

Combustion in Air Breathing Aero Engines
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Lecture – 41
Turbulent Non – Premixed Flames III

So, welcome back into this Flamelet discussion that we were doing. So, we have essentially shown you that by obtaining the by solving the continuity momentum k equation epsilon equation and then solving for the mean mixture fraction equation and the variants mixture fracture equation, we can essentially been a very powerful position.

So, that after that if you obtain a pdf of that of the mixture fraction, we can using this chamber flame assumption that at each point in the flow wherever you have a flame that essentially the whole flame is composed of numerous flame lets, and this all this flame lets obey the only chamber flame solution.

Where your enthalpy can be written as a function of Z or your reactive scalar can be written as a function of Z, and immediately we can by doing the prism shape pdf we can just go and find out the mean mixture of mean scalar of mean reactive scalar at each point in a flow using that prism shape pdf. Now that of course, the penalty is that you assume that each at each point in the flow your equation your flame let behaves in a manner which is exactly equal to the ideal one delamina flame ok.

Now, that is that can be a reasonable approximation as you have said that that is could approximation long as your flame let your fuel reaction zone thickness is essentially smaller than the Kolmogorov skill. So, that your eddys does not disturb the reactions on thickness, but well the thing is that that may that may be mostly true, but in these cases were it is not true then this assumption this whole thing fails ok.

So, will we have to find out and another better method by which we can find out psi this reactive scalar mass fraction is a function of the mixture fraction and we will see how can be done. So, will see that this lamina flame structure of a non premise flame. So, first assumption is that we will assume equal diffusivities for the chemical species and temperature.

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Laminar Flamelet Structure of a Non-Premixed Flame

→ Assume equal diffusivities for chemical species and temperature $\Rightarrow Le_i = \frac{\lambda}{\rho c_p D_i} = 1$ and $D = \frac{\lambda}{\rho c_p} = D_i$

Balance equations for scalars are:

- Mixture fraction:** (No source term \Rightarrow Passive scalar)

$$\rho \frac{\partial z}{\partial t} + \rho u_\alpha \frac{\partial z}{\partial x_\alpha} - \frac{\partial}{\partial x_\alpha} \left(\rho D \frac{\partial z}{\partial x_\alpha} \right) = 0$$
- Temperature:**

$$\rho \frac{\partial T}{\partial t} + \rho u_\alpha \frac{\partial T}{\partial x_\alpha} - \frac{\partial}{\partial x_\alpha} \left(\rho D \frac{\partial T}{\partial x_\alpha} \right) = \sum_{i=1}^n \dot{\omega}_i \frac{h_i}{c_p} + \frac{\dot{q}_R}{c_p} + \frac{1}{c_p} \frac{\partial p}{\partial t}$$
- Species mass fraction:**

$$\rho \frac{\partial Y_i}{\partial t} + \rho u_\alpha \frac{\partial Y_i}{\partial x_\alpha} - \frac{\partial}{\partial x_\alpha} \left(\rho D \frac{\partial Y_i}{\partial x_\alpha} \right) = \dot{\omega}_i$$

Assumptions

1. Low Mach number
2. Constant c_p

$$\dot{\omega}_i = W_i \sum_k v_{ik} \dot{\omega}_k$$

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So, Le_i is essentially λ which is Harmon conductivity divided by $\rho C_p D_i$ is equal to 1 and D_i is equal D , essentially and D is equal to λ by ρC_p . So, it is a generalized diffusivity which is also equal to the D_i . So, that is the thing now we have shown that of course, using the different Y_i is we can obtain a we can obtain an equation for the mixture fraction and this is the mixture fraction equations.

So, which we have essentially averaged and found out the set till then the set variance of set now of course, we can obtain a mixture fraction equation like this. So, this is a mixture fraction equation and this is our temperature equation whereas, this α is essentially the repeated indices on the right hand side you have the heat release you have the radiation you have the pressure fluctuation term and this is the species mass fraction equation ok.

So, these are all the equations and of course, you have to you have the continuity and the momentum equation also along with it and. So, those needs to be solved in the enter flow of course.

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→ Surface of stoichiometric mixture fraction: $Z(x_a, t) = Z_{st}$.
 Combustion occurs near the vicinity of this surface.
 → Therefore, a coordinate transformation (Crocco Transformation)
 $((x_1, x_2, x_3, t) \rightarrow (Z, Z_2, Z_3, \tau))$

$$\psi_i = \psi(z, z_2, z_3, \tau)$$

$$\frac{\partial \psi_i}{\partial t} = \frac{\partial \psi_i}{\partial \tau} \frac{\partial \tau}{\partial t} + \frac{\partial \psi_i}{\partial z} \frac{\partial z}{\partial t}$$

$$+ \frac{\partial \psi_i}{\partial z_2} \frac{\partial z_2}{\partial t} + \frac{\partial \psi_i}{\partial z_3} \frac{\partial z_3}{\partial t} = 0$$

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial \tau} + \frac{\partial \psi_i}{\partial z} \frac{\partial z}{\partial t}$$

$$z = z_{st}$$

Now what we do is that we want to first define a surface of stoichiometric mixture fraction that we call essentially as our flame.

