

CFD APPLICATIONS IN CHEMICAL PROCESSES

Prof. Arnab Atta

Department of Chemical Engineering
Indian Institute of Technology Kharagpur

Week-11

Lecture 52: Turbulence Modeling

Hello everyone, welcome back with another lecture in CFD applications in chemical processes. We are discussing turbulence modeling. And in turbulence modeling in the last lecture we discussed the genesis of Reynolds stress and why it is necessary to discuss about the strategies in order to close this quantity or in order to model this quantity. So, this Reynolds stress we will be back again with this equation, but the Reynolds stress

So if I define Reynolds stress as this quantity that we are trying to model this is essentially if we see if we expand it. Now, this Reynolds stress is symmetric that we see. and since it is symmetric what we have is that $u_1 u_2$ is essentially $u_2 u_1$ u_3 so $u_1 u_3$ So, if I say $u_1 u_3$ is equals to $u_3 u_1$ and $u_2 u_3$ is essentially $u_3 u_2$. And there are three normal stresses that we see this one, this one and this one which is minus ρu_1 ρu_2 .

So, we have three normal stresses. and with this equality which means we have three shear stresses which are these are the unknowns essentially. So, what we see that if we have to evaluate this term the Reynolds stress we have to know the information on 3 Reynolds normal stress and 3 shear stress which means it contains 6 unknown terms. We have 6 unknown terms in this Reynolds stresses that we have to evaluate. one of the ways is that we directly derive a transport equation for Reynolds stress, but what happens when it has been seen that while doing this it would result in a third order moments of the velocity components.

And then again if you try to resolve that The third order moments further results in an equation that contains the fourth order moments and such things goes on and that is referred as the closure problem. And that is why in this Navier-Stokes equation conventionally when they say that the closure equation it directly means or most commonly means that which kind of model you have used to close this Reynolds stress star. but analogous to that we have used the same term in multiphase flow as well the closure for the interface coupling term.

So, this analogy we have to be very clear that conventionally closure model means the model by which we address this Reynolds stress terms. So, at high Reynolds number which are of actually were of concern at the high Reynolds number cases this Reynolds stress terms are way higher than this our conventional viscous stress terms. Which means the viscous stress terms if

I write in this way. these are much greater than the viscous stress terms. In fact, in the range or higher than 100 times or 1000 times larger than this viscous stress term.

which means this at higher Reynolds number viscous stress terms are that is why usually neglected and not considered during solution or the modelling strategies. And that is why you possibly unknowingly have done fully turbulent simulations without considering this viscous stress terms. But we have to be careful for the near wall situations when we apply this modeling strategy because near wall we have a viscous sublayer. So, and that is why the near wall corrections and near wall treatment in turbulent model with the RANS models is extremely important. But here we will not discuss that in details if you are interested you can look into the near wall treatment or the wall function how those boundary layers in flow.

this Reynolds models are applied or how the wall function or wall treatments are taken in order to overcome this sharp gradient near the wall because in the wall or on the wall you generally apply no slip boundary conditions. So, the boundary layer grows the viscous sub layer exist and in the viscous sub layer you no longer cannot neglect this viscous stress term. So, in those cases there is some equality near wall cases. So, this near wall treatment I suggest you to explore on your own wall function for turbulence modeling using this RANS model.

The image contains handwritten mathematical derivations and diagrams. At the top right are logos for IIT Bombay and NPTEL. The main equations are:

$$\frac{\partial \langle u_i \rangle}{\partial t} + \langle u_i \rangle \frac{\partial \langle u_i \rangle}{\partial x_j} = -\frac{1}{\rho} \frac{\partial \langle p \rangle}{\partial x_i} + \nu \frac{\partial^2 \langle u_i \rangle}{\partial x_j^2} - \frac{\partial \langle u_i u_j \rangle}{\partial x_j}$$

$$\frac{\partial \langle u_i \rangle}{\partial t} + \langle u_i \rangle \frac{\partial \langle u_i \rangle}{\partial x_j} = -\frac{1}{\rho} \frac{\partial \langle p \rangle}{\partial x_i} + \mu \left(\frac{\partial \langle u_i \rangle}{\partial x_j} + \frac{\partial \langle u_j \rangle}{\partial x_i} \right) - \rho \langle u_i u_j \rangle$$

Below the equations, there is a note: "flows that are statistically steady RANS. do NOT resolve any dynamics of turbulence on mass, momentum, and/or heat transfer." A circled term $-\rho \langle u_i u_j \rangle$ is labeled "2nd order Tensor" and "Reynolds Stress". A note explains "mean ↔ fluctuating component velocity".

