

**Combustion in Air Breathing Aero Engines**  
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**Lecture - 37**  
**Reacting turbulent flows VI**

Welcome back. So, next we take up as we said that dissipation and scalar transport of a non-reacting and reacting a linearly reacting scalar. So, we will show that how this kind of moment, this moment methods can be useful for a non reacting scalars and then we will show for a simplified scalar that how this can fail. And then we will go into this the simplified modeling for the source terms and with that that will close this class or this module on turbulent combustion. In the next modules we will take up more advanced modeling approaches for turbulent non premix flames and turbulent premix flames.

(Refer Slide Time: 00:59)

Dissipation and Scalar Transport of Non Reacting and Linearly Reacting Scalars.

Modeling for closure of the turbulent transport term  $\overline{v''\psi''}$

Gradient transport Assumption:-

$$\overline{v''\psi''} = -D_t \nabla \tilde{\psi}_i$$

↑ turbulent diffusivity  $D_t = \nu_t / Sc_t$

$\psi_i''^2$   $k = \langle u_i u_i \rangle$

$\psi_i'' \psi_i''$   $\tilde{k} = \overline{u_i u_i}$

Transport eqn. for  $\psi_i''$

$$\frac{\partial \psi_i''}{\partial t} + (\tilde{V} + v'') \nabla \psi'' + v'' \nabla \tilde{\psi}_i = \frac{1}{\rho} \nabla \cdot (\rho D_i \nabla \psi_i) - \frac{1}{\rho} \nabla \cdot (\langle \rho D_i \nabla \psi_i \rangle)$$

$$+ \nabla \cdot (\langle \rho \overline{v'' \psi_i''} \rangle) + S_i''$$

$$S_i'' = S_i - \tilde{S}_i$$

So, here we take up this, dissipation of non reacting and linearly reacting scalars. So, as we have seen previously that this term is also unclosed and this also is a major term major problem.

(Refer Slide Time: 01:48)

Moment Methods for Reactive Scalars.

$$\Psi_i(\bar{x}, t) = \tilde{\Psi}_i(\bar{x}, t) + \Psi_i''(\bar{x}, t)$$

On averaging the governing Evolution equation for the reactive scalar  $\Psi_i$  we get.

$$\langle \rho \rangle \frac{\partial \Psi_i}{\partial t} + \langle \rho \rangle \tilde{v}_j \cdot \nabla \Psi_i = \nabla \cdot \langle \rho D_i \nabla \Psi_i \rangle - \nabla \cdot \langle \rho v'' \Psi_i'' \rangle + \langle \rho \tilde{S}_i \rangle$$

$\omega_i = \rho S_i$

Modeling the mean chemical source term is the most difficult problem in the moment methods in turbulent combustion.

Most difficult term to model.

Unclosed.

34

This turbulent transport term, turbulent transport of the species which is essentially the similar to the Reynolds stress terms, but here it is in terms of the species essentially this is the covariance of the velocity fluctuations and the species fluctuations and a Favre averages of that. So, how we can introduce a model for this?

So, as we said that the modeling for this. Now it is a general practice in turbulent combustion to employ this gradient transport assumption. So, what is the gradient transport assumption you will see that and, but you will see that that is mainly useful for reactive non reactive scalars, and we will see what are the problems that you face when you apply them for reactive scalars. So, the gradient transport assumption is that is that this  $v$  prime  $\psi$  prime covariance is equal to minus  $D_t$  times this one.

So, it is similar to the Reynolds stress closure. Where we saw that this Reynolds stress was essentially the Reynolds stress tensor essentially closed by the by this kinematic viscosity kinematic turbulent eddy viscosity times the strain rate the strain rate tensor the Favre average strain rate tensor. So, similarly here instead of the kinematic viscosity we introduce this turbulent diffusivity. And it is a modeled in analogy to the to the turbulent eddy viscosity. So,  $D_t$  is the turbulent diffusivity, and we define turbulent diffusivity is essentially  $\nu_T$  by the turbulent Schmidt number.

Now, we want to show that that the gradient transport assumption may not be acceptable for reacting scalars. And for that we need to essentially derive an equation for this thing

that is the with the variance of the of the this reactive scalar itself. And this once again you see is analogous to the turbulent kinetic energy our turbulent kinetic energy is the variance of the is the essentially the variance of the velocity fluctuation cy or. So, k is essentially; if you remember ui ui this one and for a k tilde it was like ui ui tilde this way.

So, here it is essentially this was this is essentially the psi i prime. So, here we have this thing is essentially psi i times psi i, but here i is not in terms of the direction size in terms of species. So, this is essentially these terms. So, it is analogous to this turbulent kinetic energy. So, we need to have an equation for that also, but first we have an equation for this thing, that is we have an equation for a transport or an evolution equation for psi i prime and that is given by is equal to 1 by rho.