So, once we have solved for this. So, we define a surface of stoichiometric mixture fraction $Z \times \alpha$ or this $Z \times \alpha$ at any position x is equal to Z_{st} and because the fact is that the combustion occurs is at the vicinity of the surface because Z_{st} is essentially that an location where the your mixture fraction is at stoichiometric value and that is as we have seen before that the flame always stabilizes at the point, where your scalars reactive scalars the fuel and oxidizer are essentially meeting at a Stoichiometric value ok.

That is apparent from the fact that the flame temperature is adiabatic flame temperature in an non (Refer Time: 04:19) as well. So, what we do is that we do this by this thing by this assumption that the flame is essentially the located at the point where adios mixture fraction is at stoichiometric value.

We can essentially want to do want or we want to do a coordinate transformation so that we go from the physical space of x, x_1, x_2, x_3 or that is xyz and time into this space which is the mixture fraction Z and Z_2 and Z_3 . So, what we do is that we said that say this is our any generalized structure of a flame. So, say the fuel is coming from the central part and this air is coming from outside ok.

So, of course, then the mixture of fraction Z value is equal to one and in the centers Z is equal to 0 outside and then you have the flame stabilized like this. So, we say that at any point in the flame. So, our Z is perpendicular to the flame surface, because this is the Z equal to Z stoichiometric this is the flame surface. So, of course, if this is the iso contour of Z then of course, Z cannot vary along the iso contour.

So, then Z must be varying perpendicular to the iso contour, and this is Z and this is also we define a local coordinate system which is essentially x_1 and then we have the other two coordinate system 2 coordinates x_2 and x_3 and which are also like Z_2 and Z_3 also. So, Z is not equal to x_1 , but x_2 is equal to Z_2 and x_3 equal to Z_3 .

So, this is the our local coordinate systems whereas, x_1 , x_2 and x_3 are essentially our is essentially Cartesian coordinate system whereas, this set is essentially the mixture fraction, but you see the idea is that that here its always perpendicular to the to the flame surface, because we have defined the flame surface to be essentially Z is equal to Z_{st} where the mixture fraction is constant.

So, now what we want to do is that we want to express all this quantities temperature and y_i as a function of Z , and that will follow this, this different transformation rules that is we will see that this transformation rules will be followed now why is that. So, then we can be shown in a simple manner by the following that is if we define a quantity like this that say f or ψ_i is a function of Z , Z_1 , Z_2 , Z_3 and τ ok.

So, this is the transformation this x_1 , x_2 , x_3 , t is equal to Z_2 , Z_3 and τ . So, then $\frac{\partial \psi_i}{\partial t}$ is essentially $\frac{\partial \psi_i}{\partial \tau} \frac{\partial \tau}{\partial t} + \frac{\partial \psi_i}{\partial Z} \frac{\partial Z}{\partial t} + \frac{\partial \psi_i}{\partial Z_\alpha} \frac{\partial Z_\alpha}{\partial t}$.

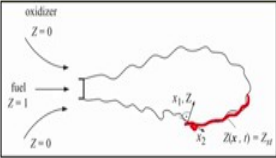
Of course you see this because and of course, you see that there is the or assumption is that that x_2 is equal to Z_2 and x_3 is equal to Z_3 and t is equal to τ . So, then this is of course, equal to 1 and this since Z_α is independent of t this is equal to 0. So, then we are left with this part. So, we can write that $\frac{d}{dt}$ by partial duo duo t is to essentially duo duo τ plus $\frac{d \psi_i}{dz} \frac{dz}{dt}$ times partial duo Z duo t .

So, this is essentially the transformation of according transformation where you go from physical spacial coordinates to variable to a coordinate which is essentially one of the dependent variables of the system itself which is Z and. So, this is how you do the

coordinate transformation and its essentially done was inspired by the crocco transformation which is applied for boundary layers ok.

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→ Surface of stoichiometric mixture fraction: $Z(x_\alpha, t) = Z_{st}$.
 Combustion occurs near the vicinity of this surface.
 → Therefore, a coordinate transformation (Crocco Transformation)
 $((x_1, x_2, x_3, t) \rightarrow (Z, Z_2, Z_3, \tau))$



$\psi_i(x_1, x_2, x_3, t)$

↓

$\psi_i(\bar{z}, \bar{z}_2, \bar{z}_3, \tau)$

↓

$\psi_i(\bar{z}, \tau)$

Express T and Y_i as a function of Z implies with transformation rules as below:

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial \tau} + \frac{\partial Z}{\partial t} \frac{\partial}{\partial Z} \quad (1)$$

$$\frac{\partial}{\partial x_\alpha} = \frac{\partial}{\partial Z_\alpha} + \frac{\partial Z}{\partial x_\alpha} \frac{\partial}{\partial Z} \quad (2) \quad \alpha = 2, 3, \dots$$

$$\frac{\partial}{\partial x_1} = \frac{\partial}{\partial x_1} \frac{\partial Z}{\partial Z} \quad (3)$$

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So, this is the thing and using this type of approaches you can obtain the other thing also this is what we just derived and you can derive, this ψ_i also in terms of z . So, essentially your transforming what you want to do is that that ψ_i is written in terms of x_1, x_2, x_3 and t and you want to basically transform into ψ_i that is the reactive scalar in terms of Z, Z_2, Z_3 and τ

Essentially and we will show that this variation along this the only variation that will be important is essentially variation along Z and variation along Z_2 and Z_3 will not be important because ψ_i is also a flame property right is also a reactive scalar and ψ_i will vary only perpendicular to the vary direction of the flame ok.

