CFD APPLICATIONS IN CHEMICAL PROCESSES
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Week-10
Lecture 50: Turbulence Modeling

Hello everyone, welcome back to another lecture on CFD applications in chemical processes. We are discussing turbulence modeling. How do we think of simplifying the resolution of the smallest scales or the smaller scales of turbulent eddies in a situation. So that we can do our modeling effectively, or I would say, depending on the objective, more efficiently. Now, what I mentioned in the last lecture is that

the scenario would be to resolve the Navier-Stokes equations as they are, incorporating the fluctuating components, even for the smaller scales. But for high Reynolds number cases, we now understand that there would be different scales of eddies, and resolving those would require an enormous amount of computational resources. So, the point is that is why the models several with the several assumptions are incorporated here or we do that where we do not require such all detailed information of all the fluctuating components or all the fluctuating scales. So, instead of simulating the exact governing equations, these equations are manipulated in such a way that the small-scale, high-frequency eddies are filtered out.

And as a result, the modified set of equations are developed—a modified set of equations which are computationally less expensive. But due to this manipulation, what happens is that this modified equation contains several unknown terms or unknown variables. and these unknown terms we have to resolve or we have to address and we require the closure model in turbulence as well like we have seen for the multiphase case it is

analogous to that where in multiphase case for the interphase coupling or interphase drag exchange terms in case of Eulerian model was done or was addressed by this closure models here also Since, we are not solving all the scales as it is we require some unknown variable in order to modify this equation that would be less computationally intensive. Now, this turbulence models so, we call these are the turbulent models. that are required to solve this unknown variables. So, that is why you can think of this turbulence models as the closure of the Navier Stokes equation when the turbulence situations occur.

So, turbulence models are essentially that is why are called also the closure models to close the Navier Stokes equation. So, now the selection of this turbulence model as I discussed in the last lecture are crucial for effective simulations or successful simulation, because the point is it requires the tradeoff between your objective and the computational resources that happened with the multiphase modeling case also. Now, there exist different models I will just at this moment would name them and we will discuss slowly. So, to start with as I said the ideal scenario would be that if any problem can be solved without any approximation and

that is we call the direct numerical simulation, which is called the DNS modeling. where we do not require no any turbulence modeling is necessary for this case. Then we have large AD simulation. or we call LES in short. So, what are those we will discuss later, but at first understand that the DNS does not require any turbulence modeling or turbulence model the Navier Stokes is solved even for all fluctuating scales as it is.

In the large eddy simulations what is done large to moderate scale ADs are solved directly as it is done in the DNS, but the small scale ADs are modeled in a different way or those are filtered out and it requires the subgrid scale modeling or so it requires subgrid turbulence models. are necessary where in DNS nothing was required. So, that means, we understand that in this direction from DNS to LEAs we require more level of or higher level of approximation, but at the same time that

provides us some cushion on the computational resources. That means, this process LES is less computationally intensive than the DNS. So, level of approximation I would say increases ok and in the other direction naturally the computational demand or the computational cost increases or the level of resolution is higher when we move from large eddy to direct numerical simulation.

And then it is still for some problem alias is still difficult because we solve a large number of large to moderate scale eddies directly or the time then scale directly. And so, in fact, which consists of say around 80 percent of the eddies that is there in the system. So, only 20 percent or around near that number. are the small scale eddies that exist those are filtered and solved through this sub grid turbulence model. So, for a problem or large scale problem where with very high Reynolds number LES is still computationally very expensive.

It is not used regularly until and unless your level of resolution you require of that accurate. So, what we have in the next set this is further with the help of other approximations we have RANS based model which means Reynolds averaged Navier Stokes based models.

So, Reynolds averaged Navier Stokes we this actually has a foundation on the Reynolds decomposition. you I have shown you that how the Reynolds decomposition works with the help of any parameter and particularly with the velocity that in general we consider with the Reynolds decomposition that there is a mean flow on which there is a superimposed velocity fluctuation

which are separated from the mean flow considerations. And then this set is used in the Navier-Stokes equation in order to find out or to separate the fluctuating components and then model those fluctuating components in different ways. Those different ways are in the Reynolds-based models because once we apply this U as the overall U that we considered earlier, the turbulent velocity is essentially plus the fluctuating component.

Once we use this U in the Navier-Stokes equation, we will see that several terms consist of what are called the Reynolds stress terms. Those Reynolds stress terms have to be resolved or modeled, and those models are done by different strategies, such as the Reynolds stress model, or the RMS model. We also have, based on what we will see, why this name comes: the two-equation model, one-equation model, zero-equation model.

