

CFD APPLICATIONS IN CHEMICAL PROCESSES

Prof. Arnab Atta

Department of Chemical Engineering
Indian Institute of Technology Kharagpur

Week-11

Lecture 54: Turbulence Modeling

Hello everyone, welcome back to another lecture on CFD applications in chemical processes. We are discussing turbulence modeling and how to apply it in various systems. So, we are going into a bit more detail on the k-epsilon model that we started—basically a two-equation model—and here we are discussing the k-epsilon model. In the last class, we started this topic where we realized that it takes two quantities to define the velocity scale and the length scale. The velocity scale, based on the hypothesis of Prandtl and Kolmogorov, can be represented by the square root of the turbulent kinetic energy. And this length scale also has to be resolved.

So, this in this case we have taken different variations we have shown a chart in the last lecture that how this epsilon the dissipation rate comes into the picture while changing the indexes of K and L if we consider in the arbitrary parameter phi that phi then becomes the rate when alpha and beta become $3/2$ and -1 . So, the point is, we reached a stage where we realized that to solve this transport equation of k, we require the estimation of epsilon. We also noted that the production of turbulent kinetic energy

is modeled as the product of turbulent viscosity and average velocity gradients, as seen in this expression. Now, the exact equation for epsilon can be written in a quite lengthy form. So, please bear with me, but it is worth understanding this expression. Minus plus x_j So, what we have here is the exact equation of epsilon where we see that we have one term, this is the second term, this one is the I would consider this part is the third part ok, this one is the fourth part. this is the 5th term 6th term 7 8 and this is the 9th term. So, physical interpretation is that this is again the accumulation this is the convection of epsilon by mean velocity we have the mean velocity here.

this 3 and 4 these are the interaction due to within the mean flow and the products of turbulent fluctuations. So, that happens that results in the production of dissipation. So, this dissipation has a production mathematically speaking is that and that comes from these two expression that the production of dissipation due to the interactions between the mean flow and the product of turbulent fluctuations. 5 and 6 these are the destruction rate of dissipation due to turbulent velocity fluctuations.

$$\frac{\partial k}{\partial t} + \langle u_j \rangle \frac{\partial k}{\partial x_j} = - \langle u_i u_j \rangle \frac{\partial \langle u_i \rangle}{\partial x_j} - \nu \left\langle \frac{\partial u_i}{\partial x_j} \frac{\partial u_j}{\partial x_i} \right\rangle + \frac{\partial}{\partial x_j} \left(\nu \frac{\partial k}{\partial x_j} - \langle u_i u_j k \rangle - \frac{\langle u_j p \rangle}{\rho} \right)$$

Accumulation of k Convection of k by mean velocity Production of k Dissipation of k by viscous stresses Molecular diffusion of k Turbulent transport by velocity fluctuations Transport by pressure fluctuations

Closures are essential:

- production
- dissipation
- diffusion (velocity, pressure)

$$\langle E \rangle = \bar{E} + k$$

$$- \langle u_i u_j \rangle = \nu_T \left(\frac{\partial \langle u_i \rangle}{\partial x_j} + \frac{\partial \langle u_j \rangle}{\partial x_i} \right) - \frac{2}{3} k \delta_{ij}$$

$$- \langle u_i u_j \rangle \frac{\partial \langle u_i \rangle}{\partial x_j} = \nu_T \left(\frac{\partial \langle u_i \rangle}{\partial x_j} + \frac{\partial \langle u_j \rangle}{\partial x_i} \right) \frac{\partial \langle u_i \rangle}{\partial x_j} - \frac{2}{3} k \delta_{ij} \frac{\partial \langle u_i \rangle}{\partial x_j}$$

for incompressible flow

is the viscous distribution of epsilon like we have seen in the equation for k. The term 8 that we see is the turbulent transport of epsilon due to velocity fluctuations and this is similar to the k expression like we have seen earlier is the turbulent transport of nu due to the velocity pressure fluctuations. So, this is here a bit different that we have the velocity pressure coupled expression here and due to that this fluctuation whatever it is transported that thing is here. This is the transport due to the velocity fluctuations. So, in this case also we find several things unknown such as

this term is unknown this term is unknown this 6, 8, 9 all these terms are eventually unknown for us and we have to estimate those before we can solve this equation. So again that means it requires several closers in order to solve this part. And there has been introduction of several closures, but let us skip that part. What is of importance is that after several closure fittings and all that we can see, the general form of epsilon—a modeled epsilon, I would say here. Because assume the several parts or the steps that we are skipping here, because all these terms in the blue circle that you see are unknown.