So, if this is the flame you have fuel this is fuel this is the mixture fraction iso contour. So, the fuel will not vary to the fuel mass fraction will not vary too much along this flame surface right it will vary perpendicular to the flame surface. So, that is make sure that these variations along this will be small and essentially it will become an equation for like this well that is the idea.

So, we saw that in the previous presume shape pdf approach what we did was that we wrote that ψ_i is just a function of Z as it is in a 1 d chamber frame. So but here what we

want to do is that we want to derive an equation by which we can write the variation of ψ as Z as an independent variable.

So, we want to write ψ as a we want to find out a governing equation by which ψ can make source as a function of that. So, that is what we are trying to do here and for that we have introduced this thing where essentially your that is perpendicular to the is perpendicular to the Z varies perpendicular to the flame which is the iso contour of the Z itself and that is that is defined by that z_{xt} is equal to z_{zt} .

So, this is the approach and to do that we introduce this coordinate transformations and which are obtained by like this that is $duo\ duo\ t$ is essentially $duo\ duo\ \tau$ plus $duo\ Z\ duo\ t$ plus $duo\ duo\ Z\ duo\ duo\ x\ \alpha$ is essential is equal to $duo\ duo\ Z\ \alpha$, α going for 2 to 3 this plus $duo, duo\ Z\ times\ duo\ duo\ x\ \alpha\ times\ duo\ duo\ Z$ and $duo\ duo\ x\ \alpha$ this very important, x_1 that is the in the direction of the perpendicular to the x_2 and x_3 is essentially $duo\ Z\ times\ divided\ by\ duo\ x_1\ times\ duo\ z$.

You can just the way we showed that the first transformation you can do the other transformations also.

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Transformed Energy Equation

$$\rho \left(\frac{\partial T}{\partial \tau} + u_2 \frac{\partial T}{\partial Z_2} + u_3 \frac{\partial T}{\partial Z_3} \right) - \frac{\partial(\rho D)}{\partial x_2} \frac{\partial T}{\partial Z_2} - \frac{\partial(\rho D)}{\partial x_3} \frac{\partial T}{\partial Z_3}$$

$$- \rho D \left[\left(\frac{\partial Z}{\partial x_\alpha} \right)^2 \frac{\partial^2 T}{\partial Z^2} + 2 \frac{\partial Z}{\partial x_2} \frac{\partial^2 T}{\partial Z \partial Z_2} + 2 \frac{\partial Z}{\partial x_3} \frac{\partial^2 T}{\partial Z \partial Z_3} + \frac{\partial^2 T}{\partial Z_2^2} + \frac{\partial^2 T}{\partial Z_3^2} \right]$$

$$= \sum_i^n \dot{\omega}_i \frac{h_i}{c_p} + \frac{\dot{q}_R}{c_p} + \frac{1}{c_p} \frac{\partial p}{\partial t}$$

X
X
X
X



Now after do the transformations you can have a transformed energy in equation, you get a complicated equation like this is all the transient term the transport terms, but you see

now you have your this mixture on the left hand side your this is eliminated your x coordinate is eliminated and you have transport convection in the Z space ok.

But of course, you will have this x coordinates also and then you have this term and then you have all these different terms on the right hand side remains same which is essentially the heat raising radiation and pressure fluctuations. But it can be argued that essentially these variations that dd duo duo Z in terms of x 2, duo duo Z and x duo duo duo Z duo x 3, duo Z duo x 2, duo 2 t duo 2 Z 2 and duo 2 t duo 2 Z duo Z 3 square.

I mean these will essentially can be neglected because this will be small. Because the reason is that this is your flame and the temperature is mainly varying like this on the two sides of the flame say this is the fuel side and this is oxidizer side. So, on these variation this is the this is the temperature. So, the temperature is much strongly varying on the one along this direction than along this direction.

So, this temperature variation is much stronger as a result we can be able to neglect all these variations that is happening along the along the iso contour of Z itself. So, that is the idea and this all can be neglected and once you do that this what we will see is that the dominant term that will emerge is essentially this term.

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Transformed Energy Equation

Important for extinction type problems

$$\rho \left(\frac{\partial T}{\partial t} + u_2 \frac{\partial T}{\partial Z_2} + u_3 \frac{\partial T}{\partial Z_3} \right) - \frac{\partial(\rho D)}{\partial x_2} \frac{\partial T}{\partial Z_2} - \frac{\partial(\rho D)}{\partial x_3} \frac{\partial T}{\partial Z_3}$$

$$- \rho \left[\left(\frac{\partial Z}{\partial x_\alpha} \right)^2 \frac{\partial^2 T}{\partial Z^2} + 2 \frac{\partial Z}{\partial x_2} \frac{\partial^2 T}{\partial Z \partial Z_2} + 2 \frac{\partial Z}{\partial x_3} \frac{\partial^2 T}{\partial Z \partial Z_3} + \frac{\partial^2 T}{\partial Z_2^2} + \frac{\partial^2 T}{\partial Z_3^2} \right]$$

$$= \sum_i \dot{\omega}_i \frac{h_i}{c_p} + \frac{\dot{q}_R}{c_p} + \frac{1}{c_p} \frac{\partial p}{\partial t}$$

