

CFD APPLICATIONS IN CHEMICAL PROCESSES

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Lecture 57: CFD in Reaction Engineering

Hello everyone, welcome back to another lecture on CFD applications in chemical processes. We are in the middle of discussing CFD in reactions, or particularly reactive flows. So, what we are discussing here is how turbulence or mixing is essential for the reaction to happen, because we understand that for this reaction to occur, mixing is essential, and for mixing, we have seen one of the best possible ways is turbulence. So, that is why it is closely related to turbulence modeling, plus the complexity that would involve having the reactions.

The point is, in the last lecture, we have seen the different length scales that are involved in turbulence. Also, in order to generate these smallest eddies for the mixing—the molecular mixing to happen—we have seen the different steps that are involved, okay? The different steps that are involved are starting with the convection by mean velocity. So, the point is, we started this discussion in the last lecture: say a tracer is injected into the bulk flow or the base fluid that is flowing into the reactor.

Now, the reason I am mentioning this tracer is that it essentially would be replaced by a reactive species for the reaction to happen. But in order to understand this different length scales reduction and associated time scale this tracer is used for the discussion to understand those length and time scales and how they control the states. So, the point is when this tracer is injected eventually this lump of tracer that we are putting into the base fluid which is flowing to

the reactor, is convected initially by the mean velocity of this base fluid. So, it goes into the reactor zone by step 1. Then what happens, or subsequently what is happening, or simultaneously what is happening is that there is turbulent dispersion. This turbulent dispersion happens due to the large eddies.

So, we have seen these large eddies that form from the turbulence, extracting energy from the mean flow. We have discussed this: the energy transfer, the cascading effect. So, these larger eddies eventually take this the lumps of the stretcher into the reaction zone, and the reduction of the segregation length scale takes place. That happens mostly through vortex stretching.

So, the convection and turbulent dispersion by the larger eddies actually create the macro-mixing input. It does not influence or create the micro-mixing, but it lays the foundation by

enabling the macro-mixing at this scale. So, because we understand there are different regimes of flow in turbulent flow, like what we have: the inertial-convective, the viscous-convective, and the viscous-diffusive ranges. So, initially, the inertia carries this tracer into the main zone, and this inertia, along with turbulent dispersion by larger eddies, creates the macro-mixing.

Subsequently, what happens to this macro-mixing? The larger eddies then, with the help of vortex stretching, The vortex stretching is a phenomena this vortex stretching that the way we can understand is a kind of say the sheet that is being stretched and after a critical point after a certain point that sheet is splitted into many parts and that eventually is the reduction of the length scale.

Now, this vortex stretching that helps in reduction of this segregation length scale in the this step 3 that you see. It increases the interfacial area between segregated lumps of the tracer and the base fluid because as the smaller part that happens the interfacial area for the contact between this base fluid and the tracer or in actual case you can consider the interaction between reactants that enhances that increases.



But the point is for the molecular diffusion to happen it is not that sufficient reduction of the length scale or that sufficient increase or enhancement in the interfacial area. So, what happens is that in the viscous convective regime or the regime that happens with the engulfment and the viscous stretching of this smaller eddies. So, with this say reduction of this segregational length scale in step 3 that we are mentioning here, we eventually get the Kolmogorov length scale eddies. Now, here still

we have a better situation than the macro mixing, but not the desired micro mixing and that is what we call that as the meso scale mixing or the meso mixing. So, this meso mixing that happens is at the Kolmogorov length scale and that happens by the vortex stretching. So, further this scales is reduced by this engulfment and viscous stretching method and that generates the Batchelor length scale it is ok. And we have seen this relation between the Batchelor length scale and the Kolmogorov length scale in our previous lecture. The point is this Batchelor length scale then

facilitates this molecular diffusion which is followed by the reaction as the final step. Now, why we are discussing all these steps? Because the reactor engineers or the chemical engineers essentially understand the extent or the degree of mixing by the two parameter one is the intensity of segregation and the scale of segregation. So, what we are discussing here or have discussed till now is this based on these two parameter that is the scale of segregation and the intensity of segregation.

