CFD APPLICATIONS IN CHEMICAL PROCESSES

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Week-01

Lecture 01: Introduction

Hello everyone, welcome to a new NPTEL online certification course titled CFD Applications in Chemical Processes. I am Arnab Atta from the Department of Chemical Engineering, IIT, Kharagpur. So, in this course, this is a new course that is being offered. So, in this course what we will cover that I will discuss with you today, so that you get a brief overview. that what is coming. We will also look into the application of this course because CFD is a word that you have possibly heard. And, some of you are interested in the CFD applications and this course is mostly would be focused towards the chemical processes. So, as a prerequisite it is expected that you have the basic understanding of fluid dynamics, you have the basic understanding of transport phenomena that are the core courses in chemical engineering and several other branches similarly. Now, as the name suggests this is CFD that is the computational fluid dynamics its application in various chemical processes. So, computational fluid dynamics as the name suggests as you can understand that it models the flow dynamics that

means, there has to be some flow in the system. And, you have heard the famous Navier-Stokes equations. The genesis of this CFD is that to solve this Navier-Stokes equations in various complex situations where it is not trivial or non-trivial to solve the Navier-Stokes equations analytically. In various complex cases this Navier-Stokes equations cannot be solved analytically and in those circumstances CFD comes handy. So, there are other modeling and simulation techniques. So, why CFD is basically important or why we should be learning CFD? The reason behind that most of the traditional modeling or the simulations that we do those are mostly based on the empirical or semi-empirical correlations and that is for a specific data set or a range of operation. Now there are situations when you will encounter that you have a data set, but you have to predict the scenario or several flow dynamics beyond that operational ranges that you are already aware of.

In such cases a validated model by that you develop in CFD comes handy to predict those scenarios. Now, we will discuss several scenarios where those are important and why we should be learning CFD because it has now become a day to day modeling tool for various operations. As chemical engineers or other branches you may be familiar with the term that is called unit operation. Several unit operations any industry, chemical industry, process industry and all are composed of several unit operations. which means that those are having a similar kind of physics or chemistry involved, but at a different scale or for different applications. Say for example, separation distillation various reactions that are involved, but in different scales or for different purposes. but the basic principles of this operations remain same. So, those unit operations unit processes are basically targeted to be solved by the CFD at a certain scale.

Now simply put this CFD becomes popular or have become popular in late 90s, but it started in 1960s also or even before that mostly in the aerospace industry. They started doing their validations, their aircraft drag predictions, several automotive industry they started to understand how the structure of the car should be to reduce the drag to gain the maximum speed of the car. flow physics or even inside the car how the AC temperature or the air flow happens everything they that is their regular use that happens to the CFD. And slowly it has become very popular with the advent of supercomputers and high-end workstations because it is computationally intensive process in several complex scenarios. So, as the computational hardwares are developed and it has become very very sophisticated, CFD is a kind of now daily tool used in several process industry and several other industries as well.

So, in this course that we will cover the some topics is that initially in the first week or in the second week we will discuss this introduction and the fundamentals of fluid flow and heat transfer. because the three things are the pillar of this simulation technique is that the equation of continuity, the continuity equation, momentum equation and energy equation. And then addition to that there are as I told you that different unit operations involve different processes for example, mixing reactions etcetera those are then coupled with these equations and the scenario becomes more complex and so the simulation strategy that becomes very intensive. So, initially we will look into this introduction that we have. We will look into the fundamentals of fluid flow and heat transfer. And then this CFD is not a magic, it essentially solves partial differential equation. A set of partial differential equations are solved, but again solving partial differential equations are non-trivial. So, that has to be simplified or approximated to a set of algebraic equation, so that it can easily be solved.

