Say for example, here you had 10,000 number of cells or grids. You got some result X versus Y. You plot it X versus Y, you get some result or some trend. you have your experimental data against which you are validating your result say these are your experimental result. For 10,000

number of cells you have this strain ok which is reasonably ok when compared to say your experimental data and that you can also calculate taking the percentage deviation at each and every location. But then whether this is your grid independent solution or not to check this you have to increase the number of grids

to further higher level or sometimes at a lower level. Say for example, you reduce this number of grids to 5 k in your next iteration, in other iterations you increase it to 15 k and 20 k. That means, 5000 cells, 10000 cells, 15000 cells and 20000 cells. Then when you plot all those 4 simulations, you say then started to get this kind of a result. This is for the 5k, this is 10k, this is 15k and this is 20k. it clearly shows that as you increase your number of sales you are marching towards or having more accurate result when you compare with your experimental data or the analytical data which means your results are still not grid independent. after having 20 K you increase it to further 30 K or 40 K and see that the result is lying there itself that this line has hardly increased and giving you this green continuous line for 30 K.

Then you can understand that you have reached a limit after which if you are increasing your number of sales by 10k your accuracy hardly improves. There comes the trade-off between your hardware resource, computational time and the accuracy that you are looking for. This trade-off is then critical. And at this juncture, if I am okay or fine with this sensitivity of the 20K number of cells simulation, I can say that I have reached a grid independent result at 20,000 number of grids. After which, if I increase my number of grids, the accuracy improves by 2 to 3 percent or maybe 5 percent at max. and which is acceptable for me. So, that is why in order to solve the simulation or to solve the problem quickly because as the number of cells grows your simulation time increases for a specific hardware resources.

So, for me 20,000 is sufficient and I call this as the grid independent simulation or the result. which is the first thing that we require in the post processing part. And after that there are other several aspects that you have to look into which slowly we will discuss in the next topics as it comes. Because this is the quantitative analysis that at first we have to do in terms of grid independent solution, but then there are other certain aspect that whether the model is capturing correct physics or not. Okay because if my trend that is required is say experimental data are of polynomial in nature and I am predicting a straight line then there must be something wrong. So whether we are capturing the correct physics whether we are accurate enough these are the essential immediate part in the post processing unit.

With this, I will stop here today. I will see you in the next class with a new topic related to this fundamentals and we hope that you will be learning it as smoothly as I am trying to convey. Happy learning. Thank you.