So, the point is the scale of segregation if we try to say it in a different way the scale of segregation is the measure of the size of unmixed lump. it is the measure of the size of the unmixed lump. But the intensity of segregation is the measure of difference in concentration between neighboring lumps of fluid. So, in a certain zone you have concentration gradient or concentration profile that is what we understand the intensity of segregation. If it is uniform then it is the best possible mixing.

So, lower the intensity of segregation more the extent of molecular mixing. So, as we lower this intensity of segregation what we have is higher extent of molecular mixing ok. So, by these parameters we actually try to categorize this turbulent mixing process in the reactive flow. Now, the point is why we are discussing all these different steps of length scale reduction.

The reason is that not only this length scale reduction is important, but also the scale of the turbulence of this tracer that we are injecting into the waste fluid. So, how does this molecular mixing happen? We have understood that with the help of length scale mixing, but we also understand that each step would take its own sweep time. So, each step has its own characteristic time scale as well.

So, the point is this time scales are also equally important because the reason what why we are understanding all these states are we have seen the two extremes of mixing: one is the macro mixing or the macro fluid, and the micro fluid in our last lecture. Macromixing or the macro fluid conditions what happens we have although homogeneity at the and the aggregates very large scale or uniformly mixed condition apparently, but it is not mixed at the molecular level. On the other hand, this microfluid condition we have the homogeneous mixing or I mean the possible the

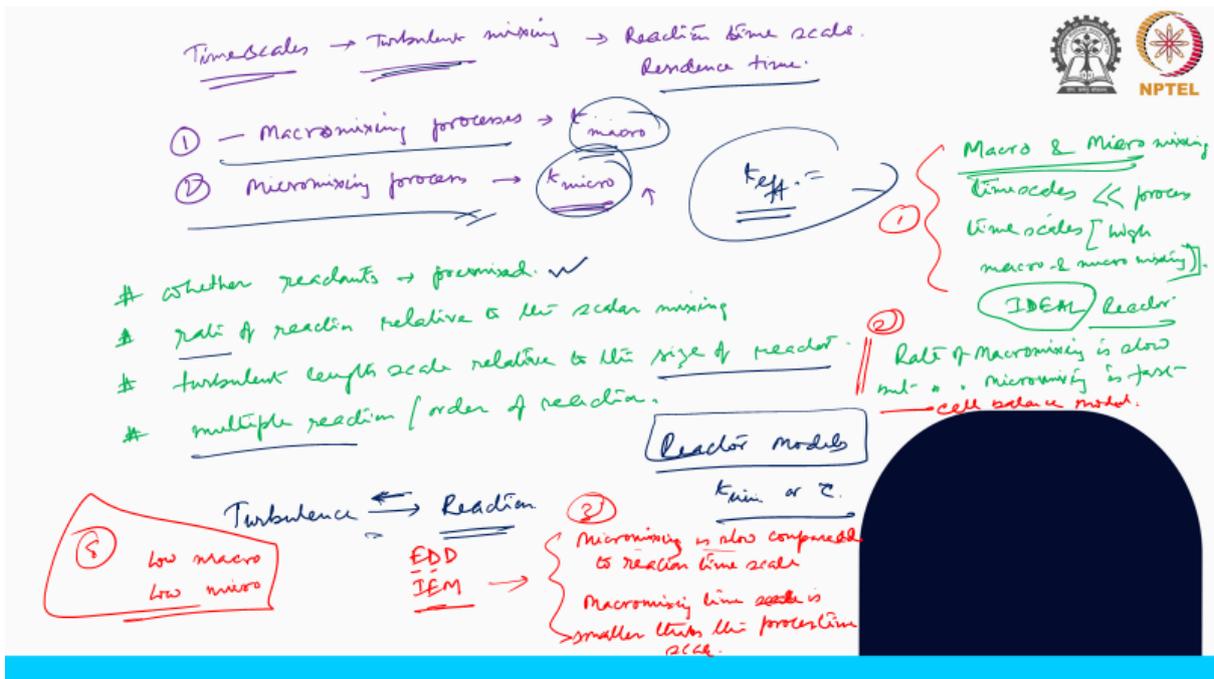
greatest possible extent of mixing at the micro scale or the molecular scale, ok. So, that was the microfluid condition. So, we had the two extremes where the reaction would happen and where the reaction would not happen in the case of macrofluid. But the real reactors or the real reacting systems operate somewhere in between these two processes or these two extremes. And to understand these two extremes, we need to understand the rate-controlling step.

