CFD APPLICATIONS IN CHEMICAL PROCESSES

Prof. Arnab Atta
Department of Chemical Engineering
Indian Institute of Technology Kharagpur

Week-12

Lecture 60: Validation and Troubleshooting in CFD

Hello everyone, welcome back for the final time on this course that is CFD applications in chemical processes. We are discussing the validation and troubleshooting in CFD, and specifically in the last lecture, we discussed what verification and validation are. The key difference between these two terms, or the technical difference between these two terms, is verification and validation. Also, we have understood why we often, or in general, say that the validation of the CFD model is only mentioned, despite the fact that verification is also equally important. Again just to reiterate to refresh your memory the validation is essentially tracks or it is the quantification

whether you are solving the right set of equations or the right set of governing equations. It actually quantifies the uncertainty in your model, and that uncertainty is generally caused by the lack of knowledge. We have discussed several factors regarding what can incorporate uncertainty in your model or what can add uncertainty to your model. Taking an example of the input uncertainty, physical model uncertainty, the submodels uncertainty, or the closure model uncertainty, etc. At the same time, verification is also important because it quantifies the error, and this error is not caused by the lack of knowledge.

Again, the lack of knowledge means the lack of knowledge in developing the governing equations or the flow physics in order to track that. This errors essentially comes from say the coding error or say the wrong choice of the differencing schemes a differencing scheme may not be suitable for that particular kind of problem. So, those are actually quantified by verification. And one of the key steps in order to make sure that you do the model verification is by the grid sensitivity study or the mesh sensitivity study.

So, verification is about checking whether the solution process of the developed equations is correct or not. Validation essentially ensures whether you are solving the correct set of equations or the right set of equations. Now, the point is, there are a few things that we can suggest, in fact, to those who are doing research in these areas. They usually come up with some recommendations that one can follow, so that the initial that are associated with your, say, first simulation, if any of you are doing the first time the simulation in a software,

in a CFD software, how to ensure that you go smooth on that. So the point is, we have seen the preprocessor, there are three parts, that is the preprocessor, then the processor part and we have post processor. So, the pre processor part that we understand in fact, we have learned by now that in the pre processor part what is happening we draw the geometry. Now, this drawing of the geometry

can be done in a third party software or say in a different software or a different module. Although the commercial CFD softwares have their own pre-processing unit where you can develop it, but if it is not done, if say it is done in any CAD softwares. We have to make sure that the CAD geometry is complete for the flow simulation. That is the first recommendation. That the geometry has to be accurate enough in order to replicate what you are trying to simulate.

Because you have a real geometry, you are trying to emulate that in a drawing. So the CAD drawing should be as perfect as to the real drawing. Now, sometimes it is not possible, so we try to keep it simple. Now, when we do that sometimes we tend to make it extremely simplified design. In that case, naturally we may omit several parts of it, several internals of it, several critical junction of it and

then the CFD prediction accuracy is lesser compared to what could have been done if the geometry is made properly. The point is, smaller details in those CAD geometries sometimes matter. So, if there is some junction, some bifurcation, some convergent diverging area those intricate details are also that actually matters when you try to simulate or emulate that drawing at first in a CAD geometry. We have to make sure that the placing of the boundary conditions, the appropriate boundary conditions, is correct for the geometry.

So, initially, we are talking about the part which is the drawing geometry and the grid design, because this is the part that is done in the preprocessor. So, what are the useful recommendations or useful suggestions? Say, for example, symmetric boundary conditions. Be careful while using the symmetric boundary conditions because of the reason I mentioned several times that despite the geometry being axis symmetry or has a if the flow symmetry does not exist or you do not anticipate flow symmetry, then that can lead to wrong

kind of calculation or not the actual flow—it would not track the actual flow physics. So, this symmetry boundary condition restricts the solution to the symmetric solution kind of, and no transport is allowed across that symmetry plane. So, if you place the symmetry boundary condition, be sure that—or you are ensuring that—across that plane, nothing is transported. So, you are ensuring that. If you are doubtful about that, then you cannot use the symmetry plane for that boundary condition.