For very thin flamelet in Z direction: Use order of magnitude analysis (similar to B. L. Theory)

Similarly, an equation for species transport can be obtained

So, the dominant term that will emerge is essentially this term and all of the terms can essential neglected. So, will talk about this dominant terms later. So, this is the

assumption of a vary with thin flame let in Z direction and use order of fine drawn analysis similar to the boundary layer theory. So, essentially what will have is that we will have this term transient term for extension drew problems and this term.

And conviction of course, we have also will also neglect, because we are only interested what happens in the vicinity of the flame. In the where the temperature gradients where the scalar gradients are very very strong, but only the scalar gradients in the normal directions are very very strong that is along our scalar gradients along the Z direction are very very strong.

So, will neglect only keep the transient term will keep the which is important for extinction or ignition type problems will keep this term and will keep the source term. So, will see what can be done with that. So, similarly the equation of species should convey also found out.

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Introduce stretched coordinate ($\xi = \frac{Z-Z_{st}}{\epsilon}$) and fast time scale ($\sigma = \tau/\epsilon^2$) where $\epsilon \sim O(\ell_R)$

- Flame structure up to leading order is described by,

$$\rho \frac{\partial T}{\partial t} - \rho \frac{\chi_{st}}{2} \frac{\partial^2 T}{\partial Z^2} = \sum_{l=1}^k \frac{Q_l}{c_p} \omega_l + \frac{\dot{q}_R}{c_p} + \frac{1}{c_p} \frac{\partial p}{\partial t}$$

$$\rho \frac{\partial Y_i}{\partial t} - \rho \frac{\chi_{st}}{2} \frac{\partial Y_i}{\partial Z^2} = \dot{\omega}_i$$
- Where $\chi_{st} = 2D \left(\frac{\partial Z}{\partial x_{st}} \right)^2$ instantaneous scalar dissipation rate at stoichiometric conditions: Represents inverse of diffusion time

- This transformation includes convection and diffusion normal to the surface of stoichiometric mixture.
- As $\chi_{st} \rightarrow 0 \Rightarrow$ Homogeneous reactor
- Valid in thin reaction zone near $Z = Z_{st}$

So, then we can introduce the stretch coordinate by Z minus Zst, and the fast time scale and like this and we can obtain an equation for this like this.

So, the term that will see is that as we said that the transient term is retained, and this the other term that is this term is retained that is the first term on the there is the first term of this third brackets is retained, and this right hand side source term is retained and this

equation is essentially called the this equation of the reactive scalar in Z space, where we have essentially removed all convection.

So, you have retained the transient term we have retained the diffusion type of term, but in Z space you must remember that and you have retained source term same for the y_i also. Now you see that there for the diffusion of temperature in the Z space there is a characteristic diffusivity that is emerging, and that is essentially the scalar dissipation rate ok.

Which is given by $2 D \frac{d^2 Z}{dz^2} \times \alpha^2$ and instantaneous scalar dissipation rate at the stoichiometric conditions and this presents essentially the universe inverse of the diffusion time. So, this will the χ is essentially is as a dimension of one per second. So, it made just essentially as the inverse of the diffusion time scales.

So, this essentially gives you the flame structure of course, with simplifying assumption, but now you do not need to essentially, but with this equations with these governing equations we do not need to go back to the one d chamber flame, but of course, if you go you can obtain the 1D chamber flame from these equations also, but with these equations you have you can obtain how temperature varies with Z independently.

As long as you are you know this what if this χ_{st} , which is the function of this $\frac{dz}{dx} \alpha$, which is a function of Z again and $x \alpha$ again. So, this as long as you know the local characteristic diffusivity in terms of this scalar dissipation rate, and you are one can find out how the temperature varies with Z without having this simplified one d chamber flame assumption.

So, the flame let this is another refinement of the flame let assumption, but we can follow those other steps as has been shown before. So, this transformation essentially what has it includes the convection and diffusion normal to the surface of the stoichiometric mixture, and as χ_{st} goes to zero that is as the scalar that is the mixture fraction gradients disappear, it approaches homogeneous reactor ok.

And it is valid in the thin reaction zone near Z is equal to stoichiometric of course, you where you go far away from this then all those things that things varying the reactive scalar varying only normal to the iso surface of Z, those type of assumptions will not be valid anymore ok.

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Time Scales in Nonpremixed Combustion

Chemical time scale at extinction:

- For a diffusion flame: $t_c = Z_{st}^2(1 - Z_{st})^2 / \chi_q$
- For a premixed flame: $t_c = \frac{\delta_q(\rho\lambda/c_p)_{st}}{2(\rho u S_L)_{st}^2}$

} Fundamental relationship between premixed and nonpremixed flames

From the above comparison: At extinction

| | |
|--|--|
| <p>Nonpremixed flame: Heat conduction towards lean and rich side just balances the heat generation by chemistry</p> | <p>Premixed flame: Heat conduction towards the unburnt mixture just balances the heat generation at that burning velocity</p> |
|--|--|

∴ A diffusion flame can exist at lower χ and lower characteristic flow time

- Flexibility to chose the convective to the reactive time
- Therefore, nonpremixed combustion is controllable and diffusion flames are stable in comparison with premixed flames

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So, time scales in non premixed for combustion you just have a check comparison between premix and non premix flames.

