CFD APPLICATIONS IN CHEMICAL PROCESSES

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Week-11

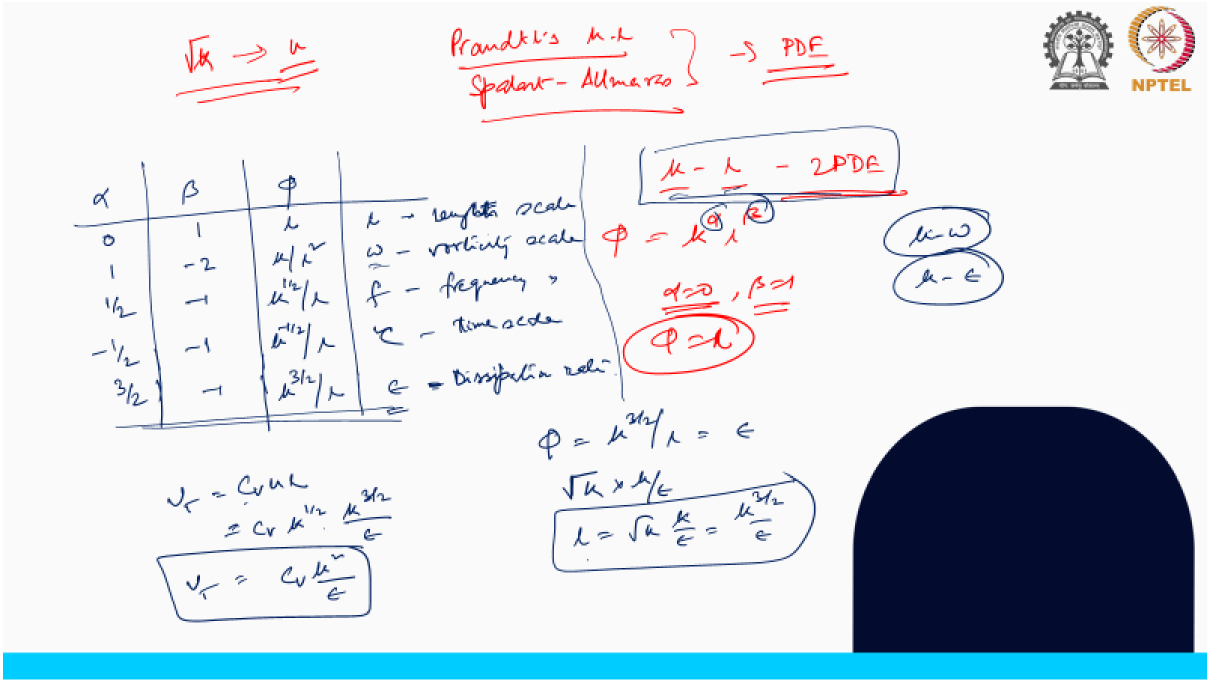
Lecture 53: Turbulence Modeling

Hello everyone, welcome back with another lecture on turbulence modeling in CFD applications in chemical processes. So, till now whatever we have discussed on the turbulence modeling part that accounts for the concept of DES, ADS and the genesis of RANS based models. Inside the RANS based models now we realized that we have to resolve the Reynolds stresses and how do you resolve Reynolds stresses for that we have several different strategies in the RANS based models. And that is why we have started understanding that what is the zero equation model that we have seen in the last lecture

that is the Boussinesq approximation one equation model in order to address this Reynolds traces. We must also understand at this point or during this turbulence modeling cases that these Reynolds stresses are not alike the conventional viscous stresses that is a fluid property and this Reynolds stress is essentially a turbulent property. And also we have to understand the difference between the molecular viscosity and the eddy viscosity or the turbulent viscosity. So the point that we have discussed till now is that from that you can understand that the turbulent eddies have a certain lifetime, they have certain history.