Whether it is 2D or 3D, the point is, a 3D geometry that you see in real applications, we try to simplify it in a 2D manner and with an axis-symmetric domain. By doing so, you make sure whether we are losing because we definitely are reducing the domain dimension and whether for that we are losing any critical or vital components that is not captured by such 2D or 2D axis symmetry domain of a full 3D one. Say for example, this bubble column. It is a fluidized bed.

Although these are done in a 2D cases but specifically for the bubble column and all you would not have say the accuracy or say real flow trained if you do it in a 2D bubble column the simulations. although laboratory scale 2D bubble column exist with a thin width very minimal width and a vertical column but the point is that for the real case it does not make any sense when inflow and outflow are not known exactly so if your inflow and outflow are not known exactly, then from the geometry standpoint those say faces or planes should be placed as far from the point of interest as possible. So, say for domain this domain you do not know how much inflow and how much outflow is going out or say one of those

you do not know how much it is and your point of interest say this plane here on this plane what is happening. So, it is that you extend your geometry and try to place the inlet or the outlet far away from the zone of interest. With constant pressure outflow, this outlet condition with a constant pressure specify the direction of flow or the outflow. For example, say normal to this plane, this actually would ensure or it would minimize the pressure difference across the surface. So, the direction of flow is also important.

And this is typically is associated with this boundary condition. When you try to assign that from a default software, you will have, there are two options. One is placing the value as well as the flow direction. So, you must ensure that the default option which is there already is according to your expectations. If it is not, you have to change it.

So, if there are multiple outflow boundaries ok, if there are multiple outflow for a particular design or a particular case that there are multiple outflow or multiple collection zone, then it is desirable to or it is recommended to use the pressure outflow option the boundary condition. We should avoid or try to avoid non-orthogonal cells close to the boundary. So, avoid non-orthogonal cells or meshes near boundaries. The angle between the grid line and the boundary should be close to 90 degrees.

Okay, we should try to make ensure that, but that is the point that happens that when you apply mesh generation button that takes the default mesh generation scheme of the safety solver, you do not ensure that. To ensure that a particular zone will have your defined type of meshes, cells, etc., you must have complete control over the grid generation. This becomes very critical or important in the case of complex geometries.

Although the flow problem may be simple, a single phase flow but if the geometry is complex then even you are not able to capture that accurately by the CFD solutions because your grid generation or the mesh generation are not appropriate. Usually, several software tools take into account a factor called the skewness value or skewness factor of the meshes. This skewness of the mesh or the factor gives you a value—if it is closer to one (this depends on the software; you must follow their guidelines).

But typically, the range varies from zero to one in several software tools, and one is not desirable. A skewness factor closer to zero is recommended for that particular software. So, this factor you have to identify where it exists, how it works for the software tool that you are using or if you are developing your own code then you have to follow or cannot avoid completely—the placement of non-orthogonal cells near the boundary.

So, this skewness is a measure that skewness value or skewness factor. So, usually the angles of this grid line and the boundary line or say wherever you are placing it near the wall or somewhere the skewness would be defined by that angle and it is generally kept in between 40 to 140 degree. So, maximum skewness should not be more than 0.95 ok, the maximum skewness value should not be not more than 0.95. The average value can be in the order of 0.3, if it is lower than that it is very good, extremely good quality meshing.

Make sure after drawing the geometry and generating the grid you check the grid quality and the grid quality would be resulted by this kind of factor depending on software to software or solver to solver so grid check is important which most of the time we forget those who are doing it they can realize that hardly they check the grid quality but as a beginner if you are a beginner make sure you Do this practice that once a grid is generated you check the grid quality and ensure that no portion where the say any convergence divergence exist or any sharp edges exist.

