

CFD APPLICATIONS IN CHEMICAL PROCESSES

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Lecture 55: Turbulence Modeling

Hello everyone, welcome back to another lecture on CFD applications in chemical processes. We are discussing turbulence modeling, the final part of it, because we have seen most of the strategies that are widely used. We have seen starting from the RANS based models and we also have seen very high resolution turbulence modeling that is the DNS or alias fundamentals although we have not gone into the very details of those. But, we have an overview of the DNS, LES, RANS based approaches and in RANS based approaches, we have seen

the genesis of 0 equation model, 1 equation model, 2 equation models. Out of those 2-equation models, we are specifically discussing the k-epsilon model—the standard k-epsilon model we have discussed. Because of its widespread use in several applications not only for the chemical engineering but for any engineering applications usually whenever the turbulence is there to start with the simulations it will apply the k epsilon model. Now, this k-epsilon model has different variations.

In the last lecture, we realized or understood why such variations are needed, and one such variation is the RNG k-epsilon model. We briefly discussed how it differs from the standard k-epsilon model. Today, we will discuss another variation of the standard k-epsilon model, which is the realizable k-epsilon model. Now, this realizable k-epsilon model—the name stems from the idea that this model features a realizability constraint, a realizability constraint on the predicted stress tensor, and that is why it is called the realizable k-epsilon model.

So, the difference actually comes from the correction of k equations that we have seen in the standard case where the normal stress can become the negative for flows where we have very large amount of strain rates. So, if you look at it, its expression is essentially now this normal stress. must be larger than 0 by definition because it is the sum of squares. But the point is if the strain is sufficiently large this normal stress can become negative ok.

From this expression we can see that this strain rate is sufficiently large then this value can become negative. So, this realizable k epsilon model uses a variable this C_μ that actually prevents this happening. So, it ensures that this does not become negative even at a high strain rate condition. So, the point is the C_μ the constant that or the variable that we are considering here in order to ensure that it cannot be a constant, but this is a function.

So, this becomes a function or it is essentially a function of the local state of flow that ensures that the normal stresses are positive under all flow conditions. To ensure that the normal stresses it ensures that the normal stresses are say positive under all flow conditions. That means, in other word to ensure realisability.

and hence the name is the realizable k epsilon model. So, this realizable k epsilon model ensures that the normal stresses are positive that actually neither the standard nor the RNG k epsilon model is realizable. So, this realisability also means that the stress tensors satisfy this condition which is we called in equality that has to be fulfilled. So, that is why we expect that this realizable k epsilon model would provide us a better performance than the standard k epsilon or its variation RNG k epsilon model.

Realizable k-ε model
Realizability constraint on the predicted stress tensor:

$$\langle u_i u_i \rangle = \sum_k \langle u_k^2 \rangle = \frac{2}{3}k - 2\nu_T \frac{\partial \langle u_i \rangle}{\partial x_j}$$

C_{μ} → function of the local state of flow - ensure that the normal stresses are positive under all flow conditions.
 → to ensure realizability

$u_i^2 \langle u_i^2 \rangle - \langle u_i u_i \rangle^2 \geq 0$ Schwarz's inequality / fulfilled.

Also involves a modification of the ε equation. This modification involves a production term for ε that is not found in either standard k-ε or RNG k-ε model.

Standard k-ε model → spreading rate of planar jets.
 ↗ axisymmetric jets.
 ↘
 Realizable k-ε model → large strain rate.