So, this is the time scale for non premix combustion Z_{st}^2 by times $1 - Z_{st}$ square divided by this scalar dissipation rate and for a non premix flame of course, this is the quenching essentially is there is a scalar dissipation related quenching. So, of course, when you have the very high scalar dissipation rate you will see that the flame is essentially will be quenched and.

So, this, but this thing is of course, we need to take care and then for a non premix flame of course, we will see that the premix flame the time scale is essentially given by this and that is the one point of deviation between relationship between non premix and premix flames ok.

So, of course, if you compare between the compare the above at from the above at extinction, you see that the non phoenix flame its essentially the heat that is conduction at the is essentially the heat that is conducted towards the lean and the rich site balances the heat generation by chemistry. So, that is what non premixed that is what a non premix flame is essentially ok.

So, for a non premix flame you is flame is situated between the fuel stream and the oxidizer stream and it conducts heat towards the lean and the rich side and that is

balanced by the heat generation by chemistry, but as for the premix flame the heat conduction happens towards the un burnt happens towards the unburned mixture and it just balances the heat generation at that bonding velocity.

So, diffusion flame can exist at lower χ and has lower characteristic flow time. So, of course, the of course, it is then it also has the flexibility to choose the convective to the reactive time because as such because there is no flame speed for a non premix flame, there is no constraint on the fact that how it should balance with the flow.

However for the non premixed that means, that the non premix combustion is essentially controllable and diffusion flames or non premix flames are stable in comparison to the premix flame. So, that is one advantage that has apart from the fact that though despite the fact that non premix flames are more polluting the premix non premix are more stable and that is one good thing about non premix flames ok.

So, of course, but at large χ at χ quenching the flame quenches and that is one thing we have to be careful about.

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Different Flamelet Models

1. Stretched Laminar Flamelet Model (SLFM) - Peters (1984) and Lentini (1994)
2. Eulerian Particle Flamelet Model (EPFM) - Barths et al. - 1998
3. Lagrangian Flamelet Model (LFM) - Mauss (1990), Pitsch (1998, 1999)
4. Conserved Scalar Equilibrium Model (CSEM)

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Now then we go to this different flame let models where we have essentially discussed this stretched flame let model by peters and Eulerian particle flame let model Lagrangian model and the conserved scalar equilibrium model.

And that is what we have essentially discussed just before this conserved scalar equilibrium model, which is where we had in the presume shaped pdf; we have essentially just plugged this conserved scalar equilibrium assumption or this thing. So, this one deep non premix flame into this presumes shape pdf ok.

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Laminar Flamelet Equations

- Flame surface is defined by setting $Z(x, t) = Z_{st}(x, t)$
- The reactive-diffusive structure of the flamelet near $Z(x, t) = Z_{st}(x, t)$ is governed by,

$$\rho \frac{\partial \psi_i}{\partial t} = \frac{\rho \chi}{Le_i^2} \frac{\partial^2 \psi_i}{\partial Z^2} + \omega_i$$
 - χ Instantaneous scalar dissipation rate; at flame surface $\chi = \chi_{st}$
 → External parameter on the flamelet structure because of Z
 → Inverse of diffusion time scale (diffusivity in Z -space)
- $\psi_i = f(\chi, Z, t) \Rightarrow$ Reactive scalars are constant along Z -constant surface
- The fields of reactive scalars are aligned with Z and both are transported with the flow
- Both Z and χ are fluctuating quantities \Rightarrow To calculate statistical moments consider the statistical distribution

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Now, going back to this what we were discussing that we have obtained this laminar we have obtained a flame surface which is essentially defined by Z is equal to Z_{st} , and the reactive diffusive structure of the flame let at near Z is equal to Z_{st} is given by given by this equation which is we have obtained by transforming from the physical coordinate into Z space ok.

Again we just recapitulating the discussion that we just had 5 minutes ago, and now that reactive diffusive structure of this is given by this you have this wire of this reactive scalar we have this by $d\rho d\psi_i/dt$ and this is ρ divided by Le_i where we can use also that this non unit loose number of assumptions and ψ_i by 2 times $d^2\psi_i/dZ^2$ square plus the of course, the source term is also there, this is in the reactive scalar.

So, from ψ_i we have gone onto ψ_i area also and this is ψ_i the scalar dissipation rate is at the defined at the flame surface ψ_i is equal to $\psi_{i, st}$. And this is an external parameter essentially on the flamed structure because of Z and its essentially the inverse of diffusion time scales and is represents the diffusivity in Z space. Now one thing is that the the most important thing that allows us to reduce to this simple equation this very

elegant and beautifully equation of ψ_i in terms of Z space is that, the reactive scalar are constant along Z surface ok.