So those are transported by convection and is not essentially can be defined by the local condition, but it depends on the history of the eddies. So, the limitations that we have in zero equations model that does not account for such scenario and that is why it is less accurate it is extremely simplified model is that instead this turbulent viscosity that we are trying to relate with. because, there we directly had some relation. But, the point is this turbulent viscosity if we can relate that with the transported turbulent quantity instead of relating that with

the mean velocity gradient that we did in the Bosons approximation or once that is the zero equations models. So, in contrast to this zero equations model this one equation model we have also seen yesterday or in the last class that one equation model allows to take into account the history And, that is independently proposed by Kolmogorov and Prandtl that the square root of the time averaged turbulent kinetic energy is best described by the characteristic velocity scale. So, k should be this square root of k that is the turbulent kinetic energy, this should be employed as the characteristic velocity scale.



And that example is taken care or this kind of scenario has been proposed by Prandtl's KL model. Or in the one-equation case, we have also seen the Spalart-Allmaras model. So, these models are essentially the one-equation model, and we have to understand that the transport of the turbulent kinetic energy is taken into account by these models. But then there, we have one that comes with the expense of one additional PDE, and that is why these are called the one-equation model. Now, this characteristic velocity

is determined from this transport equation, but the length scale we have to resolve or express in a different way, specifically in this case, in an algebraic manner. So, that is why we have one PDE for this one-equation model, and the velocity scales are determined by algebraic equations or algebraic relations. So, which means it is still inaccurate. So, that is why we require

another equation or essentially a minimum of two equations in order to resolve the velocity scales as well. But, this 0 and 1 equations model people still use this because these are for the general purpose simulations or say the proof of concept simulations that can be the influence of turbulence. But as the number of equations increases, we can understand that the computational effort or cost also increases. And therefore, these two-equation models that we will discuss today are computationally intensive, but they are more inclusive.

Or these can be called the complete models for turbulence. Because we understand that it takes two quantities to characterize the length and velocity scales for turbulent flow. So, the point is, these transport equations when we try to describe those, the turbulent production, dissipation, all those things are expressed in a localized rate. Now, without the turbulence mechanism or the transport mechanism, this turbulence has to instantly adjust to these local conditions.

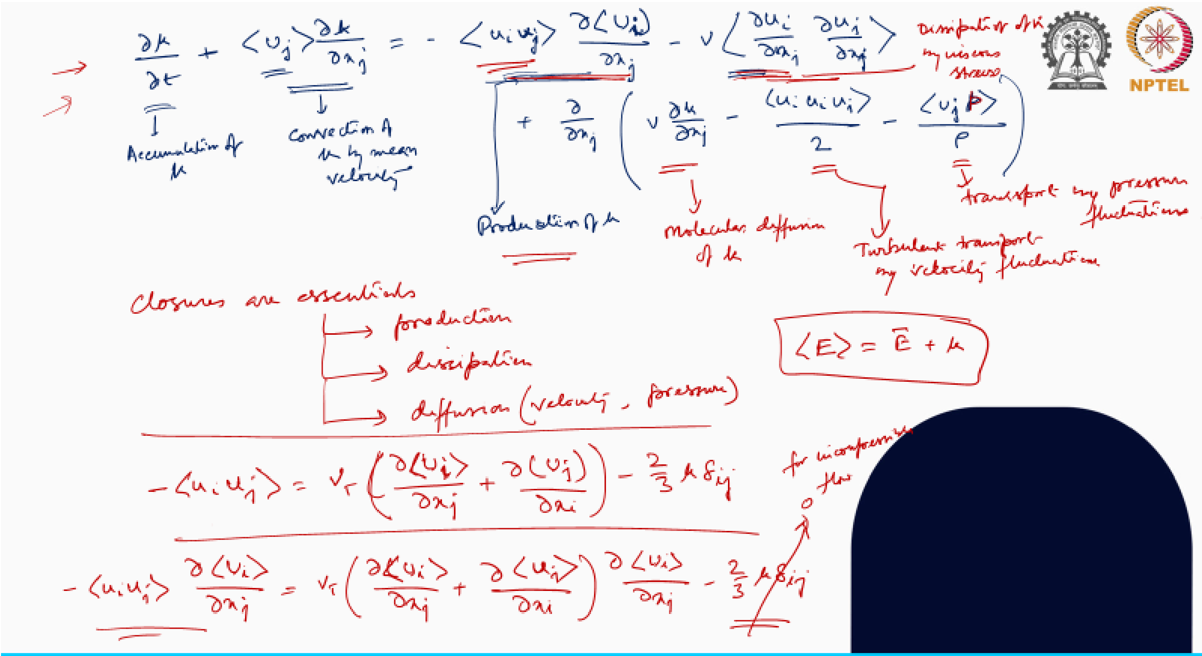
So, the point is, Then what happens is, it gives unrealistically large productions or dissipation rates when there is no transport mechanism. And in fact, in many cases, what happens is that high local values of turbulence are due to the convection of upstream-generated eddies. So, the point is one way to look into it is to model the turbulent velocity and the length scale to solve the k equation for the velocity scale and the L. So, that means, the k and L we use two PDEs to resolve this.

