CFD APPLICATIONS IN CHEMICAL PROCESSES

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Week-12
Lecture 58: CFD in Reaction Engineering

Hello everyone, welcome back with the discussions in CFD in reaction engineering in CFD applications in chemical processes. We are essentially discussing how to model reactive flow system and which model would be applicable or how to do that. While doing so in the last couple of lectures we discussed about the understanding on the length scale and the time scale of different key steps that are involved in the reduction processes or the segregation that will happen. Because we realize that not only

So, the macro mixing it is the micro mixing which is the key step behind the reaction to happen and this segregation of scale and that time scales associated time scale how those are important. Now, the point is when we try to model this reactive flow system, since it is closely associated with the turbulent flows, we have understood that in turbulence modeling, we have seen DNS, LES and RANS based models. And we have discussed those in the turbulent modeling section in detail, particularly the RANS based model. Now we have also by now realized that why RANS based models are most popular.

And in fact due to the further level of complexity of incorporating reactions in the flow system and if there is multiple reactions then it further gets complicated. So, in such system it is the practically we have seen that RANS based models are most frequently used and widely used. because DNA itself it's very computational intensive process added to that the reaction part. It is extremely difficult or in fact near impossible to have results for an industrial scale operation. LES, it requires SGS models, the subgrid scale models.

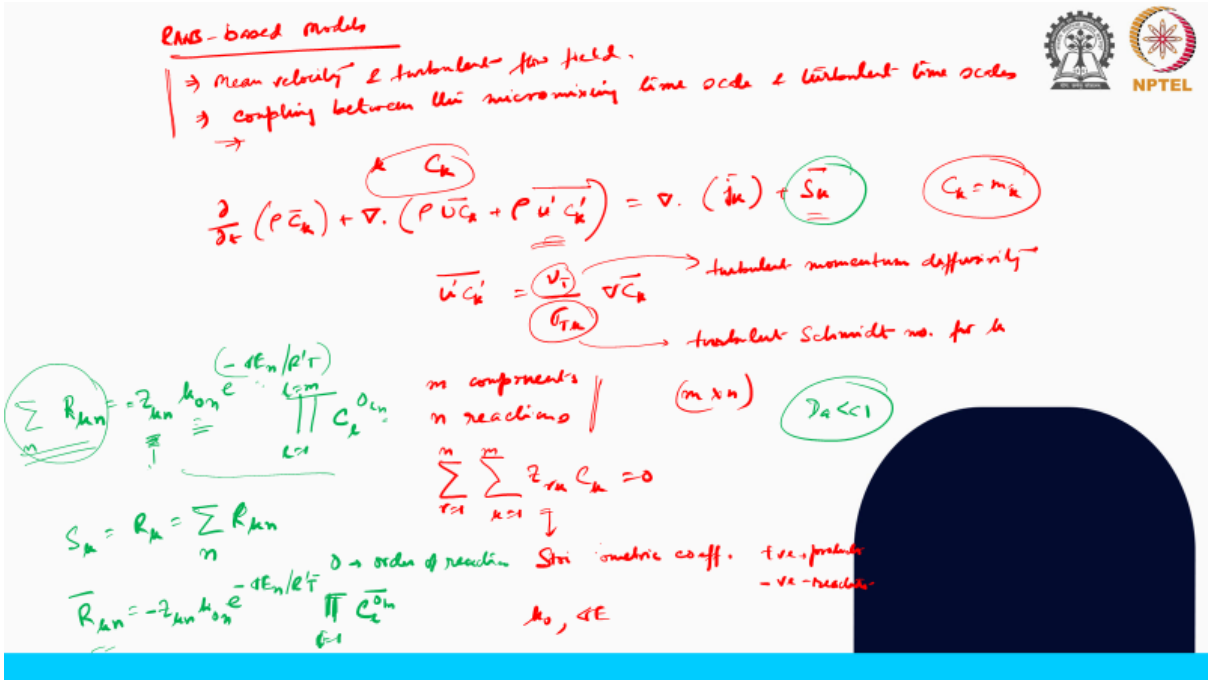
So, subgrid scale model drastically reduces the computational effort compared to the DNS. But still, LES SGSs that are used for reactions to incorporate are also required. Not a viable approach for commercial-scale applications. So, we are actually left with the RANS-based approach, and we have seen that Reynolds-averaged Navier-Stokes equations The same equations are used but in conjunction with the reaction rate that acts, or the reaction part that acts as a source term to the Navier-Stokes equation.