There usually the mesh quality tends to be awkward or not very good quality. So, in those places whether it is really smooth or refined meshes you have used and the skewness values are less than the desirable one or less than equals to the desirable one. The choice of equations will not go into that details because now I realize that you understand what is validation because validation checks whether you are solving the right equations to track the actual physics. So the choice of equations, developed equations, we are not going to details.

Now we realize that you have clicked the simulate button or you have started the simulation. you have to make sure that you check certain criteria to ensure the simulation has converged. Because we generally say whether the simulation has converged or not. So the convergence are dependent on the criteria that you set. So, poor convergence is the most common numerical reason for poor predictions.

The reason is that the residual that you define and completely trust varies from problem to problem. And that residual value, by which you ensure convergence, is also problem-specific. So, you cannot rely on the default values. So, the point is, for a steady-state simulation, you might see that there is a convergence problem, which means the steady state does not—so the solution does not exist, which is not right in those cases.

The residual should always be combined with other measures of convergence. It is not that you completely trust only the residuals. So, not only on the residuals but also some other parameter to ensure convergence. So, what are the different convergence criteria that can be used? Say, the different criteria can be mass, concentration, or any other variable of interest, okay.

So, that ensures you reach the pseudo-steady state for a transient condition or transient simulation, or you may have reached convergence of the solution, although your residuals are not converging to the desired level because you may have set very low values. We have to monitor the integral quantities of the solution-sensitive variables. So, it is recommended that you check integral quantities. of solution-sensitive variables. Monitor at various planes or points.

It is not only at the outlet or at the inlet. Monitor at various points or planes. Plot the residuals to evaluate whether the solution is poor or in some region in the computational domain. So, global balances are important, as I told you, along with the residuals—the mass, momentum, energy, etcetera—you can check whether these are balanced or not. In order to enhance convergence, if there is poor convergence, you have to ensure that you are using the robust numerical schemes because now we have seen in several places we apply different differencing scheme different solution algorithm say for example solution of matrixes and etc so say for example we should always try to solve a system with higher order this differencing scheme, not just first-order. If it is not solving with the first-order, try to go with the higher-order schemes, and you will see that it actually enhances the convergence and reduces the under-relaxation parameters.

You should try playing with the under-relaxation parameters that we have also discussed. Under-relaxation parameters in commercial software are of a default value. try changing those in order to reach the convergence try to reduce it once you reduce it which means you are taking more of the previous time step value in the case or iteration values and lesser of the next iteration values that helps in converging the inner iteration loops faster.

So, try to solve the steady-state problems transiently because, in transient simulations, the steady state would be attained if it is a steady-state problem. Solve for only a few variables at a time. that if you are developing a complex model that has multiphysics or multiphysics involved, or different variables involved, try to develop that first with the simple basic construction or the single physics of the model.

And once it is predicting well with a benchmark problem, then try to augment that, enhance that, or make it complicated with the other flow physics. It is a kind of one-by-one approach: if you have a variable density problem, first try developing a model with a constant density to see whether it is working or not. Once it is working fine, then you change the density to the variable density. This is one example that I am giving. So the point is also sometimes when you initialize the problem—this is all about the chances of converging in order to enhance it. So you initialize the problem.

Now, that initial value also dictates the speed of convergence. So, try with different initial guesses, if because the default options in the commercial softwares are sometimes the initialized from the inlet, from the outlet, from the whole domain such options are available. You should try to examine with those options or maybe your own intuitive values. Now, use the coupled solver for high-speed compressible flow.

