CFD APPLICATIONS IN CHEMICAL PROCESSES
Prof. Arnab Atta
Department of Chemical Engineering
Indian Institute of Technology Kharagpur
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Lecture 59: Validation and Troubleshooting in CFD

Hello everyone, welcome back to another lecture on CFD applications in chemical processes. Today we will discuss few recommendations although I told you during the lectures the previous lectures that there is no uniform or generic CFD model that can be applied to all the relevant problems. it is entirely depending on what you have in your wish list or what is there in your objective, the kind of computational resources that you have and accordingly you decide what is the best CFD model for you.

But still, the point is, for a certain class of problems, you can have generic recommendations because Extensive research has been done. So, instead of starting from the scratch, you can always do the literature survey or literature review and take up the recommendations or guidelines in order to start from a point where it need not be that tedious which would have been if you start from the scratch. Now, you have chosen your model.

You have set up the grid and the problem. If you remember, I told you that in a classical CFD solver, there are three parts. One is the pre-processing, one is the processing, and the other is the post-processing part. Now, in the pre-processing, what do you do? You draw the geometry, the computational domain.

You define or simplify your complex computational domain into a domain where the calculations will take place. And to do those calculations, you have to create meshes or grids in that computational domain. Now after that comes the processing part. In the processing part, you apply this

discretization models or discretization schemes be it finite difference finite volume or finite element method or the advanced method such as other boundary element method and all these the point is in that processing the calculation takes place Once the calculation is done, then comes the post-processing part. What happens? You have the XY data or XYZ data of different variables that you intended to calculate. That means the pressure, temperature, concentrations, turbulent intensity, or whatever the components are.

So those data you have to post-process, either in terms of graphical representation, bar chart, contours, or mesh plot, etc. That you can do. That means it has to be interpretable, those data, or you have to analyze the data. So in this background, the point is you encounter several problems during the simulation, and that is where troubleshooting is required. At the same time, once you have the data or the result from the post-processing, you have to make sure that data

that you have generated or predicted are in line with the experimental observation or actually in line with the physics analytical solution that can be. Now since the application of CFD is intended for situations where experiments have not been done, or it's a new situation where conducting experiments would be difficult, or you want to have some proof of concept without the laborious experimental processes. So in those cases, the CFD models act as predictive models. So, how do you validate that, or how do you make sure that your results that you are having are practical or physics-inspired, that it is not deviating from the physics?

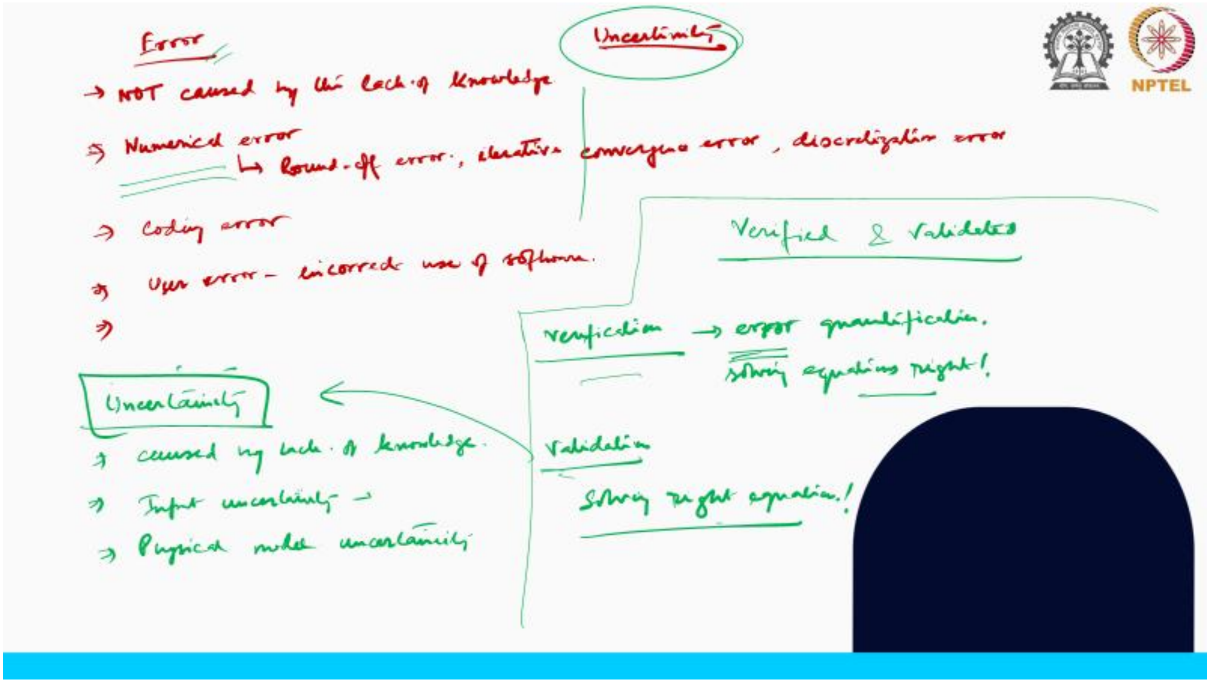
So, that happens. So, that there are two things that you have to take in into account one is the error in result that how much error you have, what are the errors in your predictions and the other thing is the uncertainty in your prediction. There are two different things which we often intermix, OK. So, the errors that happen are examples of error, say, the numerical error, the coding error—whatever you have possibly coded—that is, there is some bug in the software or, say, the user error.