And that is why these names that we are seeing—1 equation, 2 equation, 0 equations, etcetera—these are logical. So, the 2-equation model essentially models K and L, where we have K as the velocity scale because this is the hypothesis that Prandtl and Kolmogorov independently proposed, that the square root of turbulent kinetic energy should be a representative of the velocity scale. So, the velocity and length—these two are of great importance in turbulence, those are what we are countering with the help of K and L: turbulent kinetic energy and the length scale. So, generally, what happens if we say an arbitrary property, which is say, phi,

and it is related to the length scale in the following way: k to the power alpha and L to the power beta. So, the point is, depending on the value of k and L, say when alpha is 0, what we see and beta is 1, what happens is, phi is essentially 1, or this is not on it is L—basically only the length scale. So, the point is Depending on the value of alpha and beta, we can have various two-equation transport models. So, say for example, if we now consider this alpha and beta here these two.

So, if alpha beta corresponding phi then we consider that say alpha is equals to 0 beta is equals to 1 and then phi is essentially L. And so, the symbol by which we designate that is itself L and that is the interpretation of the length scale. If alpha is 1 and beta is minus 2, what happens? The phi becomes k divided by L squared, and this we say is the vorticity. If alpha is half and this is minus 1, we have k to the power half divided by L. This is essentially the frequency scale. If this is minus half and this is 1, the beta is 1, then what we have is k to the power minus half divided by

L, and this is what we have as tau, which is the time scale, OK. So, yeah. So, this is the minus 1, then becomes k divided by L. In other cases, say if I have 3 by alpha is 3 by 2 this is minus 1 then what we have k 3 by 2 and L and this quantity we say as the dissipation rate which is in fact most commonly used in this variables. So, what does this mean is that we have already found several two equation model or we can see there can exist several and the names of those two-equation models depend on this alpha and beta.



So, if alpha is 1 and beta is minus 2, what you get is omega, which is the vorticity scale. And that brings us to the naming of this two-equation model as the k-omega, OK. Similarly, This is the situation that would happen if we resolve the dissipation rate based on this 3 by 2 and minus 1 of alpha and beta. This would be the epsilon, which is the k-epsilon model. So, this k-epsilon model describes the turbulence using two variables: one is the kinetic energy, and the other one is the dissipation rate.

Similarly, K-omega defines the turbulence model by two variables: one is the kinetic energy, and the other one is the vorticity. So, this K epsilon is actually a very famous or most widely used in this I would say the standard versions or its variations that we will discuss today are most widely used of these RANS based models. So, the relation between the turbulent length scale and energy dissipation rate that we now have understood is that phi equals k to the power of 3/2 divided by L, which is epsilon. So, the length scale is simply the turbulent velocity times

turbulent velocity because, again, remember the proposition of the hypothesis that Kolmogorov and Prandtl independently provided: the square root of k represents the velocity scale. It is multiplied by the lifetime of turbulent eddies, which is k divided by epsilon. So, the length is essentially the square root of k multiplied by k divided by epsilon. In fact, from this relation, we also realize that we require two additional PDEs to resolve k and the length scale, which represents the velocity. So, U times L essentially comes out to be k times L, and L in that we are changing that variable or representing it by either one of these variables.

where L is represented by k to the power of 3/2 divided by epsilon. The turbulent Is essentially C V U L. We have seen that this is earlier, where C V is the proportional constant, the proportionality constant. So, this essentially what we can write is K to the power half, and this

