CFD APPLICATIONS IN CHEMICAL PROCESSES
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Week-01
Lecture 03: Introduction

Hello everyone, welcome back to another class of CFD applications in chemical processes. I am Arnab Atta. Today also we will continue with the introduction the very basics of few governing equations, but before that I would like to further reiterate the applications of this course that we started in the last two lectures. So for the chemical processes as a chemical engineer immediately the application is focused on the reactors. Now, as a reactor engineer this is one specific applications, it need not be just this application, it is those who are directly from the chemical engineering branch can directly related to is that for any reactor design that we have in chemical processes, one of the imminent processing is that the chemical reactions that are happening. Now, when we talk about this reactor modeling, there are mainly two aspects of it.

One is that of course, the reactor performance that the how the reactor is behaving, what is my conversion, what is my selectivity of the product, how the product quality of a successful safety is of paramount importance whether the reactor is safe to operate and in that regard the thing that comes here is definitely the stability and operability. So, these are in fact closely related. Then comes whether the cost viability, whether the kind of quality that you are preparing that justified the operating cost or the other costs that are involved. And finally, but not less important is that the environmental impact of this reactor operation.

There must not be any hazardous emissions, it has to be properly recycled, rectified or separated the hazardous material and then the discharge should go out of the factory or the reactor. So, reactor performance is definitely one of the path one of the critical thing that we look as a reactor model. But at the same time all these things That is the conversion what is it the 90% conversion is happening. The selectivity if there are multiple products or byproducts are there you have to choose your desired product and how much its selectivity when this extra reaction the side chain reactions are happening. Now all these parameters of this reactor performance are closely related with the reactor configurations of the reactor hardware and its operating protocol.

So, reactor hardware and its operating protocol these two are interrelated or dependent. That means, if something goes wrong on the left hand side this box that you are seeing or this column it affects the reactor performance. So, reactor hardware and operating protocol it also has several parameters such as how the reactor look like that means, the size, shape, what is the feed rate or the throughput that it can handle, what is the inlet outlet configurations that means, the nozzles that are there. what is the inlet outlet configurations that means, the nozzles that are there, All these are important. or actually affect or influences the reactor performance. The other parameters that are significantly important in the reactor hardware and operating

are the mode of operation, operating condition, whether it has internals and how those internals behave and of course its startup and shutdown procedure. So, mode of operation is that how the reactor is being operated, is it in batch mode, is it in continuous mode or is it in semi batch mode. Now these terminologies you are expected to be familiar with from your reaction engineering courses or maybe from other chemical process engineering calculations etcetera. But still let me quickly take you through this operations is that batch means that you put everything all the reactants in a reactor. together at a certain time you give it some time in this reactor that is operating at a certain temperature pressure and after time t you take out the product.

So, this is the batch operations you put everything together and then after some time you take out the product and that product If again here depending on the conversion of the selectivity of the system there are chances that some unreacted reactant would be there, products would be there, byproducts would be there that the separation has to take place. The other scenario that can happen that you have a reactor there is a continuous flow of reactant some reactant are coming. A and B getting reacted and you are continuously taking out the product C from the system. That means there is a continuous flow that is happening and this is the continuous mode of operation.

So, now we can clearly understand that the how the mode of operation can influence the reactor performance and mix of these two can be with the semi batch mode of operation. That means, some reactants are put in together at a certain time and the product are you are taking out at a certain interval regularly or maybe continuously. or maybe one reactant you are putting it continuously slowly, but another reactant is there in sufficient quantity at the initial period you kept it in the reactor and the product is continuously you are taking out. So, from the perspective of certain reactant this is a batch operation from the perspective of the certain other reactants it is the continuous reaction from the product it can be the batch or maybe the continuous operation. So, this is how the semi batch works. Now, depending on the residence time and etcetera that we will not discuss here. Now, this is the part where

This reactor modelers or the reactor engineers requires interdisciplinary help or the knowledge. It requires the extensive understanding of the chemistry of the system. They can collaborate with the chemist, how the conversion, how the selectivity of the reaction is happening, what is the rate of the reaction. They have to understand what is the residence time distribution so that they can understand whether the reactor is working perfectly, there is no dead zone or there is no hot spot formation. Regarding the safety and environmental impact, they have to work with the structure or the stability and operability of the system. They have to work with the structural engineers and the environmental engineers regarding the hazards and the safety of the whole system.

So, now depending on various aspect there are several interdisciplinary understanding has to come in. Now, in this part or in this particular course what we are focusing as I told you at the initial classes is that this is regarding the computational fluid dynamics. So, flow dynamics is being modeled. So, there has to have some flow So, that we can apply certain governing equations that we will see later. And the system should have a continuous flow or say there is a movement of the flow, the flow dynamics exist. So, now the point is the third point is the operating condition, the flow rate and regime.