A graph shows "velocity" vs "time" with a smooth curve labeled "DNS" and a noisy curve labeled "RANS". A small "LBS" label is also present. To the right, a diagram shows a flow over a curved surface.

Now the point is so that means, we have we are left with still resolving this Reynolds stress term that how do we do that. Now the point is in order to do that stress terms since the total number of unknowns are higher than the total number of equations. So, unless and until we do some assumption or somehow get those values of some parameters some quantities it is not possible to solve those equations these equations. So, one of the simplest approximation to

express this Reynolds stress is in terms of the velocity itself because it contains the fluctuating component,

but that would require some approximation and that is why the solution of RANS or its different variations are always an approximate solution. So, RANS solutions are always the approximate solutions not the accurate solution of the governing equations. So, now based on this background there is one famous approximation that works pretty well for several scenarios and it is widespread use till some time ago because of its simplicity is the Boussinesq approximation. Now this approximation is based on the assumption that the Reynolds stress this Reynolds stress terms are proportional to the mean velocity gradient.

So, it suggest or it proposes that the transport of momentum by turbulence is a diffusive process and this Reynolds stress terms can be modeled using turbulent viscosity that is also we called the eddy viscosity. and that is analogous to the molecular viscosity. So, this approximation mathematically tells us this τ_{ij} which is the Reynolds stresses that we have seen is essentially this is the Reynolds stress that we have seen that we say this is the eddy viscosity or the turbulent viscosity or we can further simplify it or we can further write it in this way that S_{ij} we write this

where this is the quantity is compactly written here which is a stress tensor which we say as the stress strain and tensor and this K that we know as the turbulent kinetic energy per unit mass and this is further defined as half of the trace of the Reynolds So, the point is although it is analogous to the molecular viscosity, but it is not the same because it is not a fluid property. Molecular viscosity is the fluid property, but the turbulent viscosity depends strongly on the state of turbulence and it is not a fluid property. this term here on this equation or here in this equation represents the normal I mean here in this case is essentially is the normal stress terms.

So, this is also can be represented analogous to the pressure. and usually this also is accounted in the governing equations like this that if I write again that governing equation, but in now accounting for this analogous normal stress. $\rho \mu_t \nabla^2 u_j$. So, this term is also usually is absorbed in this with the pressure term and that finally we can write when we separate out again $\frac{2}{3} \rho k$ and this term that we have multiplied by $\frac{1}{\rho} \nabla_j u_i$. So, what we see here is that if our which means now we can see that if we can estimate somehow

this turbulent viscosity then we can solve this problem or this we can resolve this equation. Now the point is if the specific detail is not required in of turbulence then we can interpret this whole modeling approach like this that as if there is a pseudo fluid with an enhanced viscosity and that viscosity effective viscosity is this. So, this equation presents the physics in such a manner if we look at it that it presents the Navier-Stokes equation with an fluid that has an effective viscosity of the molecular viscosity plus the eddy viscosity kind of a scenario.




Reynolds Stress

$$\tau_{ij} = -\rho \langle u_i u_j \rangle$$

$$= \begin{bmatrix} -\rho \langle u_1 u_1 \rangle & -\rho \langle u_1 u_2 \rangle & -\rho \langle u_1 u_3 \rangle \\ -\rho \langle u_2 u_1 \rangle & -\rho \langle u_2 u_2 \rangle & -\rho \langle u_2 u_3 \rangle \\ -\rho \langle u_3 u_1 \rangle & -\rho \langle u_3 u_2 \rangle & -\rho \langle u_3 u_3 \rangle \end{bmatrix}$$

Symmetric

6 unknowns!