So, in this RANS-based model, what we see is that, in order to solve, because this RANS-based approach actually decouples the fluctuating part and the mean part. So, this fluctuating part still requires closure models, along with that, we will require several closure models for the reaction

part. So, these models essentially require the knowledge of mean velocity. So, these RANS-based models for reactive flow Those actually cannot be used in a standalone manner.

They require the knowledge of mean velocity and turbulent field. It also requires the coupling between the micro-mixing time scale and turbulent time scales. The clear information is required, but this is quite difficult to comprehend. This coupling between micro-mixing time scale and the turbulent time scale.

This we have discussed in the last couple of lectures, the utility of this coupling. The requirement of macro fluid condition or the micro fluid condition. And since this is a very complex flow in homogeneous flow where the reactants can be partially mixed or react partially, that makes the situation further complex. So, the point is these RANS-based models help to account for this field or these areas or to circumvent these areas, and that is why it is frequently used or has widespread use.



Because along with those equations that we have seen earlier—that means the mass conservation and momentum conservation during turbulent flow modeling. here like the Reynolds averaging for the concentration of the species say K is the species and C K is the that species concentration that is there that or the reactant species is K, and this is the C K. Then what happens? The time-averaged conservation equation for species K is also solved together, which happens for each and every species involved in the reaction, so that happens through So, this is what we have seen if we consider the Reynolds averaging technique for the concentration because it has a mean part as well as a fluctuating part due to turbulent fluctuations.

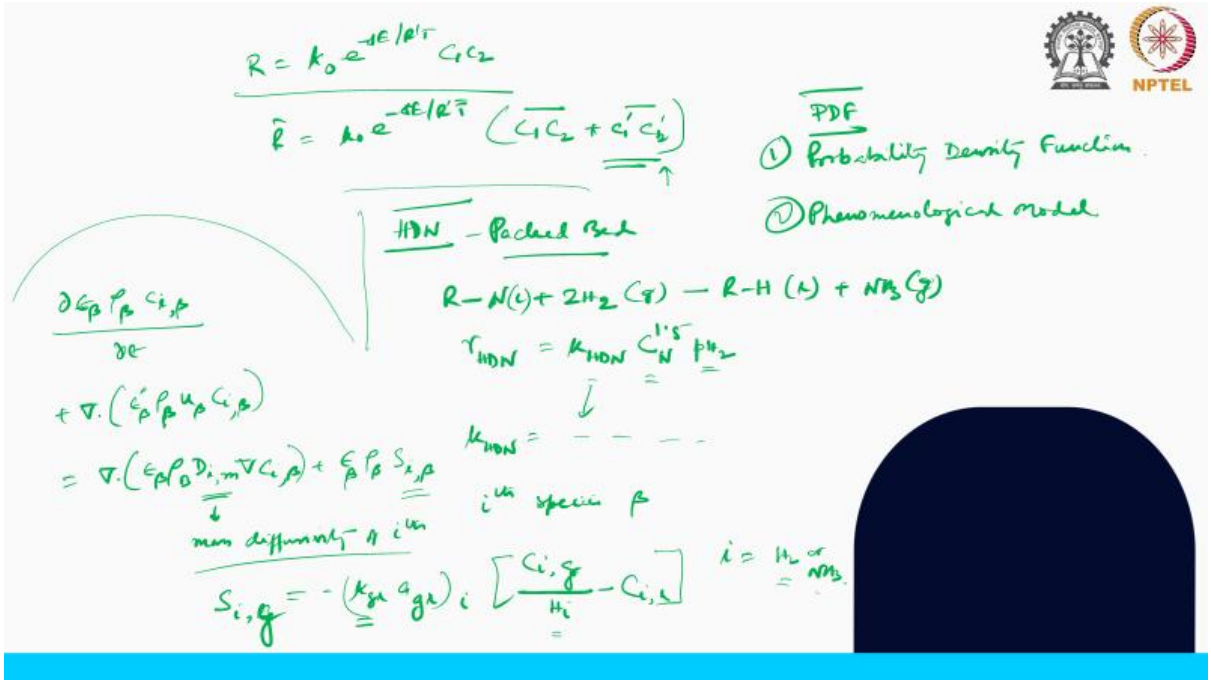
So, here this equation that we see is actually written in terms of the mass fraction. So, where essentially Ck is essentially mk. Now similar to the momentum equations this time averaging actually introduces unknown terms here and that requires further closer and particularly this fluctuating component that is the difficult part to handle or this is actually the new terms that comes due to this Reynolds averaging technique. So, the point is this also has to be closed or requires a closure model before we can actually solve such equations along with the conservation, the continuity, and the momentum equation.