So, that means, there are several numerical techniques available those we will also briefly discuss and mostly we will discuss one of such strategy called the finite volume method. So, we will go a bit details into the finite volume method that is one of the strategy that are used in computational fluid dynamics. to solve the partial differential equations because you have seen the structure of continuity equation, momentum equation, energy equations in fluid dynamics or transport phenomena. Now, those equations how those are approximated to a set of algebraic equations that is basically the key step and that step we call as discretization. So, discretization technique we will look into that. And then briefly I will show you one or two maybe the structure of how a commercial CFD software looks like or the packages that are available in the market and how those are set up for a solution. But before that in these steps we will go into the basics and we will have a look that how those steps are essentially incorporated in those softwares. Which means those softwares must not be used as black box that I do not know what is happening inside I just feed in my parameter and they are giving me the solution and I trust those.

That is the worst case scenario if that is how the CFD is practiced. Then that is why several people have called that in that case if you do that if you use that as the black box that you do not know what the software is doing or how the equations are solved, then this computational fluid dynamics that this CFD essentially then becomes colourful fluid display or colourful fluid dynamics. that means, you will have several colorful pictures, contours, very attractive pictures, but that may not have any meaning. So, to understand that these are the key steps we will which we will look into certain details. And while doing that we will see few case studies that how those are applied or how then the single phase systems are solved, how multiphase systems are solved, how the turbulence modeling in a chemical process which is extremely essential because most of the industrial chemical processes are not laminar in nature. most of them are having turbulence or inherent turbulence is there. So, how turbulence modeling because for reaction to happen the mixing is essential and once you start mixing and that is vigorously or intensively turbulence is inherent.

So, turbulence modeling understanding we will touch upon that as well and we will at the end we will see that how this whole thing is clubbed and can be augmented for a reaction system or a reactive flow. That means, we will build up slowly that we will look into the single phase system and that too possibly for the laminar case. Then we go for the multiphase system, then we look into the turbulence aspect and then we see that how everything is essential or everything are essential in the case of the reactive system. And although we parallelly will discuss that what is model validation and how it should be done, but at the end from my experience as well as the experience gathered from the several textbook, I will discuss with you few important aspect that what how the validation typically should be done or ideally should be done and the troubleshooting in the CFD simulations. And although we parallelly will discuss that what is model validation and how it should be done, but at the end from my experience as well as the experience gathered from the several textbook, I will discuss with you few important aspect that what how the validation typically should be done or ideally should be done and the troubleshooting in the CFD simulations. So, essentially you have to remember that this is a course that simulates the real process. We try to simulate the real process by computational fluid dynamics and its pillar are the flow equations. Along with that we will look into the energy equations because all the operations or most of the operations involve temperature. And then there are certain cases where we will look into the concentration profile or the species transport equation.

Further those would be augmented by few specific cases wherever that is applicable say for example, multiphase cases where multiple phases exist and how to solve such scenarios. Further those would be augmented by few specific cases wherever that is applicable say for example, multiphase cases where multiple phases exist and how to solve such scenarios. Now, the point is when we have such cases. So, as I told you that we have the flow is essential. the other one is the turbulent and in between we have the transition flow which is difficult to understand because sometimes it behaves as laminar sometimes it behaves as turbulent. So, ideally we either operate in the turbulent region or in the laminar region. Now the turbulent region or the laminar region in CFD in even with the current infrastructure two interesting thing that happens.

Even for a single phase laminar flow can accurately be predicted by the CFD simulations with the current hardware infrastructure that we have, but for turbulent flow even for a single phase a full say the direct numerical simulation of a industrial scale operations of a single phase still is considered to be impossible because it requires too much of computational power. So, what is done usually it is the turbulence is simplified or approximated to a different levels that all the because in turbulence you have seen in the fluid dynamics or in transport phenomena that there are different length scales that are involved. So, while modeling turbulence those all length scales the Kolomogorov starting from the Bachelors scale Kolomogorov scale all the scales are basically not resolved that means, all those scales are not considered or not fully understood by the simulation. So, for the industrial scale what happens those scales are filtered. ok.