So, the errors that happen are not caused—you have to remember— by the lack of knowledge. Now, lack of knowledge means I am talking about the flow physics. I am not talking about the coding language, etcetera, because if you had that knowledge, possibly there would be no coding error. But the point is, this error in the context of CFD modeling, we tell that there is the chance that this error is not caused by the lack of knowledge.

That you correctly have anticipated that the flow physics would be like this, and accordingly, you have adopted a model or you have developed the governing equations, and while executing it, there can be numerical error. Numerical errors—the example, say, the round-off error. There can be iterative, because we have seen these processes are iterative in nature. So, iterative convergence error or, say, the discretization error.

Remember we used different say differencing schemes during the calculations in a particular discretization scheme. Say this upwind first order second order these differencing schemes also introduces the truncation error. okay or say the error associated with consideration of certain terms of the Taylor series expansion and that is why we said the first order accurate second order accurate etc. So, this upwind central differencing first order this kind of things are actually comes under this numerical error where it is not your fault. while developing the governing equations because you obeyed the physics the flow physics is intact.

But while calculation this rounding of error of considering certain number of decibels or say this differencing schemes the choice of differencing scheme etcetera that can introduce this numerical error. As I said that there can be some bug or coding error. and this error that happens due to the user error. That means, the incorrect use of software ok, but this uncertainty This uncertainty is essentially caused by lack of knowledge.



for example, input uncertainty. That means, say you had limited information for a problem and you used some approximation that is not in line with the physics of the problem. And you set say the boundary conditions in a different way than what it should have been. That is your lack of knowledge about the problem or about the physics of the problem. So say physical model uncertainty.

So this input uncertainty that can happen due to limited information and your approximation to represent the geometry. Say you had a geometry which is say axis symmetry. But the flow physics would not be because there is certain scenario. For example, the temperature change and etc. where and that there is a gaseous state or the gas is flowing.

So, naturally there will be natural convections or some other phenomena by which the flow symmetry would not be there. But you have assumed the geometry to be axis symmetry and you have modeled accordingly. So, that is the input uncertainty. the boundary conditions the wrong boundary choice of wrong boundary conditions also the material property you didn't consider the material of the proper phase that is the gas liquid

and etc or even their properties physicochemical properties you have chosen it in a wrong values that is the lack of knowledge and that results in uncertainty of your model the physical model uncertainty Actually, that happens when there is a discrepancy between real flows and your CFD adaptation of it or the model adaptation due to inadequate representation of physical or chemical processes. For example, turbulent combustion, etc. or due to oversimplification of the problem.