The time scale involved in the mixing and the time scale that is there with the reaction—the reaction time scale. So, all these processes that we see—the steps and the reduction length scale phenomena—there, each step, say t_1 , t_2 , t_3 , t_4 , like this, takes its own time. And we know that the rate controlling the whole process is limited by the slowest step. It takes the longer time. So, accordingly, for all the steps, if we find out which one for your process is the limiting or the rate-controlling step, that helps us in categorizing your problem.

to a best suited model because each process when there is a fast reaction is happening again fast that means related to or compared to the reaction time scale the comparison between the mixing and the reaction time scale. So, whether it is a fast reaction or whether it is a slow reaction, etcetera, those have their different models that we have to choose. And which one to choose? This is the basic understanding that we require we analyze the system that this is my the rate controlling step and this is higher than the reaction time scale or lower

than the reaction time scale or it is in the macro fluid extreme or the sides towards the macro fluid or towards the micro fluid system and accordingly we choose the reactive flow model. There exist several such possibilities. So, the point is these time scales that are involved in the turbulent mixing. So, those here all the states that I have mentioned, say t_1 , t_2 , t_3 , t_4 , detailed research has already been done. And it is possible that you can also devote time to researching those points.

And what will happen is you will come up with the estimation or correlations of these t_1 , t_2 , t_3 , t_4 time scales. So, for each step, you can find out the time scale that is involved, and there also exist several correlations, and those have been proposed by researchers for understanding those time steps. Now, these time scales for the turbulent mixing processes, we have to analyze because for the comparison with the reaction time scale or say the residence time that it that the amount of time it is comparable, whether the reaction would happen if we understand those time scales.



So, all these steps that are here we have discussed, that is the convection by mean velocity followed by turbulent dispersion by large eddies. The reduction of segregation length scale followed by laminar stretching of small eddies. These small eddies mean at the level of Kolmogorov length scale. Which results in Batchelor length scale eddies, and these eddies eventually help in molecular diffusion, and that results in the molecular mixing, subsequently the chemical reaction happens. So, all these steps can be broadly categorized into two processes: one is the macro mixing process, the other one is the micro mixing process.

And if we assign a certain time scale with those, say macro mixing processes, that are characterized by T_{macro} , and micro mixing processes are characterized, say, by T_{micro} . Now, when one of the micro mixing steps is rate-controlling. So, micro mixing steps essentially the step 3 and 4 if we look at it that when the Kolmogorov length scale it generated the generates the Kolmogorov length scale, and from Kolmogorov length scale we have the Batchelor length scale. So, those are the smaller ones, or the micro mixing processes.

So, in those micro mixing processes if any of those are is the rate controlling then we can assign that time scale as the T_{macro} T_{micro} for this micro scale mixing process or if multiple steps or both the steps that steps we have 3 and 4 if both are controlling if both have comparable time scale. And then what we can also analyze or find out is an effective time scale. This effective time scale again has correlations proposed; it has several expressions for it by which you can estimate what the effective time scale is. Now, the reason it is important again

to reiterate that these time scales helps us to classify this different reactive flow processes to add up suitable model to adopt the suitable modeling strategy for the CFD modeling of those reactive processes. This comparative analysis would give us insight into whether the reaction

would happen, whether the reaction would not happen, what would be the extent of reactions, etcetera. Not only that several other factors actually determine this extent of turbulence on the mixing process or the extent of turbulence on the effective rates of chemical reaction. and those are say one can be whether the reactants are premixed, whether it is premixed or it is mixed in the reactor zone at the very beginning.

So, the objective is to understand that whether those are flowing together for a certain period. So, it automatically get some time for the mixing to happen and then the if the reaction rate the reaction time scale is comparable with the mixing how the reaction extent of reaction that is happening. The other thing that can be the rate of reaction relative to the scalar mixing. This comparative analysis would also give significant information on the modeling strategy.

The rate of reaction compared to the scalar mixing that is happening the at the rate it is happening. The length scale comparison the turbulent length scale relative to the size of the reactor which is essentially that the size of the reaction zone. Usually we consider the largest eddies are in the range of this reactor characteristic length of the reactor or the reaction zone. And whether the system involves multiple reactions and what is the order of the reaction.