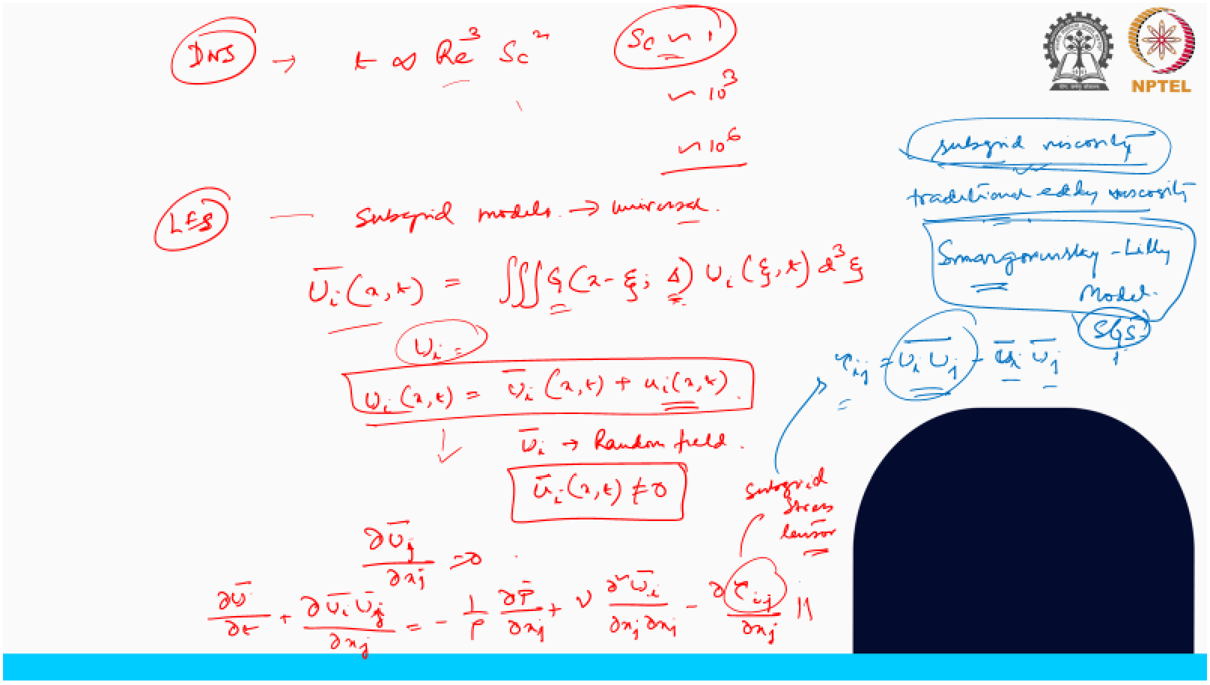
The example of a two-equation model is the very famous or most widely used k-epsilon model or k-omega model. Two equation say this these are the two equation model one equation model example is the Splart Almaras, Splart Almaras model. The zero-equation model is the Prandtl mixing length or the uniform turbulent viscosity model. Now, the point is again as per the way I have written here. So, if we go from Reynolds stress model of 2 equations, 1 equations, 0 equations the level of approximation increases if we go from 2 equation to 1 or 0 or in other words if we move from 0 to 1 equation or 1 to 2 equations the computational cost increases and our level of resolution of turbulent eddies are higher. So, this overall this set this RANS based model is also the one point statistical modeling, several order of dilution that we actually the turbulent is. The turbulent is not really the one point statistical average quantities or the can be estimated like that, but in order to model it computationally model it. These are in fact the very popular method because it requires much lesser computational power or computational resources than the LES model.

Forget about the DNS, DNS is extremely computational power or computational resource demanding process. So, we will slowly discuss one by one of these examples, these methods and mostly we will focus on the most popular the k epsilon model in a bit detail. But, the point again I would highlight that we will go through a brief overview of these models. We will not go into the extreme deep or details of each and every part of it because that would again consume say whole lot of hours in the lecture and itself the turbulence modeling can be as I told earlier can be offered as a separate course.

So, within the scope of this course we will just have an overview of this models which one to choose when to choose. So, such kind of scenarios we will discuss, but we will also go into the certain details to understand that why the naming is so for example, the k epsilon model k omega model etcetera. So, coming to this DNS ok, the DNS is definitely the favored model if we try to resolve it to the highest level of accuracy. And it seems the most obvious choice because we would not require any turbulence modeling any other modeling or any other closer if we can do the DNS modeling. But we understand that this DNS would involve

of course, the 2D 3D modelling inherently because turbulence is inherently 3D modelling. So, unsteady 3D Navier Stokes equations would be solved directly without requirement any turbulence model and the difficulty comes with the higher Reynolds number. Because we have again I would reiterate that we have wide range of scales at higher Reynolds So, the scale of resolution that we require from the Kolmogorov length scale and the time scale to the domain length or the time scale. Now, also the Navier Stokes equation there are several terms that would be the non-linear terms and the computational domain

if it is also complex then this solution algorithm the solution of the whole thing would be very time consuming. And in order to give you an estimate say the DNS the time it requires to solve is proportional to the Reynolds number Q and Smith number square. So, gases usually we have the Smith number in the range of 1, but for the liquid cases this Smith number goes say for example, water in the range of 10 to the power 3 and for the viscous liquid this Smith number can go up to 10 to the power 6 or in the range of 10 to the power 6. So, then you can think of the time would that would require for the liquid phases even for the particularly for the case of high Reynolds number.



