

CFD APPLICATIONS IN CHEMICAL PROCESSES

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Lecture 56: CFD in Reaction Engineering

Hello everyone welcome back with a new topic in CFD applications in chemical processes and that is an CFD in reaction engineering so what we have seen till now is that the CFD So the background of it that how do we discretize or simplify the complex partial differential equations to a set of algebraic equations. So that we can solve those equations because essentially the flow governing equations are of those complex PDEs. So, and specifically the Reynolds number involved in the flows in case of high Reynolds number when the flow becomes turbulent we have seen the turbulence modeling also the overview of turbulence modeling.

We have also seen that multiphase modeling which is frequent in any industrial operations or real world applications is that nothing happens usually in single phase although there are plenty of applications for the single phase as well. But the point is multiphase cannot be avoided in our day to day life. So, multiphase modeling strategies also we have seen. So, we have seen these all the things now in bit of the clusters that how the equations are discretized. This discretized equations are in fact from the partial differential equations which are the flow governing equations.

And, in those flow governing equations when we have multiphase flow we have seen how to solve it, when we have seen turbulence we have seen how to solve those or how to model those rather. Now, from the chemical engineering perspective one of the major job that the chemical engineers do is the reactor modeling. Now, this reactor modeling involves this all concept of the multiphase flow turbulence as well as the reaction mechanism, but the traditional task of the reactor engineers is to enhance the performance of the reactor to look into the safety features its day to day operations.

And this also requires the analysis of the results or the product output. Now, in reaction engineering or the reactor engineers heavily rely on the concept or mostly two concepts, which are the residence time distribution and the mixedness coefficient or the mixedness factor. So, this is the residence time distribution. and this is the mixedness coefficient or the mixedness factor because we have to understand that for a reaction to happen, we have to mix multiple reactants, ok.

So, the mixedness coefficient or the mixedness factor comes from how well the system is mixed. This mixing dictates how the reaction would happen or what would be the efficiency or the effectiveness of the reaction, and that eventually dictates the reactor operation. At the same time, these are also clubbed with how much time these reactants are getting in the reactor to mix with themselves or to react with each other. That is measured by the residence time distribution—how much time it resides inside the reactor before it goes out as unreacted or in product form. So, the classical reactor engineers heavily depend on the concept of this residence time distribution and mixedness.

RTD - Residence Time Distribution
Mixedness - fluid mechanics / mixing / diffusion / reaction

Degree of segregation → of mixing on the molecular scale.

Microfluid
↓
completely mixed on molecular scale

Macrofluid
↓
No mixing on the molecular scale but will mix macroscopically.

Reaction Microfluid
A-rich
B-rich

Macrofluid
Aggregates where No Reaction.

Batchelor scales
 $\lambda_B \rightarrow$ penetration depth of the scalar by diffusion in ϵ_k
 $\lambda_B = \frac{\lambda_K}{\sqrt{Sc}}$ $Sc = \frac{\nu}{D} \rightarrow$ Molar diffusion coeff. (compared to mixing)
Kolmogorov scales
 $\lambda_K = \left(\frac{\nu^3}{\epsilon}\right)^{1/4}$ $t_{K1} = \left(\frac{\nu}{\epsilon}\right)^{1/2}$ ν - kinematic viscosity (molecular diffusion)

Now, the point is this residence time distribution is directly linked with the flow or the flow dynamics of the reactor. And also, the mixedness is dependent on the mixing factor or the mixing efficiency by the way you are mixing the reactants. And we have seen that turbulence essentially enhances the mixing of the reactor, and that is why it is primarily used for the reactors. So, for start tank reactor we have stirrer to induce turbulence. For other kinds of reactors, we use baffles and all in order to have better mixing of the reactants, and that is actually induced by the onset of turbulence in the system.

So, this concept of flow dynamics, turbulence, and if multiphases are involved, then for reactor engineers, it is essential to understand all the concepts. or the modeling concepts when we try to do that. Now, the point is there also exist some consideration or in fact, the major considerations are also devoted towards the relative time scale of this mixing and the reaction time scale. So the rate at which these components are getting mixed they are mixing time and the reaction time scale.

So this relative analysis of the time scales that how this mixing the molecular transport is happening in order to mix the two components two molecules and by the time if the reaction is happened. So, that actually this complex system has to be clearly understood for this reactor engineers in order to design and to operate a reactor efficiently. So, a detailed CFD model can help us to achieve these objectives because in any reactive flow process this molecular diffusion Its job is to bring the molecules of different species together in a chemical reaction if that has to happen.

Now, mixing of some form of interspecies this contact that is essential for mutual molecular diffusion. this reactive process. So, we can understand is controlled by the fluid mechanics ok. So, it is essentially controlled by the fluid mechanics. mixing ok. So, it is the diffusion and the chemical reaction that happens.