So, the point is the term related to an integral part of turbulence these are the terms, the new terms that are there, and they are essentially independent of molecular diffusivity. So, the gradient diffusion model is sometimes, or most often, used in order to relate the scalar flux to the mean field in this way. where we know this term is the turbulent momentum diffusivity or turbulent viscosity that we have seen earlier. This term sigma tk is the turbulence meet number

for component K or species K. Now, although this gradient diffusion model assumption may fail in several situations, it is typically used to carry out simple calculations or most of the engineering simulations for reactive this complex reactive flows. the most difficult term that we have to close is the reaction term and that reaction term is essentially this source term here. So, this reactive system is again mostly represented by a lamp mechanism. Now, where we consider only a few species not all the species in order to simplify the process or using the lamp parameter model.

So, say we have m components involved in n reactions. There are multiple reactions happening in the system. So, we have m number of components and n number of reactions are happening. So, the point is this the whole system is then usually represented by a 2 dimensional matrix of m by n of stoichiometric coefficient and order of reaction this and a two one dimensional say vector of frequency factors and activation energy.

So, n chemical reactions basically can be written in this way. So, r is equals to 1 to n number of equations again taking a summation of k species from 1 to m Z r k C k is equals to 0 where this Z r k is essentially stoichiometric coefficient. and is considered positive for products and negative for the reactants. Now, for each chemical reaction associated with kinetics representing the dependence of the net rate of reaction on the concentration of participating species and temperature. So, the dependence on the concentration of participating reactants or participating species is represented by the order of reaction, say this O, if I say the order of reaction.



And this rate of reaction is essentially represented by two parameters: one is the frequency factor, which is say the K0, and an activation energy delta E. So, the net rate of formation or consumption of, say, species K due to reaction N can usually be written in this form. Nth component. L equals 1 to L equals m, m number of components C L, this is the order, and this is the nth component. Where this is the molar stoichiometric coefficient for species K, this term K0 n.

is the frequency factor, the pre-exponential factor, activation energy of the reaction n, ok. So, this is the stoichiometric coefficient followed by. your frequency factor and exponential is the activation energy for reaction n. R prime is the universal gas constant, and this product is taken over all participating reactants with this 0 ln or say here O, essentially O stands for the order of the reaction. So, O L N O, to be very precise here, L N at the subscript is the order of reaction N with respect to reactant L, ok.

So, it is the order of reaction N of the species or the reactant L. So, the net rate or the net reaction source for species K can be calculated as a sum of this thing. If we take the sum of it for all the reactions, that means for all the N. So, essentially this source term here would be. The total rate of formation or generation of the species k or the consumption of species k is essentially rkn for all the n. This includes whatever unknowns we have: activation energy, stoichiometric coefficients, order of the reactions, etc.

For any typical system that we have to either estimate from the laboratory or if you have correlations or the values available, we can use them and substitute them in order to close this. So, in many cases, different types of kinetic models are used or have to be followed, and it is not possible to represent all the known kinetic terms in a single format. So, when the chemical

reactions are slow, again, slow with respect to mixing, ok. So, then it is not necessary to employ additional model to close this reaction source term because for the slow reaction that means,

the Damkohler number is much less than 1, the turbulent mixing will be complete before the reaction can take place. So, the contributions of the fluctuating terms can be neglected or may be neglected. Therefore, your time-averaged temperature and species concentrations—that means the thing that will have RKN average—can be represented by this term, such term is that what we have seen earlier. by r prime t bar where this is now the time-averaged value.

So, this is for l equals 1 to m cl o ln average. can then be used as the source term in order to close the equation. So, for fast and intermediate reactions the time averaged reaction source term will contain further additional terms because it will have its fluctuating component considered in the derivations or in the development. Now, those additional terms further require

To be closed by a set of equations in order to solve these equations, and the system goes like this. So, for in such cases what will happen say if I have say single one only one reaction that is happening a second order reaction e to the power of minus delta T activation energy divided by R prime T C1 C2. So, the time-averaged reaction source term will contain a new term here due to this fluctuating component, okay. So, the fluctuating component—let us say I would designate it like this.