Now, depending on we will see in the later part that the flow regime is actually dictates the fluid-fluid interaction significantly in case of the multiphase flow. Now, most of the reactors that are there in the commercial operations works for the multiphase systems or work in a multiphase system. Even for the single phase system this understanding of the regime is important because you have to know whether it is working in the laminar or turbulent regime for the single phase case. But for the multiphase case this regime is more critical and slightly different than the simple understanding of the laminar and only turbulent. Even in laminar region when the two fluids are interacting which with each other there are several flow regimes can exist.

Say for example, let me give you a brief idea that when there is a gas and solid flow is happening concurrently in a system. Depending on the volume fraction and the velocity of this gas and liquid phases there can be bubbly flow. That means, there can be the bubble inside a continuous media of the gaseous phase or in the continuous media of the liquid phase the gas bubbles or there can be the liquid droplets suspended in the continuous gas phase. So, too extreme that can happen that means you have a gas bubble inside a continuous pool of liquid depending on as I told you depending on whether you have how much liquid you have or its velocity. Say for example, that we see in a typical bubble column reactor when you have a pool of liquid and then you inject gas.

Depending on this gas velocity there can be several flow regime that means, that the point is that there may be certain gas bubbles inside this pool that would come out. If you further increase the gas velocity it would mostly displace the liquid to pass through a different flow regime would come into play. Different flow regime means different level of interaction between the phases phases two phases and that interaction has to be mathematically interpreted while we apply that in the computational model. So, that is why understanding of the level of fluid-fluid interactions is important and that is understood by the concept of flow regime. At the same time it is imperative to say or you understand the pressure the influence of pressure and temperature of the system.

So, these are the operating condition that dictates how the reactor would operate or how the reactor performance would be influenced. So, as I told you that each and every point here on the left hand side influences the reactor performance. or in other way the reactor performance can be understood clearly if we understand these left hand side parameters or we thoroughly understand will go through the comprehensive understanding of this parameter. The reactor internals, the reactor internals, internals means say in a certain reactor you have the baffles where the flow is getting mixed. In a bubble column reactor there can be internals to have this gas bubble movements uniformly inside the liquid pool.

In packed bed reactors there is liquid distributed. So, when this reactant comes this has to be distributed over the packed bed of catalyst. So, that this reactant A and B are mixed well or they get a chance to interact with each other for the reactions that has to happen over the catalyst. Now if that has to happen uniformly there need we need a good distributor. In several system there are chances of exothermic reactions or the temperatures that have to be controlled. So, that heat box system or the quench box is also important in certain cases certain reactor. Now if that is not maintained. the system may behave awkwardly again that would influence the reactor the product quality or the conversion of the system or in fact if the heat is not properly absorbed or it is not properly removed that actually directly affects the stability and operability of the reactor.

There are systems where the startup and the shutdown protocol of a reactor dictates the reactor performance as well. Say for example, when we take a packed bed, a packed bed of catalyst. Now if it is operated in dry state that means these catalysts are completely dry you put in reactant and you take out the product and the other system is that you have a catalyst you put it overnight or give it some time with certain reactor or certain reactant So that the catalyst get wetted or it is pre-wetted before the system starts with a certain reactant. And then both of the reactants are continuously given to the reactor and the product C is coming out.

In both these two cases you would find the different quality of the product or maybe the different conversion of the product. So pre-weighting of the bed in such cases dictates the reactor performance. Similarly the shutdown procedure of a reactor of a system. So the whole point of saying all this thing is that in the specific application of reactor modeling there are not only the chemistry part or the selection of the reactor are important, but also hardware and operating protocol that needs to be fixed are equally important or that has to be clearly understood. Now here comes the application of CFD. In several of these cases and in fact in most of these cases

This CFD modeling can be applied to have a comprehensive understanding of the physics or at the same time it also that CFD model can be used for multiple iterations of setting a particular say operating condition for a desired product quality or the conversion and selectivity of the reactor. That iterative method which is sometimes costly just for the experiments or by experience usually that is set conventionally. Now these parameters are conventionally set through a lot of years of experience in the industry. But if it has to be intensified or if something goes wrong in the troubleshooting period, this application of CFD and its model development on all of these parts individually or club together becomes handy when we try to look into the individual aspect or say we try to find out or try to find out the influence of individual parameter on the reactor performance. So, application of CFD in a chemical process that is shown here for the by the example of reactor modeling is immensely important.