So, in addition to that this model generally involves the modification of epsilon equation also. Now, that modification involves a production term for turbulent energy dissipation that is not found either in the standard of the RNG model. So, this model also involves a modification of the epsilon equation and this modification involves a production term for this turbulent energy dissipation that is not found or cannot be found in either standard k epsilon model.

or even RNG k epsilon model either in standard or in k epsilon model. So this standard cape silent model predicts say it like in the previous lecture we saw that this standard cape silent model works reasonably well to predict say the spreading rate of say planer jets, but it cannot accurately predict the spreading of axis symmetry jets. So, and the reason mainly can be attributed to the modeled dissipation anomaly that we discussed that is it predicts spreading rate for this asymmetry jets as well as for the planar jets the way it resolves.

the anomaly in the dissipation equation. But in the case of realizable K-epsilon model it even resolves this round jets which actually is the axisymmetry jets quite well. And this model is actually better suited for the flow in which strain rate is large. For the large strain rate, realizable capsaicin model is better suited for the large strain rate problems. That means it includes the flow with strong curvature, the streamline curvature, and rotation, which are the limitations in the standard k-epsilon model.

So, research also shows that several results also shows that depending on such scenarios or the problem specification, realizable k-epsilon model performs better than the standard k-epsilon model or sometimes even the RNG k-epsilon model. So, the point is we have the other variation. So, these are the two variations we discussed of the standard k-epsilon model: one is the RNG k-epsilon model, and the other is the realizable k-epsilon model. Now, these are the so-called two-equation models. The other variation, or the other modeling strategy, is the Reynolds stress model.

or the RSMs. Now, what we have understood is that this Reynolds model, these turbulence models, are based on Boussinesq approximation. So, those models which were based on the Boussinesq approximations provide inaccurate results when we have a sudden change in mean strain rate, okay? Because the history effect of the Reynolds stresses persists for long distances in turbulent flows, and those are not really accounted for in those modeling strategies. And the point is, the Boussinesq approximation assumes that the eddies behave like molecules and momentum exchange happens quickly.

So, in these Reynolds stress models, So, in fact, most—in fact, all—the previous models that we discussed are based on these Boussinesq approximations. Now, the point is, this Reynolds stress model does not take into account the assumption that we have isotropic eddy viscosity, this concept. So, Reynolds approximation, the Boussinesq approximations, and this inherent isotropic eddy viscosity assumption It is not there in this Reynolds stress model.

So, this does not consider the isotropic eddy viscosity. Reynolds stress models close the RANS equations, the Reynolds-averaged Navier-Stokes equations, by solving the transport equation of Reynolds stresses. We have seen the six components of the Reynolds stresses. So, all these six are solved individually. That means it does not require any additional modeling or turbulent closure models that we have discussed for other cases.



So, this RSM, the Reynolds stress model, solves one equation for each Reynolds stress and does not require any additional modeling for turbulence. So, the Reynolds stresses that we have seen are non-linear. These eddy viscosity models are usually referred to as second-moment closure. So, the main advantage of these single transport models is their natural approach, in which non-local and history effects are accounted for. So, these models actually improve performance under certain conditions because they account for the effects of streamline curvature,

swirl, rotation, and rapid changes in strain rate in a more rigorous way than the two-equation model. So, that is why RSMs are also popular for flows with, say, particularly strong streamline curvature, strong curvature of the streamline flow, swirling flow, rotational flow, and rapid changes in the flow strain rate. So, these are essentially handled more effectively by RSM models, which are better suited for these cases. The standard case silent models actually fail, or even in certain variations, they are not as accurate as what we get from the RSM models or the general stress models.

So, in principle, this Reynolds stress modeling is should be the obvious choice because there is no further turbulence closure models involved in closing the Reynolds stresses all transport equations are used for every stresses, but the point is as the equation. So, here we solve 6 additional equations—6 additional PDEs for those Reynolds stresses. So, the point is,

It is more computationally expensive. If you remember, on the scale, it was after the two-equation model in the RANS-based approach. So, the point is, we solve 6 additional equations for the Reynolds stresses along with the other equations that we have seen in the system while solving or understanding this turbulence modeling. And that makes this approach a bit less

attractive because it is more computationally intensive. However, the recommendations are that these models should be used when the flow features of interest involve anisotropy in Reynolds stresses.