So, all have their own contribution towards this reaction engineering modeling or the reaction modeling in the CFD. So, every part plays its important role and their contribution cannot be overruled if we consider this if we try to model this a reactive system or reactive flow system. So, the point is a particular reaction. From reaction engineering, we know what the reaction rate is. Now, the same reaction rate can be classified as slow or fast, depending on the relative rates of reactions and mixing.

So, we will look into that those that when it is fast when it is slow I mean fast or slow means relative to the time this relative time scale of mixing or relative to the time scale of reaction that it happens. in all these cases one thing remains common is the solution of Navier-Stokes equation because now we understood that here the flow is there and this flow can be further augmented by the presence of multiphase and turbulence. So, multiphase with turbulence and then reaction is happening or simply multiphase and reaction is happening or single phase

case also simply turbulence is there and the reaction is happening in a single medium, but multi component. So, the point is, we have to have several informations ready before we go into this reaction modeling or reaction that reactor modeling particularly because see reaction engineering reaction modeling that would be the part is dealt by the catalyst engineers or the catalyst researcher. or the part that does not involve reactor hardware or reactor flow systems.

So, how a reaction can be intensified or how its synthesis can be accelerated—these aspects, I would say, are not part of the reactor engineer's role. Reactor engineers deal with reactor internals, reactor operations, and related aspects. They are provided with information such as how the reaction occurs, the reaction rate, the product, byproducts, etc. Classical reaction engineering deals with those aspects. Reactor engineering, on the other hand, deals with the flow or fluid dynamics part, along with related internals and operations.

So, the point is that the mixing of fluids is quantified by reactor engineers using the term 'degree of segregation.' This is a measure of mixing on the molecular scale. So, the degree of segregation is a quantifiable parameter that measures the mixing of components at the molecular scale or reactants at the molecular scale. Now, two extremes of molecular mixing are typically known or can be classified: one is called the microfluid, the other is called the macrofluid.

- ① Convection by mean velocity
- ② Turbulent dispersion by large eddies
- ③ Reduction of segregation length scale
- ④ Laminar stretching of small eddies
- ⑤ Molecular diffusion & chemical reaction



So, in microfluid, what happens is the species are completely mixed on a molecular scale, are completely mixed on a molecular scale. But in macrofluid, what happens is there is no mixing on the molecular scale, but I mean the species are well mixed macroscopically. So, what does this mean? This means that, say, I have a reactor in which species A and species B are mixed with a baffle, and these species that come are well mixed at the molecular level, and then the reaction occurs. If the mixing is not happening at the molecular level, the reaction does not occur. And in this case, the microfluid and macrofluid, what happens here the same A and B are coming, but they are, say, macroscopically mixed. So, if the greens are component A and this is, say, B, then these are well mixed; you can consider that these are mixed.

So, the points, these are the aggregates, these are intermixed; these lumps are well mixed at the macro scale, and in this case, the reaction does not occur—no reaction. So, we understand that when two miscible fluids or components are brought together the react and this reaction is completely dependent on the extent of mixing, or we can control this reaction by the extent of mixing. So, the point is Now, here the relative time scales are important.

So, when this A and B are mixed at the molecular rate at a rate which is much faster than the reaction rate, then the reaction happens to mix with each other at the molecular scale, and the reaction occurs. OK, and the reaction rate—the effective rate—would be controlled by the reaction kinetics in those cases, that is, the microfluid condition, OK. Now, when this macro condition this macro fluid condition means when reactants A and B are mixed macroscopically—they are well mixed but not at the molecular scale, OK.

Then virtually no reaction takes place, and we do not require any reactor modeling concept or something like that because no reaction is happening. So, one is the ideal condition micro, for the reaction to happen; the other one is another condition where the reaction does not happen. So, the real cases happen somewhere in between these two extremes—it is neither completely ideal, that is, the microfluid condition, nor is it the macro fluid condition. So, the point is we will have an intermediate way that would exhibit, say, kind of A-rich or B-rich zones or regions with partial segregation.

So, in several fast reactions—again, fast means if I say a fast reaction, which means it is compared to the time scale of mixing. The reaction time scale is smaller than this mixing time scale. So, for this fast reaction and the high viscosity system for example, say the polymeric reactions the polymeric systems The mixing process interacts with the chemical reaction and significantly influence the reactor performance that is the product distribution, product quality and etcetera.

So, the traditional method of finding this upper and lower limit on performance by applying microfluid or macrofluidic concepts, these are served this actually serves as the basis for the design. So, it is the foundational approach. But it requires the detailed CFD based modeling and analysis of the interactions between the reactions and the chemical reactions whatever which is happening. So, that would help us to get a better understanding of this system. Now, the point is this time scales that we are discussing.

So, if we consider because now we know that the smallest length scale for turbulence which is in fact, the mixing we are considering. The mixing is represented or the turbulence is represented by mixing say here. So, those time scale, length scale all we have seen earlier. Now, if we quickly remember those we now realize the concept of turbulence this fluid motions that exist or the fluid length scale exist at a particular region or a particular point of different scales.