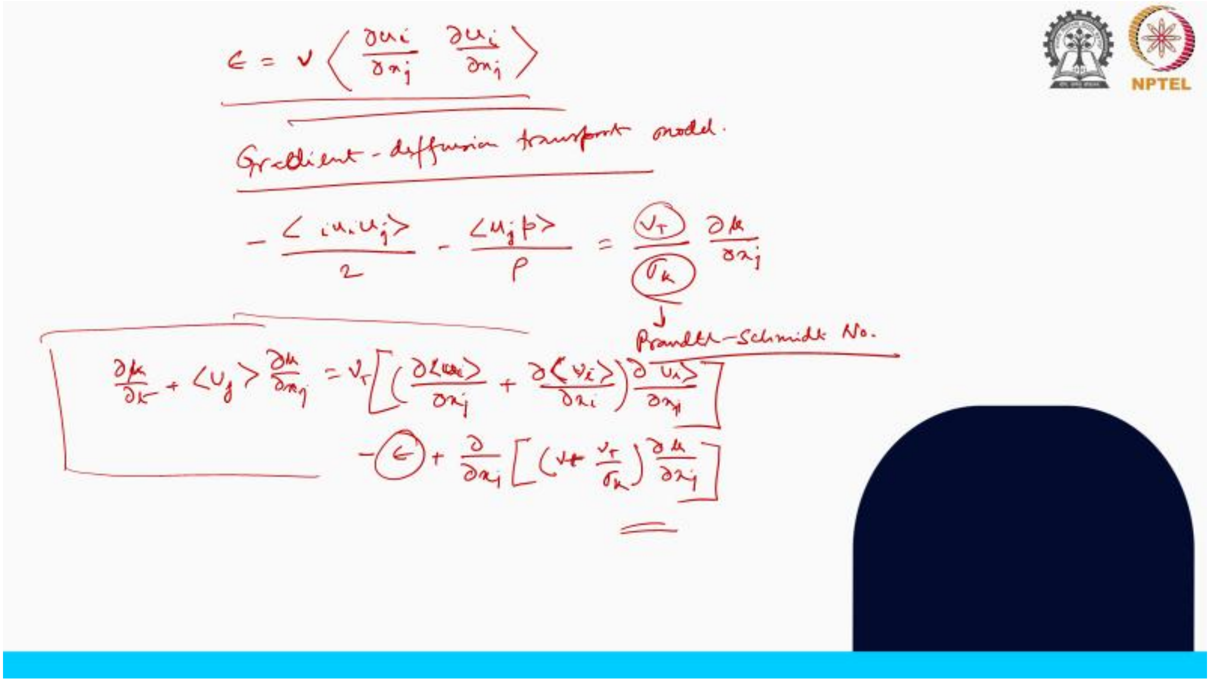
L is K to the power two-thirds divided by epsilon. So, essentially it becomes Cv k squared by epsilon.

So, which is the turbulent viscosity. So, these two-equation models are widely used for simulations, not only in chemical engineering problems but in any engineering problem. Now, although these models have some limitations, which we will see. They are actually favorable because these are robust as well as relatively inexpensive. In fact, a lot inexpensive than the DNS or the ABS model expensive compared to the 0 equation model, but that is the

trade-off we have in terms of accuracy. These are far superior to the 0 or the 1-equation models. So, this K epsilon model is very popular due to the fact that this epsilon the role it plays in the interpretation of turbulence addition to the fact that this epsilon appears directly in the transport equation of K, which we will see. And that is why it provides a good compromise between the generic applications and the economy of the CFD problems. Now, we have to be.

Careful that these equations, that this K and epsilon, the transport equations, are essentially simplifications of the exact transport equation for K and epsilon. Which means this K-epsilon model is one of the several possible closures. inside the closure of the closing Reynolds stresses that this K epsilon model is one of the several possible way for the closure by which the RANS equations are simplified even further. So, the point is this closures are not unique that we have seen such situations, but the point is it is required that all closure models have to be based on the statistical averaging due to higher-order moments that are introduced in the problem.

So, the exact transport equation for turbulent kinetic energy. We can deduce from the equation of kinetic energy by Reynolds decomposition, and that would be in this form. G, in fact, here. So, it takes this kind of form, where I will just tell you the importance of all the terms. So, the first term is the accumulation of K. The second quantity is the convection of K. By mean velocity, because here we have the mean velocity.