So, the time-averaged component would look like r prime t bar. So, C1 C2 capital and say C1 prime C2 prime average of it. So, now you see that this part comes into play here, which needs to be further closed because this is again an unknown term that has been introduced, and a closure model is necessary for this. And this— By doing such a thing or by looking at such a thing, it becomes further complicated.

And it would require further closure models and further chemistry that has to be unraveled. Various methods have been used to develop such processes. We will not go into the details of it, but those are conventionally divided into two categories. One is the conventional closure model with or without using the probability distribution function (PDF). So, the conventional model with probability density function, and the second category is the phenomenological—

Okay, so we will not discuss those here, but the way it is done, we have got an understanding of it. So the point is, such a process can eventually be applied for a multiphase system as well. Say, for example, the reaction is happening—which is, if I give you an example—that happens in a packed bed reactor frequently used, say, hydrodenitrogenation. So, HDN is a kind of reaction for which packed bed or trickle bed reactors are frequently used.

So, this HDN reaction, or hydrodenitrogenation, where nitrogen is removed from the fuels. So, that reaction typically happens see if I say R n this component whatever that I mean this is a

representative part of this compound I have to remove this n part, and that happens in the presence of hydrogen, which is a gaseous phase, and this is the liquid phase. A gas-liquid reaction that happens.

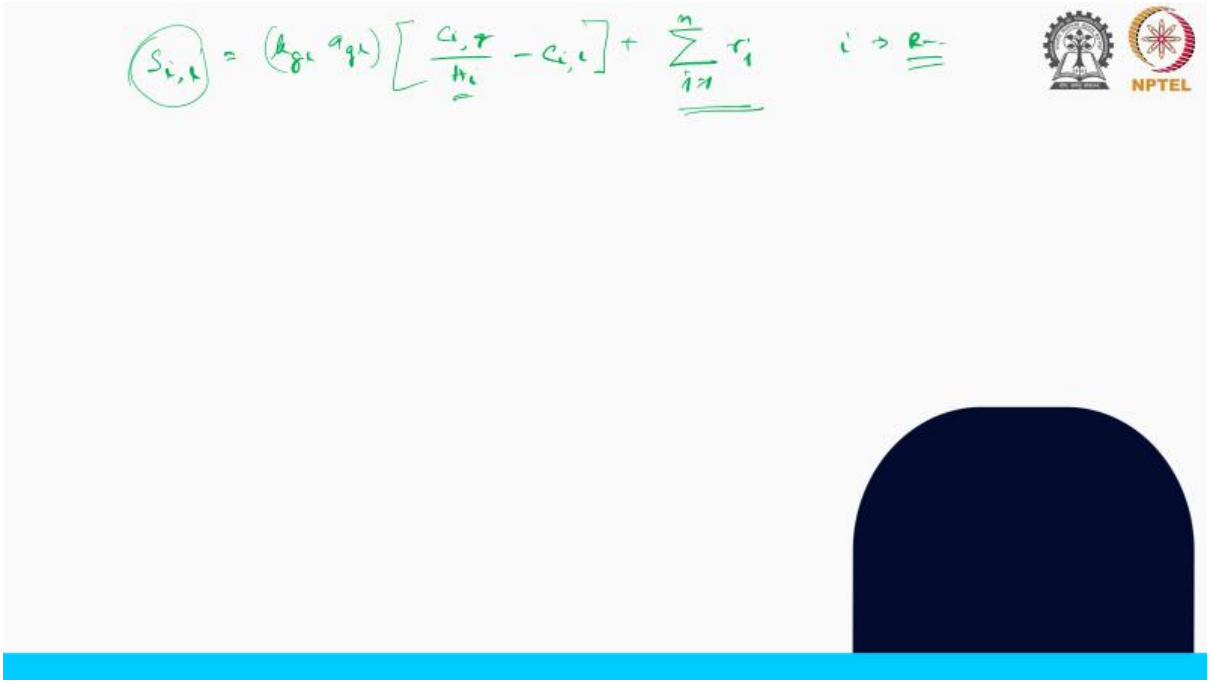
So, here, what happens eventually is we get plus NH3 in the gaseous form. So, this is a typical or representative HDN reaction—hydrodenitrogenation reaction—the gas-liquid reaction. So, the kinetic model that is involved with this. So, RHDN, if I say, is essentially KHDN—the rate constant—and it is represented by, say, C to the power (this is the concentration of N) to the power 1.5, including the partial pressure of H2O. So, C N is essentially the concentration of total nitrogen-bearing compounds.