Say there is a compressible flow happening or there is a gaseous flow happening and the density is changing but you missed that part and you considered and modeled it as an incompressible flow. Whereas it should have been a compressible flow. In practice it is a compressible flow. In reality, it is a compressible flow. So definitely, the model would not be accurate or it would give a wrong result. So this, there say we simplify or sometimes oversimplify the problem because we understand due to this

complex geometry or baffle, et cetera, in a heat exchanger, there will be turbulent motions of the fluid. But due to oversimplifications, we model that particular geometry. Considering there will be diameter flow. So that would not certainly give you the accurate result or the desired result. So wherever combustion, turbulence, etc. is happening, if those are intense, you cannot simplify those just for the sake of simplicity or just like

we say assume this thing, assume that thing, that does not work in such scenario. So, the point is input certainty there is input uncertainty as I said that the domain geometry giving the example of the flow symmetry there has to be flow symmetry in order to consider axis symmetry boundary condition or axis symmetry domain. Otherwise, you cannot. The boundary conditions, if you do not have, say, sufficient information, and instead of pressure inlet, if you define velocity or something like that,

then it would not be correct. And also the fluid properties, the appropriate fluid properties, whether it is compressible, incompressible, whether it is a variable fluid property, because if there is an exothermic reaction, we have discussed in the last lecture, that if there is a variable property due to this exothermic reaction, the viscosity density will change. But if you consider that constant throughout the domain, throughout the simulation, then that also causes problems. This physical model uncertainty is actually stem from the lack of validity of sub-models. That means, for a whole problem like multiphase flow, we require a closure model.

Now, for this phase-phase interaction closure model, there are several closure models, for example, the Gidaspow model, the Schiller-Naumann model, et cetera. Now, those are developed for a certain category of problems. So, if you do not understand and choose by default, they set a default setting where, for example, your system is operating in a liquid-liquid system. And, for example, this Gidaspow model has not been derived for this liquid-liquid system, but rather for the gas-solid or solid-solid interaction. Then certainly your model would not give you an accurate prediction.

So, then what is to be done if your system is unique? You have to develop those sub-models. That I have a multiphase model in which these phase-phase interactions are modeled like this.

And that has to be fed to the system or fed to this code as a user-defined function or user-defined equations. A complex flow may involve entirely new or unexpected physical or chemical processes that are not accounted for in the original sub-model. Because the original sub-models

they may have proposed that as a generic solution because they have operated or experimented for a range of conditions. And your situation is outside that range of operating conditions. So you are expecting and anticipating that you would find something new, unique, and that is why you are looking at that particular window. And you are using that previously proposed correlation which is outside the range of your objective.

So, in absence of a better sub model you do not have any option but to work with this less sophisticated model and that results in the model uncertainty or the result uncertainty. Now there can be situations that despite the availability of the comprehensive submodel, you may have deliberately chosen a simpler submodel in order to make your life easier. But then again the problem is that it would not give you the accurate result, because it would not account for those complex physics or it would not resolve those complex physics. Say your objective is to understand the very critical turbulent fluctuations for a small scale operations which can possibly be done say by DNS or LES at the max.

but you are doing it with a RANS based model which is further say zero equation model or one equation model. So, definitely you would not be capturing that in order to make your life simpler, but your objective is not met although you are using some kind of turbulence model. So, the point is a complex flow may include some mixture of physics chemistry as the original simple flow, but may not exactly of the same blend which requires the adjustment of the sub model constant or the empirically fitted constant. This is the example we had seen in cases of say modified Ergun equation when we spoke about the packed bed modeling case.

That depending on the shape and size of the catalyst particles through which gas and liquid are flowing, the Ergun constant values has to be tuned or adjusted in order to predict the pressure drop more accurately. So similar thing can also happen or you have to do that whatever the empirically fitted constant that you find in a correlation that could be used as a closure model. Even if you are operating in a particular or the similar window or the operating condition, but there is some new physics or a blend of physics or a multi-physics problem, then the point is that those constant, those empirically fitted constant have to be also adjusted. The empirical constant

Within the sub-models are essentially the best fit for the experimental data, which themselves have a certain level of uncertainty, and that is why those experimental data or experimental points are represented by the error bar. After several repetitions, they take the average value, and the uncertainty is presented by the error bar. So that itself is accompanied by a certain level of uncertainty. So the empirically fitted constant carries some uncertainty into the model. Also, there exists a certain lack of validity in simplifying assumptions.