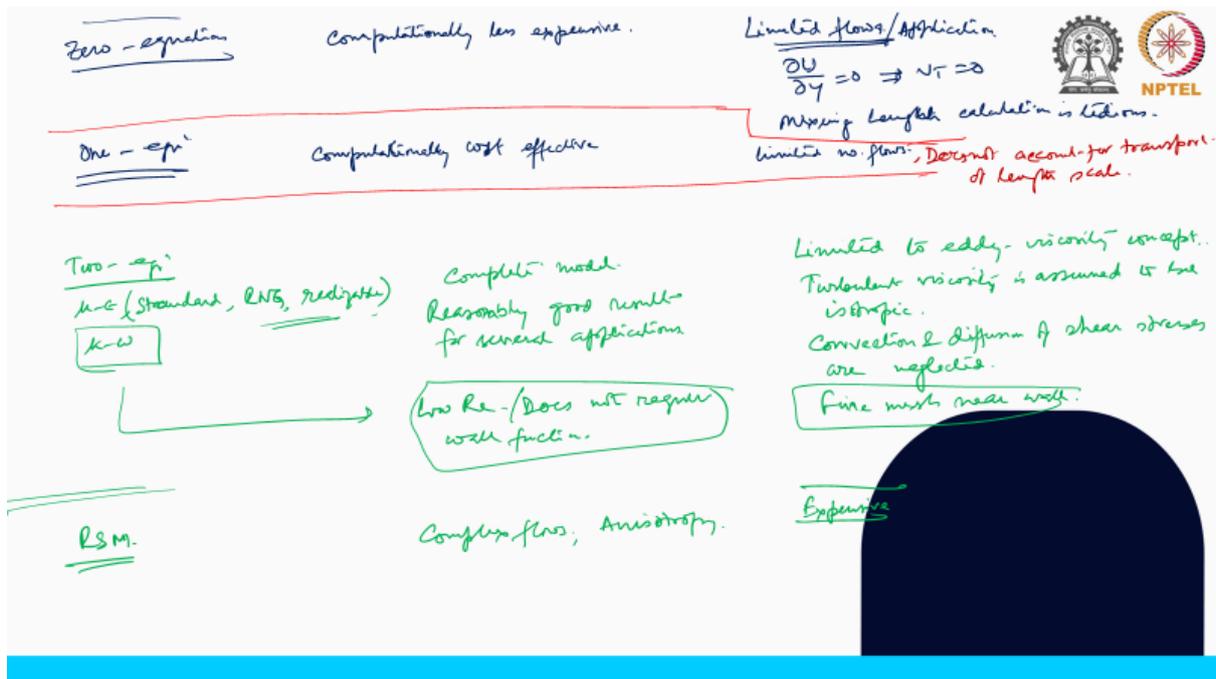
So, this is the recommended use: when we expect that the flow features are the results of anisotropy in the Reynolds stresses, then this model has to be used. So, we will not go into the details of the equations that are used in the Reynolds stress models, but instead what we will now do or we will now see the pros and cons or the summary of all the models that we have seen starting from the zero equation model. So, the zero-equation model's pro was that it was cost-effective. So, numerically speaking, it was computationally cost-effective. So, I can say that computationally,

less expensive, but it is used for a limited number of flows. So, the cons is the limited flows or the limited number of flows limited application. When say particularly it has a limitation that it should not be used in such scenario. So, lack of transport of turbulent scales because no equations are solved for the transport turbulent transport. The estimation of mixing length if we apply the mixing length concept

mixing length estimation or calculation is tedious and cannot be used as a generic turbulence model. The computationally more intensive is the one equation model. which is still cost effective computationally cost effective although a bit computationally intensive than the 0 equation model, but it is also applied for a limited number of flow. So, this is also applied for limited number of flows and it uses an algebraic equation for the length scale which is too restrictive because that is why because it solves only one PD additional PD for the velocity scale.

but the length scale is considered to be the algebraic relation of the equation which is too restrictive. And the transport for length scale is not accounted for because only one additional PDE is solved for the velocity scale ok. So, the other limitation is that does not account for transport of length scale. Then we have two equation model such as k epsilon standard RNG realizable, etcetera.