So, for all these terms like in the case of k we use the closure and then fit into the previous governing equation in order to have a modeled k. So, this is also the modeled k equation. So, then it means that the modeled E or the modeled dissipation rate is expressed in again a constant, and that is the model parameter—let us say, give it a name: 1 epsilon 1 T epsilon. minus C epsilon 2 epsilon square k plus.

So, again, this is the modeled k expression. where these are all the modeled coefficients that we have here. Again, the first term is the accumulation of epsilon; the second term is the convection, the convective term. This is the production rate—so this is the whole production

rate; this is the dissipation rate, and this is the diffusion term, the diffusion of epsilon. So, the time constant of turbulence is calculated from the turbulent kinetic energy and the rate of dissipation of turbulent kinetic energy, which we can say as K by epsilon.

So, the point is that here the source term is the same as that of the k equation that we have seen earlier but divided by this time constant k by epsilon. So, here what we had—this is the production term again—is divided by that time constant term, and that is why the epsilon k exists here in this expression. and the rate of dissipation is essentially proportional to so, this pi tau is essentially epsilon square by k. Therefore, this turbulence quantity must be calculated or the turbulent viscosity that we have this here has to be calculated before we can close or solve this equation.

Or eventually, we can solve the k-epsilon model or use the k-epsilon model. Because earlier, we modeled k, and while solving k, we required the value of epsilon. So, for that we came to a transport equation of epsilon and here we see that for solving epsilon we will require some model parameters, the coefficients, plus this turbulent viscosity that is here. So, again, this means that turbulent viscosity mu.



$$\epsilon = \nu \left\langle \frac{\partial u_i}{\partial x_j} \frac{\partial u_i}{\partial x_j} \right\rangle$$

Gradient-diffusion transport model.

$$-\frac{\langle u_i u_j \rangle}{2} - \frac{\langle u_j p \rangle}{\rho} = \frac{\nu_T}{\sigma_k} \frac{\partial k}{\partial x_j}$$

Prandtl-Schmidt No.

$$\frac{\partial k}{\partial t} + \langle u_j \rangle \frac{\partial k}{\partial x_j} = \nu_T \left[\left(\frac{\partial \langle u_i \rangle}{\partial x_j} + \frac{\partial \langle v_i \rangle}{\partial x_i} \right) \frac{\partial \langle u_i \rangle}{\partial x_j} \right] - \frac{\epsilon}{\sigma_k} + \frac{\partial}{\partial x_j} \left[\left(\nu_T + \frac{\nu_T}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right]$$

So, essentially, what happens is that this turbulent viscosity we knew is proportional to U L, and if we introduce this proportionality constant here. So, that becomes k squared by epsilon again, replacing U as k to the power half and L as k to the third by epsilon. So, what it means is that what you see here is we require a few adjustable parameters. We require a few adjustable parameters here, and those are this C epsilon 1, C epsilon 2, this sigma epsilon, as well as this C mu that we have seen there. So, those parameters have some default values.

$$\frac{\partial \epsilon}{\partial t} + \langle u_j \rangle \frac{\partial \epsilon}{\partial x_j} = -2\nu \left[\underbrace{\left\langle \frac{\partial u_i}{\partial x_k} \frac{\partial u_j}{\partial x_k} \right\rangle}_{\text{III}} + \underbrace{\left\langle \frac{\partial u_k}{\partial x_i} \frac{\partial u_k}{\partial x_j} \right\rangle}_{\text{IV}} \right] \frac{\partial \langle u_i \rangle}{\partial x_j}$$

$$- 2 \underbrace{\left\langle u_k \frac{\partial u_i}{\partial x_j} \right\rangle}_{\text{IV}} \frac{\partial \langle u_i \rangle}{\partial x_k \partial x_j}$$

$$- 2\nu \left[\underbrace{\left\langle \frac{\partial u_i}{\partial x_k} \frac{\partial u_i}{\partial x_k} \frac{\partial u_j}{\partial x_k} \right\rangle}_{\text{V}} + \underbrace{\left\langle \frac{\partial u_i}{\partial x_k \partial x_j} \frac{\partial u_i}{\partial x_k \partial x_i} \right\rangle}_{\text{VI}} \right]$$

$$+ \frac{\partial}{\partial x_j} \left[\underbrace{\nu \frac{\partial \epsilon}{\partial x_j}}_{\text{VII}} - \underbrace{\nu \left\langle u_j \frac{\partial u_i}{\partial x_k} \frac{\partial u_i}{\partial x_k} \right\rangle}_{\text{VIII}} - 2 \underbrace{\nu \left\langle \frac{\partial p}{\partial x_j} \frac{\partial u_i}{\partial x_j} \right\rangle}_{\text{IX}} \right]$$