$$\left. \begin{aligned} \langle u_1 u_2 \rangle &= \langle u_2 u_1 \rangle \\ \langle u_1 u_3 \rangle &= \langle u_3 u_1 \rangle \\ \langle u_2 u_3 \rangle &= \langle u_3 u_2 \rangle \end{aligned} \right\} \begin{aligned} -\rho \langle u_1 u_1 \rangle \\ -\rho \langle u_2 u_2 \rangle \\ -\rho \langle u_3 u_3 \rangle \end{aligned} \left. \begin{aligned} \text{Normal} \\ \text{Stress} \end{aligned} \right\} =$$

$$\rho \langle u_i u_j \rangle \Rightarrow \mu \left\| \frac{\partial \langle u_i \rangle}{\partial x_j} + \frac{\partial \langle u_j \rangle}{\partial x_i} \right\| \left. \begin{aligned} -\rho \langle u_1 u_2 \rangle \\ -\rho \langle u_1 u_3 \rangle \\ -\rho \langle u_2 u_3 \rangle \end{aligned} \right\} \begin{aligned} \text{Shear} \\ \text{Stress} \end{aligned} =$$

1000 times

Near-wall treatment - wall function for turbulence modeling



which roughly estimates the turbulent mixing process due to the diffusion of momentum and other flow properties. So, the point is that regardless of the approach by which we can determine this eddy viscosity, there are several limitations involved with this Poisson approximation. Although it is simple to implement, Because of the straightforward assumption that the Reynolds stresses can be presented or represented or modeled as proportional to the mean velocity gradient. Because this approximation is that in Boussinesq scale approximation the eddies behave like molecule.

It behaves like molecules, and turbulence is isotropic. The turbulence is isotropic, and there exists local equilibrium between the stress and strain. Now for this all these assumptions what happens that it fails to predict sometimes a very simple flow for example the channel flow measurements in channel flow show that the average quantities, say U_1 square, are not equal to these values. What Boussinesq's approximation takes into account are these things.

So, this inequality exists in practical channel flows. But the models based on this Boussinesq's approximation actually depict the scenario as if isotropic flow exists and the flows are in local equilibrium. But the point is although we have this limitations still this Boussinesq's approximation based model are several times used to the less intensive computational power or resources that it requires. It can elaborate the influence of turbulence but not to the very details because of several limitations that we have just discussed.

And that is why we require more sophisticated turbulence models that can capture these scenarios, the scenarios of turbulence and its intensity. So, the point is, These are the models that are based on Wasson's approximations, as I said, that sometimes fail to predict simple scenarios like these channel flow systems. So, the point is when it comes to turbulence

modeling based on RANS and the eddy viscosity concept. These turbulence models we can think of as a set of equations that we need to determine to find the viscosity.

Now, in the kinetic theory of gases, the viscosity is considered proportional to the velocity times the distance. So, the turbulent viscosity models are also based on that appropriate velocity, considering the appropriate velocity and the length scale that describes the local turbulent viscosity. So, to overcome this drawback that we have seen in the Bosnian approximation based RANS models, further it is developed that dimension of the eddy viscosity, which we can see, is essentially meters squared per second. That means we can write it in some proportionate format that is L square by T if L is my say the length scale and T is the time scale

is proportional to the eddy viscosity, and here we have a proportionality constant. So, here what we see is that this means U L. So, L by T is the U, and we have another L associated with it. So, this eddy viscosity is associated with the velocity times the distance, like in the kinetic theory of gases, and by this concept, we try to evaluate these eddy viscosities. It is reasonable because these scales are responsible for most of the turbulent transport.

Boussinesq Approximation

Reynolds stress \propto mean velocity gradient.
transport of momentum by turbulence \rightarrow diffusive process
turbulent viscosity (eddy viscosity).

Isotropic
 $-\langle u^2 \rangle \neq \langle u_1^2 \rangle$
 $\neq -\langle u_3^2 \rangle$

Channel flow

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

$$\Rightarrow \frac{\tau_{ij}}{\rho} = -\langle u_i u_j \rangle = \nu_T S_{ij} - \frac{2}{3} k \delta_{ij}$$

\downarrow
Strain tensor

$$\frac{\partial \langle u_i \rangle}{\partial x} + \langle u_j \rangle \frac{\partial \langle u_i \rangle}{\partial x_j} = -\frac{1}{\rho} \frac{\partial \langle p \rangle + \frac{2}{3} \rho k}{\partial x_i}$$

$$\frac{\partial \langle u_i \rangle}{\partial x} + \langle u_j \rangle \frac{\partial \langle u_i \rangle}{\partial x_j} = -\frac{1}{\rho} \frac{\partial \langle p \rangle}{\partial x_i} - \frac{2}{3} \frac{\partial k}{\partial x_i} + \frac{\partial}{\partial x_j} \left[(\nu + \nu_T) \left(\frac{\partial \langle u_i \rangle}{\partial x_j} + \frac{\partial \langle u_j \rangle}{\partial x_i} \right) \right]$$