And the fields of reactive scalars are aligned with Z the reason is that if reactive scalars are constant along Z then of course, then it varies perpendicular to the iso contour of Z , reactive scalars are not constant along Z reactive scalar is essentially constant along Z is equal to constant surface. So, iso surface of Z reactive scalars are also constant along the iso surface of Z .

And then if it is to vary this reactive scalars they must be varying along the perpendicular to the iso surface of Z , then it varies essentially along with Z . So that means, the fields of the reactive scalars are run with said and both are transported with the fuel. And now Z and ψ_i both are fluctuating quantities and to calculate the statistical moments and we have to consider the statistical distribution.

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1. Steady flamelet equations:
 If the joint pdf of $\tilde{P}(Z, \chi_{st})$ surface is known, solve steady flamelets equation to get ψ_i and its Favre mean is given as,

$$\tilde{\psi}_i(x, t) = \int_0^1 \int_0^\infty \psi_i(Z, \chi_{st}) P(Z, \chi_{st}; x, t) d\chi_{st} dZ$$

2. Unsteady flamelet equations: (Joint pdf are impractical)

- Use multiple flamelets, each of which represents different range of χ distribution
- Used in Eulerian Particle Flamelet Model (EPFM)
- Scalar dissipation rate modeled as a function of Z
- Above formulation is used in modelling conditional Favre mean scalar dissipation rate ($\tilde{\chi}_Z$) defined as:

$$\tilde{\chi}_Z = \frac{\langle \rho \chi | Z \rangle}{\langle \rho | Z \rangle}$$

Flamelet equation in a turbulent flow:

| | |
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| $\rho \frac{\partial \psi_i}{\partial t} = \frac{\rho}{Le_i} \tilde{\chi}_Z \frac{\partial^2 \psi_i}{\partial Z^2} + \omega_i$ | <ol style="list-style-type: none"> 1. Unable to predict ignition (small χ) / extinction (large χ) events. 2. Use LES |
|--|--|

So, once again we see that we need to essentially go back to this to the to this steady flame let equations that, if we now have the of course, now if we have this joint pdf of this ψ_i Z and ψ_i st surface is known then we can solve the steady flame let equation to get ψ_i and this Favre average mean is given as this whole equation ok.

This is once again that is from the joint distribution of Z and ψ_i st we can find out the mean ψ_i . Never as (Refer Time: 23:23) various point ψ_i as a function of Z this thing can

be obtained from the this steady flame let equation where of course, this term has to be neglected. So, this is then valid only under the steady case that has to be remembered.

But now if the unsteady case if you have an unsteady flame let equation then this joint pdf is becomes impractical and then one can use multiple flame lets each of which essentially represents different ranges of chi distribution, and this is typically used in the eulerian particle flame let model. And the scalar dissipation rate can be modeled as a function of Z , and the above formulation is used in modeling condition of Favre averaged of the mean scalar dissipation rate χZ which is defined like this. As you see that this difference is that it is a conditional on z .

So, it is like this means that its ρ times the scalar dissipation rate giving Z condition on Z divided by the ρ given Z and then averaged. So, then the flame let equation in a turbulent flow is then given by this quantity, then you can use basically for the unsteady flame let in this form whereas, this ψ has been replaced with which ψ tilda at Z ok.

So, then once again you have come to this equation, but now you see that the as I said that the original this model that this conserved scalar equation model of this where we have essentially plugged in the solution of this 1D chamber flame or the 1D or the equilibrium solution into at each point in space from the pdf.

And the solution was Z average it on Z variants of Z that we have realized by solving by accounting for this either this steady flame let equation or the unsteady flame let equation where we have replace ψ with this essentially ψ this Favre average of Z . Now of course, there are trouble because this one in points which involves large departure from the mean ψZ values where we encounter small Z as well as or large ψ events that is when you have when the ψ is very large you go to extinction ok.

So, then one then one has to use large de simulations for that. So, that is one thing one is to keep in mind.

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Modeling of Turbulent Nonpremixed Combustion

Two important modeling approaches to turbulent nonpremixed combustion are:

1. Conditional Moment Closure (CMC) – Klimenko and Bilger
2. The Pdf Transport Equation Model – Pope, Dopazo, etc.,

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So, next we go into two advanced concepts of modeling turbulent non premix combustion and this will just skim through, but. So, in details we have discussed this flame let approach, and these two things are more advanced and it is more complex also, but we will just discuss them and these two are essentially the conditional moment closure are approached by Klimenko and Bilger.

And the pdf transport equation model by pope and Dopazo and will just go to this.

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Conditional Moment Closure (CMC)

Reference: A. Klimenko and R. Bilger, *Prog. Energy. Comb. Sci.* (25) 1999

- Conditional moments are averages and variances etc., taken for those quantities which comply with certain condition
- Rather than taking conventional averages, condition the reactive scalars on the mixture fraction
- Klimenko: Turbulent diffusion can be better modeled in Z space.
- Bilger: Fluctuation of reactive scalar associated with fluctuation of Z.

- **Flamelet model:** Flame surface statistics and laminar reactive diffusive structure is attached to the flame surface

- **CMC:** Conditional moments at a fixed location and time **fin** the flow field.