This term is the production of K, meaning the large eddies extract energy from the mean flow. So, this is ij. So, this is the production of K, this term. This term is the dissipation of K by viscous stress. Where the turbulent energy is transformed into heat, increasing the fluid temperature.

In this term, we have three separate terms. This one is the molecular diffusion of K. This term represents the turbulent transport by velocity fluctuations. These are all fluctuations. And this final term here is again the turbulent transport by pressure fluctuation. This is the transport, again turbulent transport by pressure fluctuation; this is the P fluctuation.

So here, this production of k, the dissipation rate, then this turbulent transport, and this transport by pressure fluctuations—these are all unknown. And we have to use some approximation in order to close this equation or to solve this equation. So therefore, the closures are essential again here; closures are essential for defining production or estimating production, the dissipation, and the diffusion terms—diffusion—and that is by velocity and pressure both. These production terms actually represent the production of turbulent kinetic energy due to the mean flow rate or the mean flow strain rate.

Now, if we consider this equation of kinetic energy for this mean flow here, then this term actually acts as a sink in this equation. So, which means that the production of kinetic energy is, in fact, a result of the mean flow losing kinetic energy. Otherwise, if you remember that cascading effect of the—or the cascade effect in turbulence—which is the energy transfer cascading effect. So until and unless something is lost from the mean flow, it would not be gained by the other, which is the energy lost by the mean flow, which is gained by the larger eddies. And also, if we remember that energy would have the form in its decomposed form that this is the expression that we can have—that the mean energy that we consider. So, the production term in this Reynolds stress multiplied by the shear stress, and the maximum production will occur where both are large. So, and those happens nearly mostly near the boundary layers and that is why it is again I must reiterate that the near wall treatment in turbulence modeling particularly using this trans model is essentially extremely important. Now, the point is these Reynolds traces we can identify in the production term, and we assume that the Boussinesq approximation can be used in this model as well.

So, in that case, this is the thing that we have. So, this part again we consider that it can be represented or estimated. This is the thing that we have seen earlier as well. So, which means the production of turbulent kinetic energy can be modeled as. So, now we have this whole term here.

So, this term that we have. del xj minus two-thirds k delta ij. So, here the last term again is usually zero; in fact, it is zero for incompressible flow. Because of the continuity. So, the point is this Boussinesq approximation is applied or considered for isotropic conditions, and it is assumed that the normal stresses are equal. So, this is the consideration we are already making while modeling this production.

The second closure that we require is for the dissipation, which we need to model the k-equation—the energy dissipation rate, which is the rate of destruction of turbulent kinetic energy. Dissipation is the destruction of kinetic energy in the fluid while flowing, and this dissipation rate. We can define xj as which is here, in fact, this term. So, that is why I said earlier that one of the benefits of using K-epsilon is that this epsilon appears in the transport equation of K itself. So, this is the dissipation rate, and the third one we require is the diffusion for both velocity and pressure fluctuations.

So, now these higher-order moments that we have here—what happens is these are modeled by the assumption of gradient diffusion transport mechanism. So, these are modeled by the gradient diffusion transport model. What does it do? This assumption actually allows us to think that the turbulent transport due to velocity and pressure fluctuations can be modeled as P by rho is essentially eddy viscosity by sigma k, k by dxj, where this is a model coefficient known as the Prandtl-Smith number, and this is the turbulent viscosity we already knew.

So, once we replace this closure or fit this closure into the transport equation, what do we get? We get this form: J is nu t xj minus epsilon plus xj, and then we have this quantity inside k by T xj, but the point still remains. So, this is a consolidated form of the previous equation that we have here. The point still remains that if we try to solve this equation, we have to calculate the dissipation rate.

Now, the dissipation rate is modeled with a second transport equation in the two-equation model. The production of turbulent kinetic energy is modeled essentially as a product of turbulent viscosity and average velocity gradient. So, on this note, I will stop here because, in the next lecture, we will start from here, where we will show you the transport equation of epsilon. And in that, we will also discuss the variations of the k-epsilon model, and then we will close this by showing you some suggestions for a typical flow problem. On this note, I stop here and thank you for your attention.