For example, there are steady-state operations and unsteady-state operations. You are not solving a problem in an unsteady manner, but rather, to simplify it, you are solving it as a steady-state case, which should not be the solution just for the sake of simplicity. incompressible compressible so if there is any adiabatic problem and heat transfer across the boundaries but you are considering that as an adiabatic system that also is not right there are multiple species in the problems or in a reactive system or a multi component there are multiple phases that has to be resolved

but you are for the sake of simplicity or in the name of simplicity you are not accounting for those So all these things boil down to a situation where your model results have to be verified and validated. So there is verification and validation of the model. Verification, Actually quantifies this error. Error quantification. That means it is a process by which you determine the model implementation accuracy.

The developer's conceptual understanding of the problem. And solving the equations correctly. This is the most important part. That whatever equations you have developed actually come from good knowledge or sound knowledge of the problem. This is the error part that you are quantifying by verification.

You are solving the right equations. But whether those equations are solved in the right manner. So that these numerical errors, truncation errors, etc., are not there. So, this verification quantifies the error, while validation quantifies the uncertainty, which means whether you have correctly predicted the physics or not, the trend of the result or not. Validation checks or quantifies the uncertainty, which is a very vital part because uncertainty is caused by the lack of knowledge.

If you do not have the right knowledge about the problem, your model can go anywhere. I mean, it can go in a completely different track. So, validation is the process of determining the degree to which a model is an accurate representation of the real world. From the perspective of the intended uses of this model. So, here you are checking whether you are solving the right equations.

This is very vital—whether I am solving the correct physics, whether I am tracking the correct physics of the problem or not. Here, your governing equations are based on the correct physics. But then here, you are solving equations that you have developed correctly or not. So, here is the right equation, and here are the equations—whether you are solving them in the right manner. So, that is why validation and verification are both important.

And most commonly, we use the term 'validation of the CFD model' or 'validation of your predicted model.' The reason is that we first try to understand whether we are capturing the right physics—the flow physics—or not. And that comes from validation. And that happens through the comparison between the experimental result, if it is available, or the analytical result. Now, that too happens for some benchmark problem for which experiments have been done or analytical solutions are available.

And that is why it is extremely important that when you solve for a new system that has not been explored earlier, you apply your developed model to some benchmark problem and observe. So now, your question may be: if I have developed a model for a new situation, how can I apply it to the benchmark problem? This developed equation is essentially based on the standard equations or on the standard platform. The point is, for that base, whether your equations are correctly tracking the trend or not—you can always check by switching off those additional terms or the convoluted terms. in the code or not making the system more complex because on some base you are augmenting your problem so at first correct that

baseline or check that baseline and that is you do by validation of the model and then You have some solution. You are tracking the correct physics. You are on the right trend of the predicted result with the experimental or the analytical thing. And then you come closer to the accuracy level by checking the verification state that whether now I am accurately solving.

Because you remember in the finite volume method we essentially comes to a solution of a set of matrices AB is equals to A or AX is equals to B where you solve the AX. Now, this method, there are several methods that helps in solving those simultaneous algebraic equations and we have not discussed those because we consider those as trivial at this moment because there are several methods available, Gauss-Jordan, Gauss-Siedel, etc., TDMA. The point is which method is correct or accurately capturing that. Now your focus may be on that level or say the differencing scheme, changing the differencing scheme from first order to second order

or to some higher order in order to reduce this numerical error that you see in the verification stages. Or say refining the grids, mesh independent simulation. There you basically go closer to this verification level. And several times it has been seen that that actually works and in fact in any CFD modeling this grid independent simulations or grid independent results are essential. And because that closes down this numerical error.

If there is coding error, you have to troubleshoot. If there is any debugging that you have to do for your own code, you have to do that. And most importantly, it is very tempting if you work with commercial CFD solvers, which has a nice graphical user interface GUI. To convolute the problem, to make it more complex by switching on several parameters that you may not know why you are doing. You just augment or switch on those parameters or those problems, or say those—I would say the dropdown menu selections of those—and that actually unnecessarily convolutes the problem.

So it is recommended that you keep it simple and after that you do the verification and the validation before you go for your own problem prediction because the developed CFD model lies in the model prediction for the operations that have not been explored or done earlier. So, on this note, I will stop here, and in the final lecture of this course, The thing that we will discuss is the best practices or some recommendations that may be helpful for your research problem, coursework, or project. So, on this note, I thank you for your attention, and we will see you in the final lecture in the next lecture.

Thank you.