Modeled ϵ

$$\frac{\partial \epsilon}{\partial t} + \langle u_j \rangle \frac{\partial \epsilon}{\partial x_j} = C_{\epsilon 1} \frac{\nu_T}{k} \left[\frac{\partial \langle u_i \rangle}{\partial x_j} + \frac{\partial \langle u_j \rangle}{\partial x_i} \right] \frac{\partial \langle u_i \rangle}{\partial x_j}$$

$$= - C_{\epsilon 2} \frac{\nu_T}{k} + \frac{\partial}{\partial x_j} \left[(C_{\mu} + \nu_T) \frac{\partial \epsilon}{\partial x_j} \right]$$

$\nu_T = k/\epsilon$ $C_{\mu} = \frac{\epsilon^2}{k}$ $\nu_T = \frac{k}{\mu - \epsilon}$

So here also, we had this sigma k, if you remember it. So, in the model k equation, we have this sigma k that we discussed or mentioned, that sigma k that was introduced there. Which we mentioned as the Prandtl-Smith number, if you remember it. And here we have another one, two, three, and the fourth. These are all unknown for us or the closure coefficients, we can say.

So, 1 2 3, this is the fourth, and this is the fifth. So, if I summarize it, that would be easier for you to understand quickly. The constant, or we can say the closure coefficient, and their value. So, what are the closure coefficients? Let us start from this slide: we had C mu, and then we had C epsilon 1, C epsilon 2. So, C epsilon 1, C epsilon 2, and also we had sigma epsilon, and from the equation of k, we had sigma k, which is the Prandtl-Smith number.

These are the 5 closure coefficients that we need the values for implementing the k-epsilon model. Now, these 5 closure coefficients are considered to be universal, assumed to be universal, and therefore, these constants are usually of the same values for any problem, but those can be changed a bit. They can slightly vary in a different class of problem. So, these values are, say, this C mu is usually what you find in any conventional or commercial CFD solver.

The default set values are 0.09, this 1 is 4.44, C epsilon 2 is 1.92, this sigma k has a value of 1.0. And sigma epsilon has a value of 1.30. So this robustness and this modeling terms or say the easy interpretation of this modeling terms in k-epsilon and makes it an attractive choice or popular choice among the all two equations model in the RANS based modeling system. But the point is, the standard k-epsilon model still does not give good accuracy.

This is the standard one. And that is why there are certain variation of the standard k epsilon model exists. Say for example, flows that cannot be predicted accurately with the standard k epsilon models are the flows with streamline curvature. okay swirling flows axis symmetry jets. This cannot be predicted in general with sufficient accuracy by the standard case silent model that we have discussed.

Now, this the reason why this cannot because of the underlying Bosnian hypothesis that is there we have considered here. in the standard case silent model that imposes isotropy because Boussinesq approximation is done considering the system is isotropic in nature and the normal stresses are equal ok. So, that is one of the reason that how the dissipation was handled. And also this model was derived and actually tuned for flows for the high Reynolds number which implies that it is suited for the flows in which turbulence is nearly isotropic ok. So, k epsilon is more suitable for isotropic turbulence. or turbulent flows.

And the flows in which the energy cascade proceeds in local equilibrium with respect to generation, because those then those assumptions of the approximations holds good for this modeling strategy. Now this model parameter that we have used in k epsilon model it is a have a compromise that to give a best performance for a wide range of flow and that is why it is widely used for any class of problem people initially starts with the k epsilon modeling. The accuracy of this model can be improved by adjusting this parameters that we have listed for a particular experiment.