So, having understood this application part I hope it is clear that why we need CFD in chemical processes because say for example, if I say that this baffles distributor this quench vox the position the shape the configuration of this distributor. So, because say the distributor of say a gas liquid system typically say looks like this kind of a evenly spaced small holes through which say the gases so the liquids are coming in and there are some bigger holes again say for evenly spaced through which the gas phases are or the gases are fading. Now, the point is when it comes inside the reactor this gas and the liquid sprinkles say I am talking about a packed bed reactor. So, these catalyst are then get weighted by this liquid phase and also interact with the gas phase that are coming inside.

Now this particular distributor whether it is working evenly because we expect that there will be a even distribution of gas and liquid from the very beginning. And then also when it say the trickles down inside this tortuous path and typically this these beds are of in the meter of length in cases of commercial applications. So, what we expect that that there will be a even distribution of gas and liquid, but that does not happen because due to this tortuous path and the cylindrical reactor shape in nature there are tendencies of this liquids to go near to the wall. And after a certain length there are chances that certain portions are not at all weighted by the liquid phases.

And if that happens, that means your reactor will not work properly or efficiently for the desired product and the conversion rate. So what you need in that case? you possibly need again here another a redistributor. That means, you collect this liquids once again here and again you place a redistributor there another distributor. So, that from here wherever it is not working there is a maldistribution, the redistributor takes that and again this starts distributing evenly. Now, where that has to be placed? what is the length for your given feed rate because this position would also depend on the feed rate or the velocity superficial velocity or the flow rate whatever you call of this gas and liquid phases.

Now there comes this CFD modeling handy that instead of trial and error you can give a prediction that if I have this kind of a distributor I possibly would need another redistributor after a distance of this much from the inlet for a better conversion or for a better operation of my reactor. So, similarly in other aspect if this distributor if you see that there is not an even distribution immediately at the bottom of it or at this level, you can design your own distributor and have a predictions that how it would behave before you go for its fabrication, commercial fabrication or any other replacement. So, this is one application of one parameter taking the distributor as an example.

Similarly, this flow rate, flow regime, pressure, temperature, how these individual parameters influence your reactor performance that instead of trial and error in the experimental setup a validated CFD model can easily predict. Similarly, say for example, operation is being continuously run in an industry or commercial scale in a batch mode or in a continuous mode at a small scale or a whatever scale. But then they are interested in understanding whether if I have to go for a high throughput operation, whether my batch operation can be further converted to continuous operations without diluting the product quality. And my reactor type. That thing then can be modeled in CFD. to have this predictions that if the mode of operation changes from batch to continuous phase for the same reactor, how the product quality would be or what would be the conversion of the product.

and whether at the same time it would give us the idea that whether it would be safe to operate because the safe to operate and all these structural things would be understood by the parameters of pressure, temperature. So, whether the material of construction can withstand that much of excessive temperature if that there is an hazardous reactions or exothermic reactions happening or like I said here if there are certain dead zones where the reaction is not happening maybe the temperature is different that temperature would be different in those places than the other cases. So, the temperature distributions and all whether that your reactor can withstand. The pressure that would be generated once you change this flow rate or flow regime, the definitely the pressure drop or the pressure difference would be different whether your reactor structural safety would be there would be intact or not that also can easily be understood by the CFD model. So, in a nutshell in this particular lecture what I have extensively elaborated to you is the application of the CFD model for a particular scope although it is not limited to this only applications on this application only,

So, in a nutshell in this particular lecture what I have extensively elaborated to you is the application of the CFD model for a particular scope although it is not limited to this only applications on this application only, but similar to this there are several chemical processes where the CFD model is invaluable. a properly validated I mean why I am saying always a validated CFD model that we will see slowly in the when we go deeper into the this course that because one thing is clear that the CFD model that you are developing will have several approximations involved and how those approximations would come into the CFD model that also we will see slowly. But, since it is a numerical model there will be certain approximations to simplify a real system. So, validation is essential that we discussed in the last class also that either with any existing operating condition or experimental condition or if that is an ideal reactor then there you know what is the analytical solution of it. because for the ideal reactors, ideal results, there are existing models that are well defined and that can give you the accurate predictions analytically.

But as I said that the commercial reactors are not ideal in nature. So there are deviations from its ideality. So, first thing that typically is done that the reactor model either you validate it with the ideal reactor or if you have experimental data from the non-ideal reactor or any reactor that you validate that you check that model predictions are checked against those experimental results. And, if the model predictions and the experimental results are close enough we say this model is validated. We have trust on this model and then we go for predicting various scenarios that I have discussed today. And, in those circumstances and the utility of the CFD models are immense.

So, with this I will stop today, but before that I would like to take you through the reference books or the textbooks that you can follow is that these are these three books are of main importance I would say and then there are several other reference books whenever that would appear I will mention that to you. You can have a look at these books. These are simple to understand, but great to have these books as a beginner and also these are used sometimes for extensive research. So, with this I will thank you for your attention today and we will see you with the next lecture shortly. Thank you.