1. Conditional pdf, $P(\psi_i | Z; \mathbf{x}, t) = \frac{P(\psi_i, Z; \mathbf{x}, t)}{P(Z; \mathbf{x}, t)}$
2. First conditional moment of the reactive scalar:
$$Q_i(Z; \mathbf{x}, t) = \langle \psi_i | Z \rangle = \int_0^1 \psi_i P(\psi_i | Z; \mathbf{x}, t) d\psi_i$$

Because of (2), Q_i is a function of x, t , as well as Z

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So, the first will go to this conditional moment closure and this is just an overview are not going to the details. So, conditional moments, you see conditional moments and essentially this just we have seen that this is ψ given z . So, that is typically a conditional moment.

So, conditional moments are averages and variances taken from those quantities, which comply with the certain condition. So, if this conditional moment this conditional pdf this f if is the pdf of u is given by f_u , and the pdf of say some quantity G is given by f_G . So, the pdf of u given G is essentially pdf of u and G divided by pdf of G .

So, this is the how the conditional moment from that one can obtain the conditional averages also. So, the conditional moments are averages and variances and taking with quantities which you comply with the certain condition and rather than taking conventional averages the condition that reactive scalars and the mixture fraction.

So, we have not. So, here in this conditional moment closure we are not will not go with directly mean like mean like this like ψ_i average that we were discussing. So, what we what will go is that what we want is that, we want something like this given an average something like that the ψ_i given Z that at a particular point in if you know the value of Z what is the that given the value of that what is the average of ψ_i so, that is the conditional average of Z a conditional average of ψ_i given z .

So, that is the what we are interested in here why? Because Klimenko said that turbulent diffusion can be better model than Z space and Belger form that fluctuation of reactive scalar is associated with the fluctuation of Z . So, that is for this raise two reasons essentially both of these people both of this very highly decorated scientists and proposed this conditional moment closure models.

So, the flame let model the flame surface statistics and laminar reactive diffusive structure is attached to the flame surface. So, the what we have done is that we solve in the flame let model we solve for Z tilde, we means Z Favre mean Z we solve for the variance of Z and then we attach a diffusive reactive structure to it either by solution from 1D or by solving ψ_i as a function of Z . In the conditional movement closure at fix basically here we are obtain the conditional moments at fixed location and time in the time in the flow field ok.

So, that is the that is the conditional moment closure approach that we use. So, the conditional pdf is given by this, that is a p that is that is a pdf of psi i given Z is given by the joint pdf of psi i and Z this is the joint pdf of psi i is Z at x and t and this is the pdf of Z at x and t. So, it is a ratio the conditional pdf of psi i just be. So, sure now that is a conditional pdf of psi i given Z is essentially the joint pdf of psi i and Z at the at a particular point divided by the pdf of Z at the particular point ok.

And the conditional moment of the reactive scalar is given by this, that is a Qi Z xt is the conditional moment of reactive scalar is this essentially psi i given Z averaged is we can find out from the conditional pdf of psi i given Z and if you just get the first moment of the is given by the first moment psi i times the pdf of psi i given Z at that and we integrate between 0 and 1.

So, this is how the conditional moment of a reactive scalar is defined

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Following Bilger's approach, decompose reactive scalar into conditional mean and conditional fluctuation:

$$\psi_i(x, t) = Q_i(Z; x, t) + y_i(Z; x, t)$$

Using the above decomposition in the governing equations for a reactive scalar

$$\langle \rho | Z \rangle \frac{\partial Q_i}{\partial t} + \langle \rho | Z \rangle \tilde{u}_z \cdot \nabla Q_i = \langle \rho | Z \rangle \frac{\tilde{\chi}_z}{2} \frac{\partial^2 Q_i}{\partial Z^2} + \langle \omega_i | Z \rangle$$

Additional terms for diffusive flux and conditional turbulent transport (can be modeled by gradient flux) are neglected

- i. \tilde{u}_z : Favre conditional velocity = Replaced by Favre mean velocity
- ii. $\tilde{\chi}_z$: Favre conditional scalar dissipation rate = Calculated based on the pdf transport equation
- iii. $\langle \omega_i | Z \rangle$: Favre conditional chemical source term = Calculated based on presumed shape pdf approach

→ Higher moments of chemical source term are neglected. This implies $\langle \omega_i | Z \rangle = \omega_i(\langle \psi_i | Z \rangle)$

→ Derivation of CMC equations follow that of flamelet concept. However, CMC has an advantage that it clearly identifies $\tilde{\chi}_z$

Now in bilgers approach we decomposed the reactive scalar into conditional mean and conditional fluctuation. So, we define psi i is essentially not psi i an average plus psi i fluctuation is this is the conditional mean and this is a conditional fluctuation, and using the above decomposition in the governing equations for the active scalar, we obtain one can obtain this equation this is a very very important equation which is has important influence in the turbulent non premixed combustion modeling and I mean to some extent in turbulent premix combustion modeling ok.

So, this is the equation and on the left hand side you means to have a some temporal term of this conditional mean and then the conditional mean is transported by the mean velocity u_z , but in Z space this is not just simple velocity and then you have this same thing that the diffusion of the conditional mean in Z space.