Sometimes it happens that if you tune this parameter the accuracy may improve a bit or to a certain level. Now since this strength and weaknesses or the pros and cons of case silent models are well known and that is why there are developments of different variation of the standard case silent model. And those models we will briefly have an overview of it because there are several modifications. And say the popular ones if I name those the standard cape silent model the variation of standard cape silent models are say the RNG and realizable cape silent model.




$$\nu_T = C_\mu \frac{k^2}{\epsilon}$$

$\nu_T \propto u^2 \lambda$

Constant/closure co-efficients	Value
C_μ	0.09
C_{ϵ_1}	1.44
C_{ϵ_2}	1.92
σ_ϵ	1.30
σ_k	1.00

$k-\epsilon$ (5)
 Suitable for isotropic turbulence flow

RNG model (Renormalized Group)
 Realizable $k-\epsilon$ model

$$\frac{\partial \epsilon}{\partial t} + \langle u_i \rangle \frac{\partial \epsilon}{\partial x_i} = C_{\epsilon_1} \nu_T \frac{\epsilon}{\lambda} \left[\left(\frac{\partial \langle u_i \rangle}{\partial x_j} + \frac{\partial \langle u_j \rangle}{\partial x_i} \right) \frac{\partial \langle u_i \rangle}{\partial x_j} \right] - C_{\epsilon_2} \frac{\epsilon^2}{k} + \frac{\partial}{\partial x_j} \left[\left(\nu + \frac{\nu_T}{\sigma_\epsilon} \right) \frac{\partial \epsilon}{\partial x_j} \right] - S_\epsilon$$

Streamline curvature
 Steady flows
 Asymmetric Jets

RNG stands for renormalized group technique. renormalized. So, this is the R in G. So, the renormalized group technique that is used in the k epsilon model that can be derived from the Navier Stokes equation. So, that has been one of the popular variation of the standard k epsilon model and the other one is the realizable k epsilon model. So the main physical difference of the standard k epsilon and the RNG k epsilon model that lies with the different formulation by the renormalized group technique of course. And there is an additional source term that appears in the renormalized group model and that happens to be like this.

that this equation that we already have So, this is the expressions we have already seen. Now, this is the additional source term that appears due to the renormalization technique which is essentially is. So, this is essentially this S_{ij} So, this is the one quantity that we see.

Now, this quantity is the additional source term is modeled by again $C_\mu \eta^3 (1 - \eta) / \eta_0 \epsilon^2 + \beta \eta^3 / k$, where η is equal to k by ϵ root over of $2 S_{ij} S_{ij}$, where this S_{ij} is the strain rate tensor. There are constants involved: η_0 β , these are of say 4.38, and β is 0.012. So, this is again a kind of closure that is used here.

$$S_{\epsilon} = 2 \nu S_{ij} \left\langle \frac{\partial u_i}{\partial x_j} \frac{\partial u_j}{\partial x_i} \right\rangle$$

$$= \frac{C_{\mu} \eta^3 (1 - \eta/\eta_0) \epsilon^2}{(1 + \beta \eta^2) \mu}$$

$$\eta = \frac{k}{\epsilon} \sqrt{2 S_{ij} S_{ij}}$$

S_{ij} - strain rate tensor
 η_0, β
 $\downarrow \quad \downarrow$
 $4.38 \quad 0.072$

The additional term is the ad hoc model, which is essentially responsible for the difference in performance compared to the standard model. The standard k-epsilon is known to be much more dissipative in nature, and that is because the turbulent viscosity in the recirculation tends to be much higher, which actually damps the vortices. So, in regions with large strain rates, the additional term in this RNG formulation results in smaller destruction of the epsilon. And therefore, it augments the epsilon and reduces the turbulent kinetic energy, which effectively reduces the viscosity. So, therefore, these improvements are expected in swirling flows,

which was the limitation in the k-epsilon model and in flows where the geometry had a strong curvature. That means the streamline flow with curvature, where the standard k-epsilon model was less accurate than its RNG variation. So, this RNG model is more responsive to the effects of rapid strain rate and streamline curvature than the conventional k-epsilon model. And this RNG model is also very good for predicting swirling flows because of the reason we just discussed. So, we have also now realized why this name came: the renormalized group technique, by which this k-epsilon model is derived from the Navier-Stokes equation.

It results in different and analytical model constant and this constant that appears from this derivations the values are slightly different from that we have discussed in the standard k-epsilon model. So, this set of values actually is a bit different in the RNG model, but those again are model-specific. So, again if you use those RNG k-epsilon model, then you must look into that software solvers theory guide for those particular constant values and if you require you may tune that for your particular applications for better acquisition. So, again, on this note, I will stop here today.

We will touch upon another small section on this turbulence in the next lecture and also we will suggest the or we will show you the recommended uses of this turbulent models and then we move on to the reaction part. Because reaction essentially requires mixing, and nothing can be better than