So, this also here or in fact, there is other also K omega different variation we did not discuss, but the genesis we realized factor of the indices' values of alpha and beta that we have seen earlier. So, this actually in a sense is a complete model that accounts for velocity and length scale separately that is why two additional PDE we are solving that are predicted with the transport quantities and it shows reasonably good result. Good results for several applications, okay.



And it is specifically very good to trade off between accurate results and also computationally cost-effective turbulence modeling. So, there is a if you have a have to a trade off then this is the model is best suited for that you get a reasonable accuracy of the turbulence modeling for the turbulence modeling also and on additional with that you also have reasonably less computationally intensive model, which are the two-equation models.

But these are limited to the eddy viscosity concept. The turbulent viscosity is assumed to be isotropic, and that is the limitation. If that is not isotropic turbulence, you expect your results to reflect the anisotropy of the turbulence. Then you cannot use these models, the two-equation RANS-based models, okay. Additionally, the convection and diffusion of shear stresses are neglected.

So, these are the overall two-equation approach, the two-equation RANS-based approach, their pros and cons. And specifically when we talk about the standard k epsilon let me just repeat again which is the most widely used and validated model. but it is not good for round jets or where you require the axis symmetry results that involves or the problems that also involves the significant curvature, swirl, sudden acceleration, separation of flow etcetera or even at the low Reynolds number flows turbulent flows. So, it has several limitations, but still it is widely used and accepted or validated model.

The RNG k-epsilon model which is the modification of the standard k-epsilon model, it provides improved or say better results than the standard one and it can be used for the swirling flows. and also for close separation situations. But it is not stable as the standard k-epsilon model during the simulation and also it is not suitable for the axisymmetry jets or the round jets. The realizable k-epsilon model that we have seen which is the modification of the standard

k-epsilon model it provides much better result even in the case of swirling flows, flow separation and also can handle the limitations of the RNG k epsilon is the round jets of the axisymmetric jets.

But again the problem is so much nonlinearity involved while solving it that it is also not as stable as the standard k epsilon model during the simulation. The k omega model that we have not discussed in details this actually very much useful for the low Reynolds number turbulent flows and does not require wall function which is inherently required for this k epsilon models. It works well. So, this does not require wall functions for the viscous sub layer part near the walls.

And also works well with the adverse pressure gradients and separating flow, but the limitation is that it requires very fine mesh since it does not require the wall function it requires very fine mesh near wall. So, and the thing that we have broadly discussed are the RSM models, Reynolds stress models. These are applicable, the benefit is that it can be applied for complex flow scenarios where the standard k epsilon, realizable k epsilon, k epsilon those fails. Because, those has the limitations that cannot be used for the separating flow, high curvature, stream line flows, swirling flows, rotating flows, etcetera.

But swirling flows can be used with the can be predicted with the realizable cave-siren model. But the point is this RSM models is applicable for several complex type of flow or the complex flows. It is can be applied for the complex flows. That is the benefit. It accounts for the anisotropy. So, it is recommended that when you have anisotropic turbulent flow you use RSM models and extremely good performance for the swirling flow separation or even the planer jet.

But the point is it is computationally very expensive. computationally very expensive because several terms in the transport equation are unknown and also needs the closers. although no additional turbulence modeling is required, but we are solving say 6 additional PDEs for the Reynolds stresses, all individual Reynolds stress terms and that also further involves several unknowns. So, it also requires several quantities

the terms that has to be closed before we can solve all those equations. So, on this comparative summary of the several or various turbulence models, particularly of the RANS based approaches and separately on this Reynolds stress models that we discussed, we must choose the turbulence model wisely. And again the things I am always repeating it is in fact, in all the class all the lectures is that there must be a tradeoff between your required resolution for the result or the objective and the computational resources that you can afford.

So, on this note, I will stop here today, and this closes our discussion on turbulence modeling. In the next lecture, we will now start the reaction because reaction involves mixing, and I told

you earlier also that nothing can be better for mixing than turbulence. So, thank you for your attention. We will see you in the next lecture.