So, this is the species diffusivity term and this is the averaged contribution. This is the turbulent transport term that we are discussing about last the si the source term. So, si is the source term fluctuation is essentially is equal to si minus the Favre average design now from this, similar to the turbulent kinetic energy derivation we can derive this equation for this the variance of the Favre variance of the Favre average variance of a the reactive scalar.

(Refer Slide Time: 07:13)

$$\langle \rho \rangle \frac{\partial \overline{\psi_i'^2}}{\partial t} + \langle \rho \rangle \tilde{v}_j \cdot \nabla \overline{\psi_i'^2} = - \nabla \cdot \left( \langle \rho \rangle \overline{v'' \psi_i'^2} \right) \quad (T1)$$

$$+ 2 \langle \rho \rangle \overline{v'' \psi_i''} \nabla \overline{\psi_i'} \quad (T2)$$

$$- \langle \rho \rangle \overline{\tilde{\chi}_i} \quad (T3)$$

$$+ 2 \langle \rho \rangle \overline{\psi_i'' s_i''} \quad (T4)$$

(T1) → turbulent transport term.  
 (T2) → production of scalar fluctuations  
 (T3) → Favre averaged scalar dissipation rate  
 $\tilde{\chi}_i = 2 D_i (\nabla \overline{\psi_i''})^2$   
 $\epsilon = 2 \rho \sum_{ij} \delta_{ij} \delta_{ij} \quad \delta_{ij} = \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$   
 (T4) Covariance of the reactive scalar with the chemical source term.

And this one is given by plus is the temporal term the convective term, where the variance of psi i is transported by the mean velocity is equal to minus this divergence of the mean density the turbulent transport term. Once again you see this is that this is

essentially the production, we will see this is essentially similar to the production term the production of the scale of fluctuation done, just like similar to the production of the turbulent kinetic energy term scalar dissipation rate Favre average scalar dissipation rate just like the turbulent kinetic energy dissipation rate and the scalar reactive scalar source term covariance.

So, this we will say that this is T 1 this is T 2 this is T 3 and this is T 4 on the right hand side. And this is of course, the left hand side is of course, the transport of this  $\psi'$  square Favre average that is the on the this thing this the Favre the variance of the of the reactive scalar fluctuations, the transport of that which is the left hand side is of course, that and on the right hand side we have different terms; which of course, determines the local rate of change of this of fluctuations the variance and the and the terms and then the convection by the mean flow.

So, that this left hand side tells that about the right hand side what does the different terms. So, the right hand side terms say that T 1 is essentially the those each of this can be modeled and has different meanings for we will not go into that, but I will just say the what the terms mean essentially this is the turbulent transport term. And T 2 is essentially the production of scalar fluctuations. Actually we should derive all these equations by yourself because then the physical significance will also be clear.

And these are not very hard to derive, but of course, in a due to limited time of the class we are just showing all these equations that this can be derived we just need some algebra can be Lucians and a averaging and commutation of this average inside and outside the gradients derivatives, but you have to be careful there is could be this derivation is prone to mistakes. Production of a scalar fluctuations the meaning molecular transport term you can be neglected for simplicity, but you see that the mean molecular diffusivity term still appears in this one, which is a scalar dissipation rate and that is T 3 and whereas, T 3 is given by just like the energy dissipation rate scalar this is scalar dissipation.

So, before that this- as I said that this T 2 this is essentially the production of scalar fluctuations and that is produced by once again the mean scalar gradients and the this velocity scalar covariance. So, it behaves just like the mean just like the mean turbulent kinetic energy production and dissipation. So, the production term was there Reynolds

systems times the mean strain that I mean of a  $d$  of mean  $u_{ij}$  and here also it is exactly behaves in a similar manner. So, when there is a mean velocity gradient it produces and there is a presence of some burden on stress locally it produces that a that a turbulent kinetic energy.

So, when here we have this mean a scalar gradient it produces these fluctuations of these things, and the variance of these reactive scalar fluctuations. So, it is it behaves in an essentially similar manner. And  $T_3$  is this  $\psi_i$  is essentially the Favre averaged scalar dissipation rate. And that is given by this is the thing just to you remember it was like  $2 \nu s_{ij} s_{ij}$  fluctuation. So, here also it is like  $s_{ij}$  is the velocity gradient  $Du$ . So, just if you remember that epsilon was nothing, but mean the turbulent kinetic energy dissipation rate was nothing, but twice  $\nu s_{ij} s_{ij}$  whereas,  $\epsilon_{ij}$  it is equal to  $\rho u_i dx_j$  plus  $\rho u_j dx_i$ .