So, different scales coexist basically. And, we have also known that the vortex stretching that happens and the vortex stretching leads to the formation of the smaller eddies from the larger eddies. So, kind of a sheet you think of an imaginary sheet, if the sheet is stretched which is the larger eddies, it stretched further and this larger eddies eventually produces the smaller

eddies. and this at the smallest scale the energy is irreversibly dissipated into heat at a rate which is the turbulent dissipation rate or the energy dissipation rate ϵ . This is what we have already known about this.

So, the smallest scale we call those the Kolmogorov scales, and if we write those, say this is the λ , the length scale, if we consider to the power one-third, the time scale is ν by ϵ to the power half. So, where this is the kinematic viscosity ν , which is also called the momentum diffusivity. So, we have to be very careful or have a clear mind about the difference between the molecular diffusivity and the momentum diffusivity. So, this is the momentum diffusivity that we have, or the kinematic viscosity.

Or we say the momentum diffusivity. This λ_k is the length scale, and T_k is the time scale, say Kolmogorov time scale and the Kolmogorov length scale. Now, the strongly dissipative nature of the fluid motion at the smallest scale indicates the viscous mixing. And the formation of the smaller scales actually forms or the building blocks of the mixing. As smaller scale that would be, in fact, the essence of mixing, the building blocks of mixing.

A complete viscous mixing can occur, I mean, but it actually does not ensure the complete molecular mixing. If there is a complete viscous mixing, it still does not ensure that we have a complete molecular-level mixing. Because this momentum diffusivity and molecular diffusivity, these two are different things. Molecular mixing is usually characterized by the Batchelor length scale, ok. So, that is called the Batchelor scales.

This Batchelor length scale if we say λ_B the λ_K for the Kolmogorov, B for the Batchelor. That is the penetration depth of the scalar by diffusion in Kolomogorov time, which means we can write this λ_B as λ_K divided by the Smith number, where the Smith number is ν by D , where D is the molecular diffusion coefficient. So, Batchelor length scale and Kolmogorov length scale how these are related we can see from this expression.

Where S_c is the Smith number and D is the molecular diffusion coefficient and ν is the kinematic viscosity that we knew earlier. Now, for the gases this Smith number is in the order of 1. So, the molecular mixing is at par with the viscous mixing. So, the rate the viscous mixing happening at the same rate the molecular mixing can happen for the gaseous phases. But for the liquid phases this Smith number is in the order of 1000 the order of magnitude ok.

And if that is the case then it shows that we have a slower molecular mixing. if S_c is 1000 what you have that the Kolomogorov length scale is much larger than the Batchelor length scale, which means this molecular mixing is then the slower ok. So, typically this energy and concentration if you look at the spectra for the turbulent and this time scale analysis it gives us an idea or it gives us the classification idea that how the reaction is categorized or how the reaction is placed in between this microfluid or the macro fluid condition.

So, this is why this time scale analysis is important. The reaction time scale and the mixing length time scale. Because this gives an idea of where this reactor that you are designing, operating, or intensifying is presently located. Is it completely the microfluid condition that is in fact if that happens for the gaseous phase because the first it is the reaction time scale at the same level the mixing is happening because Batchelor length scale and the Kolmogorov length scale are comparable or you have a different scenario because for the liquid case that mostly happens.

On this foundation what happens is that if we try to understand the relative importance of or the interaction between turbulence and reaction engineering or chemical reaction, then we have to understand this various process that are involved in the reactive mixing. So, what happens when a fluid element of different components is added to a turbulent flow field? Let us say we consider it as a tracer added to a turbulent flow field to understand how this mixing happens.

So, a tracer is added. The molecular mixing that happens actually occurs through a couple of steps. The first step is that convection must happen, and this is taken care of by the mean velocity. So, convection happens, and this turbulent fluid element is essentially transported within the solution domain by the mean flow field.

And then the turbulent dispersion. Large eddies are dominant because they disperse the stressors by the large eddies. And subsequently, these large eddies, which occur through the energy cascade mechanism, transition into smaller eddies. So, basically, the reduction that happens, or the reduction of segregation, length scale occurs.

So, after convection by the mean velocity into the flow domain turbulent dispersion by the large eddies and there we see the reduction in the segregation length scale due to the formation of smaller eddies. And then, this vortex stretching and other phenomena that we will discuss involve laminar stretching of small eddies. What does it do? We will discuss each step in detail. But what happens?

The vortex stretching happens of this small eddies and it generates more interfacial area for the mixing to happen and the final step is the molecular diffusion followed by the chemical reaction. So, until and unless molecular diffusion and molecular-level mixing occur, no reaction will happen. So, we will go through all these steps. Briefly understanding the time scale and how this phenomenon occurs and how it enhances mixing.

We will continue this discussion in our next class. So, until then, I thank you for your attention, and we will see you for detailed discussions on this reaction and CFD applications in reaction engineering in the coming class. Thank you for your attention.