And then the large scales eddies are simulated or resolved or even in a gross scale or even in a in a relatively larger scale or the more popular thing that happens also as the time averaged profile of the turbulence model that comes as the RANS modeling scale. So, we will discuss those, but the point is Even for the say gaseous system and the liquid system despite being both are flowing laminar or both are flowing in turbulent the complexity in both the cases are different. This is this can be understood by a simple expression that the transport distance due to diffusion in laminar flow. ok that usually can be calculated by x is equals to root over of d t. So, the diffusivity of liquids actually is in the order of 10 to the power minus 9 meter square per second. and the average transport distance in 1 second that can happen is around 3 micron and in case of the gaseous phase where this diffusivity is in the order of 10 to the power minus 5 meter square per second. the same transport length becomes 300 micron in 1 second. So, which means that for the gaseous phase if you try to resolve this laminar flow your grid size which will also discuss what is grid.

The grid size in computational fluid dynamics the CFD cases for the gaseous is much larger can be much larger than the liquid phase if we have to simulate it for the mass transfer or for the mass diffusivity. Which means for the liquid case for the same problem say the if you have a laminar case of the same Reynolds number. The diffusive due to diffusivity difference the mass transfer simulation in liquid phase would require much denser grids than the gaseous phase, although your Reynolds number is same. So, this point has to be critically understood that depending on that what kind of simulation or what processes you are simulating not a one size fits all this kind of model does not work that I have developed it for the gaseous phase let us apply it for the liquid phase for the same case. If you do that blindly that simulation or that predictions may not work at all. Now, in the case of single phase and the multiphase case as I told you the single phase cases are much straightforward and with high degree of confidence nowadays the CFD predictions are trusted. In the case of multiphase flow the situation changes a bit because the multiphase flow several phases interact with each other. And therefore, the phase interaction changes.

So, phase phase interaction in multiphase case is a vital parameter that you have to model or how you interpret that interaction that becomes vital in the multiphase flow modeling. because we will see again different framework while modeling multiphase flow. And essentially each phase when it flows will have their own momentum equation and those momentum equation of each phases are coupled by that phase phase interaction term. because we will see again different framework while modeling multiphase flow. And essentially each phase when it flows will have their own momentum equation and those momentum equation of each phases are coupled by that phase phase interaction term. Now, as good as your model of phase phase interaction Now as I told you in the previous structure that there are several numerical methods when we try to solve this or when we try to have this. several numerical methods or the strategies that how we solve the partial differential equation to set of algebraic equations or in a different way.

Now, the methods that are involved that are broadly classified in three ways one is called the finite difference method that we call FDM. The other one is this finite volume method we call this as the FVM. The other the third one is called the finite element method or we call FEM. So, how we solve this partial differential equation inside this CFD packages depending on those strategies several softwares have been developed ok. So, to name a few the popular softwares that you see in the market for the CFD are say fluent marketed by ANSYS. there is Comsol, there is Flow3D, there is StarCD, there is OpenFOAM.

So, several such CFD solver I would say those are the CFD solvers. So those solvers are available. Some of them are licensed or having proprietary license by certain companies. Some of them are open source software. Open source software means that you can use it for free, you can download it, you can customize it on your own. OpenFoam is one such example. As I told you also that we have several strategy that based on these strategies these softwares are developed. So, based on finite difference method which is the kind of age old strategy which fails in complex geometry which are of irregular shaped that is why These softwares are built either based on the finite volume method or the finite element method. So, finite volume method is incorporated in ANSYS fluent, OpenFOAM, COMSOL incorporates finite element method. So, you have to choose the software accordingly. and in this course as I told you we would mostly discuss about the finite volume method. Because if you look at these content and if you see the other available courses you would see that itself one of these topic can be taught for the whole 12 weeks or so in greater details.

But the idea of this course is to have you through this I this summary of these things So, that you can quickly go to the application and whenever or wherever you need more details you can go back to that specific topic learn about it in more details and then go back for your research. So, in the next lecture I will discuss with you the overall strategy that how a problem is set up in a software or even in your own code what should be the steps and how it is usually solved. So, with this I will stop here today and hope to see you in the next lecture. Thank you.