So, this is exactly analogous to that term. So, production happens to this production happens to this term and dissipation happens to this term. So, it is essentially we see that analogies come out and then  $T_4$  is essentially the covariance of the reactive scalar with the chemical source term. So, that is what  $T_4$  is. So, now, we will define we will see that how this gradient transport assumption can be good for a non reactive scalar, but it can be problematic for the reactive scalar.

So, now before that we need to introduce some this introduce the corresponding integral time scale for the scalars and in terms of this scalar variance and this and this scalar dissipation rate and that can be defined as this.

(Refer Slide Time: 14:52)

Handwritten notes showing derivations for turbulent kinetic energy and dissipation rate models. The notes include:

- $\tau_i = \frac{\overline{\psi_i'^2}}{\overline{\chi_i}}$
- $\tau = \frac{\overline{k}}{\overline{\epsilon}} \rightarrow \tau = C_\chi \tau_i$  (with a note "2.0" pointing to  $C_\chi$ )
- $\frac{\overline{k}}{\overline{\epsilon}} = C_\chi \cdot \frac{\overline{\psi_i'^2}}{\overline{\chi_i}}$
- $\Rightarrow \overline{\chi_i} = C_\chi \left( \overline{\psi_i'^2} \right) \left( \frac{\overline{\epsilon}}{\overline{k}} \right)$
- $\tau_2 = \tau_3$  (written twice)
- $2(-\overline{v''\psi_i''}) \nabla \psi_i = C_\chi \frac{\overline{\epsilon}}{\overline{k}} \overline{\psi_i'^2}$  (with a note "Production = dissipation")
- $D_t \propto \frac{\overline{k}^2}{\overline{\epsilon}}$
- $\frac{m^2}{s} \sim \frac{m^4}{s^4} \cdot \frac{s^3}{m^2} = \frac{m^2}{s}$
- $D_t (-\overline{v''\psi_i''}) \nabla \psi_i$
- $\sim C_\chi \frac{\overline{k}}{\overline{\epsilon}} \overline{\psi_i'^2} \propto \overline{v''\psi_i''}$
- $-\overline{v''\psi_i''} \sim C_\chi^{-1} D_t \nabla \psi_i$  (circled in red)

just like if you remember the integral time scale can be define like this. Favre average turbulent kinetic energy divided by the Favre averaged dissipation rate. And then this can be related by tau is equal to c psi by tau i whereas, c chi is typically taken to be 2.0 in commercial softwares and using this we can essentially model.

Now, we can say that using combining these 2 things we can write that mean k by mean dissipation rate is essentially equal to c chi times and this means that. So, this way the scalar dissipation rate can be modeled. So, this is the thing. Now if you use that the concept that in this equation, if we say that this production is equal to dissipation that if we equate this T 2 and T 3, if we equate d T 2 and T 3 by this thing that production is equal to dissipation. And then we can justify essentially what we will show that that the gradient transport assumption can be justified.

How do we do that we said that, if production is equal to dissipation then the production term is this thing. So, production is equal to dissipation. And since  $D_t$  the turbulent dissipation the turbulent diffusivity can be written as this form you see by dimensionality this has got 2 meter squares per second and this is meter 4 per second 4, and this is this dissipation rate is essentially meter square per second cube and. So, it has got the same dimension. So, it is like meter square per second.

So, using that dimensionality we can write in  $D_t$  is equal to minus  $v'' \psi_i''$ . So, the whole purpose of these thing is to show basically that this gradient

transport assumption that we just introduced that is this turbulent transport term  $v' \psi'$  that is written as  $-\overline{v' \psi'}$  that this assumption is justified for a non reactive scalar, but it causes some problems for a reactive scalar. So, that is the whole thing.

So, we will see we are proceeding in that manner. So, what is the justification is that that if we write it in this form we can this guy can be written as essentially  $\overline{v' \psi'}$  can be written as proportional to  $c \chi^k$ , and  $\overline{\psi'^2}$  and this guy is essentially proportional to  $\overline{v'' \psi''}$  and therefore, therefore, if we combine these 2 things we can write what we get is  $-\overline{v' \psi'}$  is proportional to  $c \chi - \overline{v' \psi'}$ .

So, you see that the gradient transport assumption is justified in this case. Why is it what is the basic code assumption the more basic code assumption is that the probably have equated production equal to dissipation. That is this we have said that  $T_2$  is equal to  $T_3$  and that is why we can have this gradient transport assumption, but the problem is that we have totally neglected this term  $T_4$  right which is the fluctuation which is the covariance of reactive scalar with the chemical source term.

Now, when you have reactions you cannot neglect these terms and that is why, but when you do not have reactions, you see that this assumption not this thing that is the gradient transport assumption holds pretty well and it actually can describe things, the scalar the mean scalar transport equation pretty well using the gradient transport assumption, but when you have reactions then the just production equal to dissipation is not enough because you have other source terms, which is like the covariance between the scale of fluctuation and the reactions.