$k = \frac{1}{2} \langle u_i u_i \rangle$
 ν_T
 $\nu_{eff} = \nu + \nu_T$

What are the scales? The velocity scales and the length scale that we considered here, but this turbulent eddy viscosity may vary with position and time and therefore, we have to specify it before solving the equations that are associated with the eddy viscosity. So, these governing equations that we see here contain this eddy viscosity, and if we try to close these equations, we have to define the eddy viscosity first. But and then that is why there are numerous methods that provide this value of the eddy viscosity which are categorized

based on the number of equations that we have to solve in order to get this value. One of the simplest things that can be is that no transport equation is solved in order to calculate the eddy viscosity, and that could be the zero-equation model. That means no additional transport equations are required in order to resolve this eddy viscosity. So, depending on the number of additional transport equation that we require to solve this eddy viscosity that is why we have seen earlier the name that appears that one equation model, zero equation model, two equations model inside the RANS based approaches.

So, essentially, these transport equations are the PDEs. So, if we have to solve two PDEs together with these RANS equations. So, the number of PDEs that we solve along with the RANS equations. We call that the n-equation RANS-based model. The two equation model one equation model means two extra PDE's we have to solve along with the RANS, one extra PDE

in the one-equation model; and zero means that we do not require any additional transport equation in order to resolve this problem. Turbulent viscosity. But the degree of accuracy of these turbulence models depends on the validity of the assumptions behind them and our choice of the number of equations, whether it is zero, one, or two. What has been seen is that these two-equation models are most widely used because of their superior accuracy compared to the other models in the RANS-based approaches.

$v_T = m^2 s^{-1} = C_v \frac{L^2}{k} = C_v u_t$

Zero-Equation model → Prandtl's mixing length L

One-Eqn. → Spalart - Allmaras model

PDE → RANS

So, one of the most widely used zero-equation models is the Prandtl mixing-length model, OK? So, in the Prandtl mixing-length model, the mixing length that we consider It says that this L strongly depends on the nature of the flow and is generally space-dependent. So, it actually

offers improvement over the constant viscosity model and is capable of predicting complicated I mean certain degree of complicacy, but it actually is very helpful for the simple flow systems.

But the point is, this model is not sufficient for complex scenarios. OK. And there, we require some advanced model because it is very difficult to estimate the distribution of this mixing length in a system. And also, the other limitation of Prandtl's mixing length is that the eddy viscosity is instantaneously affected by the shear rate and vanishes whenever the velocity gradient is zero. But in several cases, this does not agree or does not corroborate with the experimental because what happens is that the Reynolds stresses—the turbulent stresses, specifically—are coming not only from the event of a single point but from a

the region, OK. It is not as point specific, but from a region and they are transported by convection and diffusion and they have a certain energy is dissipated, which means they have a history as well. So, this zero-equation model for which the example is Prandtl's mixing length.

The zero-equation model is unsuitable for generic use as it does not account for the effect of accumulation and transport on turbulence. So, we require a one- or two-equation model, but again, as I said, this one-equation model is the Spalart-Allmaras equation or the one-equation Spalart-Allmaras model. where we solve one equation. There, the point is. The transport of turbulent kinetic energy when it is taken into account in one equation model at the cost of solving only one

is a bit superior. However, this model only scales the characteristic velocity, which is determined from the transport equation. And the length scale, therefore, must be specified in an algebraic manner. So, the point is, to resolve this length scale, we require an additional transport equation. So, we have two things: one is the length scale, and the other is the velocity scale. So, the characteristic velocity scale is modeled by $1 \rho d$.

In the one-equation model, but for the other one, we would require another equation, and that results in the two-equation model, okay? So, the point is, we have sufficient background now to go to the two-equation models. The reason for better accuracy with these two-equation models is something I will start discussing in the next class. So, but before that, I would like to conclude today's session by saying that, by now, we have realized what the different number of equations or the naming inside the RANS-based model means—why one is called the zero-equation model, why it is a one-equation model, and why it is a two-equation model in general.

And together, we have seen how this Reynolds decomposition results in the RANS model and why we require these zero, one, and two-equation models within the RANS-based framework. On this note, I will stop here today, and we will be back with the next lecture on the two-equation models that are based on the RANS approach. Thank you for your attention.