And that is why the application of this DNS is still limited. towards the gaseous phase because we have certain degree of flexibility or reasonable value of smith number in this case which is in the order of 1. And it is not that useful or I would say not that extensively used for the any other liquid phases and particularly for the viscous liquids. So, since no information is lost in DNS it is in fact, the highest order of accurate solutions that you can get in any turbulence model. Now, since the problem in this DNS is that simulating high Reynolds number in the presence of very small length scale with high frequency eddies.

So, the logical option would be to filter out those the small scale and the high frequency eddies and that is why the development of alias happened. Where a moderate range, as I told earlier, from a large scale to the moderate range of eddies are solved directly as in the DNS. But the small-scale eddies are filtered and used or solved through the sub-grid scale modeling or sub-grid models. Now, this small scale eddies these are since again considering these Kolmogorov hypothesis and the similarity understanding what the logical deduction is that the small scale eddies are nearer to isotropic range or nearer to the isotropic scenarios at high Reynolds number cases or high Reynolds number flows.

And that is why it is logical to filter them out in order to understand or to model their effects through the sub-grid scale model. So, sub-grid scale models, that means, again based on the logic of choosing or using the Kolmogorov hypothesis, the sub-grid models that resolve these small-scale eddies should be universal, irrespective of the flow scenarios for a particular Reynolds number that is sufficiently high. So, as I told you that in general the 80 percent of the turbulent energy is resolved through the calculation of the velocities large to moderate scale velocities and the rest is done by the sub-critical model. Now, different kinds of filter functions are used; one such example, let me just tell you, is that.

Where this is the filter that we used—the filter width or the range, particularly this delta. The filter function acts to keep the values of u_i. Only when it is sufficiently large and does not fall below a certain small value that is considered as small-scale, the smaller eddies. So, this filter—that means, a user-fed function—can be used as several different functions like Gaussian functions and all, but the point is here. This velocity field that is there essentially is filtered like this.

The velocity field is then filtered or decomposed in this way, which is analogous to Reynolds decomposition, but it is not the Reynolds decomposition because here this u_i bar is a random field. And this filtered residual that we are doing is not 0 that is the main difference between this decomposition in LES and the Reynolds decomposition. So, the filtered continuity equation would look like this. This is the continuity equation and the filtered momentum equation would look like.

So, here this closure problem or the this sub grid model that we have to use appears from this stress term the residual stress tensor that we have here. This is also called the sub grid stress tensor. this actually tells us the transfer of momentum by turbulence at scales that are smaller than the filter that we are using here ok. So, this filter function that this g that we use is effectively 0 for values of u i that occurring at a small scale. for those scales this is eventually 0 and bigger than that scale this is used in order to filter those small scale fluctuations.

And eventually when those are replaced in the Navier Stokes equation it results in this closure issue that has to be addressed by the sub grid stress model. So, the filtered velocity is here. this u i u j bar those are solved by this, but the correlations that we require which is in this tau if I write here this value is essentially tau i j is u i j bar u i u j power. So, this filtered velocities these are solved, but this we require this one which is unknown.

So, that is why we require a sub grid stress model in order to solve this part and the and so, this is this appears to be say that if we try to address this that can eventually involve the modeling of the sub grid viscosity. Now, the point is the subgrid viscosity and the traditional eddy viscosity. So, the subgrid viscosity and the traditional eddy viscosity are not the same, but the difference is that this actually acts as a correction to the behavior of the small scale the sub grid viscosity and this is not a correction to

the entire influence of turbulence on the mean flow that is usually done by the traditional eddy viscosity. So, sub grid viscosity acts as a correction to the behavior of the small scales, but not to the conventional mean flow, the influence of turbulence that comes from the mean flow, which means the sub grid viscosity is small compared to the traditional viscosity. So, this subgrid viscosity has to be modeled separately in order to close this equation or to solve this alias. There are different subgrid models available, and one of the frequently used models is the

Smagorinsky-Lilly model, or we say SGS model as well—SGS subgrid scale model. And one of the frequently used subgrid scale models, which we abbreviate as SGS models—subgrid scale models. One of the frequently used, like we have seen in the multiphase cases, there are several models to close those interface coupling terms. Now, similarly here also several researchers have addressed this issue and according to based on their names those models are available and those can be explored in details for those who are interested in this area.

We will not go into the details of what that model is or what different models are available. But this is just to name one such model, the Smagorinsky-Lilly model, which addresses the subgrid scale viscosity or subgrid viscosity that helps to close the alias function. So, on this note I will again stop here today and in the next class we will discuss again the Reynolds link up decompositions which helps us to understand this Reynolds stress models, two equation models, one equation model and the zero equation model. Because these are the frequently used models, and particularly the k-epsilon model, we will take up in the coming lectures.

So, till then, thank you for your attention.