Because the thing is, the highly coupled flows with strong body forces or flows being solved on very fine meshes—in those cases, we should be using the coupled solvers. And we have to keep in mind that the coupled solver and the segregated solver—these two solvers are there. Segregated solver and coupled solver. So, as the name suggests, the segregated solver means it solves a kind of one-by-one model or equations, but the coupled one takes everything together and solves it together. So, quite normally or logically we have to keep in mind that this coupled solver requires a double of nearly double of the more memory.

than the segregated solver. So as per our computational limitations for a given problem, we can try that as well. But coupled solver is more robust. To avoid the numerical errors, this we discussed about having a better convergence. Now to have avoid the numerical error, the first thing that comes to my mind or it should come to your mind is to use the higher order schemes, the higher order differencing schemes.

The first order can be initially used. when you have this convergence issues, but always you have to make sure that the solutions are I mean the problem is solved with the higher order schemes. The point is this first order schemes may lead to the problem with the numerical diffusion. We have to also estimate the discretization error by showing that solution that it is a mesh independent. This is the thing that we discussed several times.

Mesh independency or mesh independent solutions. So, this is basically kind of a research specific recommendations also that try to use this node based gradients with unstructured tetrahedral meshes. Now what is unstructured? It is not having a uniform size or shape of the meshes, particularly the shape of the meshes. It can be combination of various structures.

also there would be you would find there is a term called the body fitted mesh ok. For the complex geometries these terms appears in the CFD simulations and those are again quite research specific, but I would say that the unstructured tetrahedral meshes when it is used we should be using that with the node based gradient calculations. the discretize at the same time of the mesh independent result our result should also be discretization scheme independent ok. That is the one check that you can do in order to reduce this numerical error.

Refinement or say the coarsening of the computational mesh. So refinement is necessary wherever we have the critical part we think we have to capture sharp edges, sharp curve, diverging, converging portions etc. And, the coarsening part say where you we this is simply simple geometry simple structure we have where we need not require that much of fine machine. So, the combination of these effectively increases the computational efficiency and also the numerical error can be minimized by refining the grids at the certain location. So, the mesh spacing mesh quality this also improves the numerical error.

The other thing that we should remember that in transient simulations particularly again there is a time step criteria we have seen. So, we should be we should use the lower value of the time step when we initially start the simulation. So, we have to start with the short time step and slowly we can increase in. There are nowadays advanced solvers which can adapt this time step that we call the adaptive time stepping method.

Initially, it starts with the minimum value that you give, and as the simulation progresses, depending on the convergence criteria or the convergence tolerance limit, etc. It generally increases step by step, although you are not doing it manually; the solver does it efficiently.

Okay, the point is regarding turbulence modeling you can start with the simple one that we discussed regarding the turbulent model simulations or different turbulence model, but again depending on the cost of your computational power and the time you have to find a trade off with your objective and the computational resources.

So, many physical phenomena may not be captured by the turbulence models, and that adjustment you have to make with your computational power, okay? The point is further the turbulence modeling depending on the model that you use it requires wall function, wall refinement etcetera those are also critical when there is a boundary layer problem exist. So, we have to be very careful about the grid refinement or say I would say the adaptive grid refinement that wherever it is necessary the grid is finer, where it is not it can be coarser.

For the reactive time step in reactive flows, we have discussed this in the reactive flows part separately, but in the turbulent flow part, we will discuss it separately. For the multiphase cases also, when we have discussed these multiphase issues, the choice of solver and how it is done. In fact, for the turbulent cases, we have already done those things. And we have now understood what the typical recommendations are—the generic recommendations we can provide. But again, you have to keep this in mind: no specific model, no one model is, in a generic sense, the best model for a class of problems.

Even in a class of problems, there may exist different complexities. So, we have to check different models or, depending on the objective—what to look at or what to resolve—we have to come up with a suitable model, an appropriate model. So on this note, I will stop here and I hope you had a nice session throughout this course that helped you to understand from the very fundamental of the CFD to

of various areas—for example, multiphase, turbulence, reactions, etc. And finally, we try to summarize this with generic recommendations. So on this note, I wish you all the best for your exams and all future prospects, and I hope to see you in a new course, another course sometime soon. Thank you for your attention.