So, the point is the chemical reactions it is not that only turbulence is affecting or influencing the chemical reaction. The other way also happens. So, it is not only the way we have discussed it should not be perceived that the turbulence is essentially affecting or influencing reaction. The other way also can happen because this reaction

sometimes in fact practically in many cases also say releases energy so reactions a certain kind of reaction exothermic reaction they also release energy and if that is sufficient to modify the fluid property then this influence of turbulence or the extent of turbulence is also altered So, this both way interaction further say augment or further make the situation more complicated. As I said for the exothermic reaction, if the energy is sufficient to alter the fluid properties, then what we can also have the variable density flow. For example, in combustion that happens.

So, most of the computational model that we see or frequently use are of the constant density model. But, in such scenario we have to be very careful that we have to use the variable density flow or the situation arises the in the compressible flow system ok. So, this what are the available reactor models that we have. These are classified as according to the assumptions about this relative magnitude of characteristic time scale of mixing whether it is macro or micro and the time scale of the reactive flow processes that is the reaction time scale that we say or say the T kinetic or say the residence time.

The relationship between this or the choice of the suitability of the model depends on the extent of macro or micro mixing. So, what happens if we have say both macro and micro both time scales are much smaller. So, let us clearly understand this situation that macro and micro. So,

this mixing time scales. So, macro and micro mixing time scales are much smaller than the process time scale of that is what we have high.

So, the situation is essentially high macro as well as the micro mixing. Then what happens? It is the ideal scenario. So, it is the ideal reactor scenario. So, the models that we adopt for such scenario are the ideal reactor model when macro and micro scale time scales are much smaller than the process time scale. when this rate of micro say now I just we say write say the rate of macro.

Macro means macro mixing is slow, but the local micro mixing is fast. So, it is slow, but rate of micro mixing is fast this scenario also can appear. So, then what happens is that the relevant mixing scale is essentially the intermediate between the micro scale and the reactor scale. Now, the point is although the reactants are locally mixed on the molecular scale, there is macroscopic segregation because we have macroscopic mixing that is slow. So, several reactor models are available in such scenario say for example, the cell valence

So, in such case there is cell balance model that are available which can be used for such scenario. Now, here what happens no special modeling efforts are actually necessary, but what happens is that due to the reaction source that is there in the momentum equation. the Navier-Stokes equation that we solve that results in some additional non-linearity in the system. So, that has to be taken care or solved accordingly. So, we have two scenario one is the ideal case and here the rate of macro mixing is slow, but rate of micro mixing is fast.

Now, it can also happen that when the local micro mixing is slow compared to the reaction time scale and the macro mixing time scale is smaller than the process time scale. So, in such so, the scenario is micro mixing is slow and that is compared I mean slow compared to the reaction time scale. And the other scenario is that the macros mixing time scale is small or smaller than the process time scale. So, in that case what happens?

The performance of the reactive flow process is essentially governed by micro mixing ok. So, in such cases although there is no say macroscopic segregation but reactants are not mixed on the molecular scale because it is also slow compared to the reaction time scale. So, it requires again special kind of methodology for the reactive for the reactive flow process balance.

Say to name a few and these models are very research specific and a specific to this set and those can be the engulfment deformation diffusion EDD model. We will not discuss those in details this if somebody is extremely interested in the research they can explore these processes or the say this is the engulfment. diffusion model. The other one is the interaction by exchange with the mean, such models, OK. So, these specific models are available and are used for scenarios when this is governed by the micro-mixing.

Essentially, the performance of this reactive flow is governed by the micro-mixing, but it is not appropriate or not completely happening because it is slow compared to the reaction time scale. The other scenario, so this is the first scenario or say the second and this is the third scenario that we discussed and can happen when the macro-scale and the micro-scale segregation exist together. That means nothing is happening there; we have a low degree of macro-mixing.

Low macro-mixing and also low micro-mixing extent. So, in such a scenario, nothing is happening, and no model is adequate as such in terms of the reactive flow process. So, on this note, I will stop here today because, in the next session, we will discuss how we can apply this whole understanding with a case study. I will take you through a set of reactions. Reactions—how they are coupled, what we require, when to apply such things—and that will happen in the next lecture.

So, until then, thank you for your attention.