All the nitrogen-bearing compounds that are there in this representative model or representative compound. And the pH 2 is essentially the partial pressure of hydrogen; KHDN is the rate constant for the HDN process, OK. So, this KHDN further will have some relation that would be known to you or you have to find out. So, this rate constant should be known to you before you can solve this process.

It will have an expression that you can estimate. So, this reaction rate has to be incorporated in the source term by some user-defined function. So, eventually, the mass balance equation has to be solved for the ith species in, say, a phase because here we have both gas and liquid phases existing. So, multiphase reaction. So, in that case, say the ith species' concentration in the beta phase. So, based on volume fraction and velocity.

So, we will have a species transport equation that you have to solve. And that would look something like, based on the volume fraction of it, including the phase density in which the concentration is present. See, the concentration of the ith species in the beta phase by delta t plus u b c i beta equals S i beta.

So, where all the things are known to us, this is the volume fraction. The epsilon is the corresponding volume fraction of the beta phase because we know in a packed bed that there is a voidage that is occupied by both gas and liquid phases. We have had these discussions; we will not reiterate further here, but the point is all the components, all the things, have a standard nomenclature. But here, this d i m is essentially the mass diffusivity. of the i-th species that we have seen here, ok.



So, the mass diffusivity d i m stands for that of the i-th species. C i beta here represents the concentration of the i-th species in the phase beta, ok, and rho beta is the density, and epsilon beta is the volume fraction of phase beta. So, what we see is that this source term is there further. So, this source term, either for the gas or liquid, has to be further explained. So, this S, either say if I say L or G, whatever that would be.

So, S, if I consider the liquid phase, say for this typical reaction, it can have KGL, AGL. of IF spaces Cij HI minus Cil, where I is either for the hydrogen or NH3. So, for the gas phase, if this is the gas phase, this is the reaction that the KGL, this is the expression KGL, AGL, CIG, HI, CIL, where I is either the hydrogen species or the NH3. So, where this KGL is nothing but the gas-liquid mass transfer coefficient, AGL is the interfacial area between the gas and liquid. CIG here is essentially the concentration of species I in the gas phase.

So, similarly for the liquid phase, there will be CIL, which is CI at the liquid phase, and HI is the Henry's constant for the i-th phase. Ok, and for the liquid phase, similarly, what we can write. So, I L the source term that will be there. So, K g L A g L C i g H i minus C i L plus j is equals to 1 to n R j where here I is that RH or the R the component in the compounds involved in the nitrogen part which are in the liquid phase.

So, the point is Eulerian two phase framework can be used such cases But here we do not consider the solid phase, the catalyst phase. It is the entire bed we are considering as a kind of a porous media situation. So, we have seen the porous media voidage condition, the porous media boundary conditions, etc., We have discussed that separately.

Now, here this S i L since if we consider only one reaction, then it would be for only one single reaction when J is 1. And this density, viscosity, etc. that will have to be evaluated as per the available correlations. Because if the temperature would change, this property would change accordingly. If the pressure is changing and it has influence on the property, viscosity, density, etc.

So, depending on the available correlations, you have to change or you have to find out those density, viscosity or those are considered as variables. The this Henry's law constant or Henry's constant this or the gas liquid mass transfer coefficient interfacial area these are also have to be found out or estimated if it is not available in the literature you have to estimate experimentally or if it is available in the literature use those expressions as a you did use a different function in order to find out those. Once it is found out, you go back to the Navier-Stokes equation where you have the source term. And this reaction, this source term would be placed on the right-hand side of this reaction, of this momentum equation, and then accordingly it can be solved.

So in summary the point is this what we have seen this simple HDN reaction example is when the turbulence is also not even considered or the situation that that I mentioned, that if the reaction is slow, the turbulent mixing has happened, and then the reaction is taking place. the consideration is that you need not require any fluctuating component, the mean velocity, the mean part can be solved along with the Navier-Stokes equation set that is the continuity and the momentum equation. So, the point is, the summary is that we can incorporate, and this is how we do incorporate, the reaction part, the reactive flow part in the process. Even with the multiphase as well as the reacting, if there is turbulence.

If we consider turbulence this similar formulation goes and the RANS based approach will have another term on the right-hand side, where this S would be estimated in this way, the source term for the reaction. So, on this note, I will stop here. And in the next couple of lectures, the final lectures, we will discuss the best practices of this CFD modeling approach and a few other tips that can help you to solve your problem. So, thank you.