And once again the Favre average is scalar dissipation rate of Z appears as the diffusivity characteristic diffusivity and then you have a closure for the may have the closure problem for the reaction rate. So, here you see that this is the Favre conditional velocity and ψ_i which is replaced by the replaced by Favre mean velocity Favre mean velocity in replaced by this and Favre conditional scalar dissipation rate and calculated based on the pdf transport equation, and then the Favre conditional chemical source term and calculated based on the presumed shape pdf approach.

So, those thing has to be integrated then the higher moments of chemical source term are neglected and this implies that we can model this ψ_i this ω_i that is species consumption or production rate at a given Z is essentially ψ_i , and then this as a function of this mean of ψ_i given z .

So, the derivation of CMC equation follow that of the laminar flame let the concept; however, CMC as advantage that it clearly defines or identify the χ_Z in it. So, this is the thing.

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The Pdf Transport Equation Model:

- Pdf transport equation for the velocity and reactive scalars- one-point statistics
- Joint pdf transport equation for velocity and reactive scalars- Infinite hierarchy of one-point statistics
- Inclusion of the velocity gradients and the reactive scalars ⇒ Solve modeling issues with viscous and scalar dissipation

And next we will go into the pdf transport equation model. The pdf transport equation for the velocity and reactive scalars for one point statistics it is at a particular point in the flow you obtain the pdf.

So, here in the pdf transport equation models you do not model the velocities or the species as such you model the pdf of that you see how the pdf is essentially is essentially changes under the effect of advection diffusion and reaction at a particular point. So, the pdf transport equation for velocity and reactive scalars and inclusion of velocity gradients in the reactive scalars and we have to solve the modeling issues with viscous and scalar dissipation ok.

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Transport Equation for the Joint Pdf of Velocity and Reactive Scalars

- $\psi \rightarrow$ Reactive scalar
- $P(\mathbf{u}, \psi; x, t) d\mathbf{u} d\psi \rightarrow$ Probability of finding velocity and reactive scalar within $\mathbf{u}-d\mathbf{u} \leq \mathbf{u} < \mathbf{u}+d\mathbf{u}$ and $\psi-d\psi \leq \psi < \psi+d\psi$.
- Transport equation for the probability density $P(\mathbf{u}, \psi; x, t)$

$$\underbrace{\frac{\partial(\rho P)}{\partial t}}_{T1} + \underbrace{\nabla \cdot (\rho \mathbf{u} P)}_{T2} + \underbrace{(\rho \mathbf{g} - \nabla \bar{p}) \cdot \nabla_{\mathbf{u}} P}_{T3} + \underbrace{\sum_{i=1}^n \frac{\partial}{\partial \psi_i} [\omega_i P]}_{T4} = \underbrace{\nabla_{\mathbf{u}} \cdot [(-\nabla \cdot \boldsymbol{\tau} + \nabla p') \mathbf{u}, \psi] P]}_{T5} - \underbrace{\sum_{i=1}^n \frac{\partial}{\partial \psi_i} [(\nabla \cdot (\rho D \nabla \psi_i)) \mathbf{u}, \psi] P]}_{T6}$$

- $\nabla_{\mathbf{u}}$ \rightarrow Divergence w.r.t three components of velocity
- $(\) \rightarrow$ Conditional averages w.r.t fixed values of \mathbf{u} and ψ
- T1 \rightarrow Local rate of change
- T2 \rightarrow Convective derivative in physical space
- T3 \rightarrow Transport of velocity by gravity and mean pressure gradient
- T4 \rightarrow Chemical source term
- T5 \rightarrow Transport of pdf in velocity space by viscous stresses and fluctuating velocity gradient (unclosed)
- T6 \rightarrow Transport in reactive scalar space (molecular mixing)

So, this is psi is the reactive scalar and this is the pdf of finding the velocity and reactive scalar this is joint pdf of velocity and psi of the reactive scalar, and the this is essentially the pdf P times du times d psi is essentially the probability of finding velocity and reactive scalar within u minus du and u plus du and psi minus psi probability of finding psi within psi minus t psi and psi plus t psi.

And the pdf transport equation for the pdf the transport equation for the probability density can be obtained you can see popes book for this derivation it is an important derivation and. So, here we have the different terms, and you see that this divergence of u is respective the three components of the velocity this means this angular brackets are the conditional averages with respect to fixed values of u and psi.

This is of course, much more involved as you can see that this T 1 is the local rate of change at time T 2 is the convective derivative in physical space, T3 is the transport of velocity by gravity and the mean pressure gradient by the forces and T4 is the chemical source term one advantage of this pdf equation is that this term is fully closed, and the transport of pdf in velocity space T5 is the transport of pdf in the velocity space by viscous stresses and fluctuating velocity gradient this is unclosed.

And the T6 is the most difficult term to handling in this thing is essentially the transport in reactive scalar space and this is the T 6 term.

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Continued..

- Because of higher dimensionality of pdf transport equation, finite volume and finite difference methods are not suitable.
- Therefore, Monte-Carlo techniques are employed
- Lagrangian particle tracking algorithm (Pope, 1985) to overcome the difficulty of Monte-Carlo methods

$$\frac{dx^j}{dt} = u^j(x); \quad \rho^j \frac{d\psi_i^j}{dt} = \omega_i^j$$

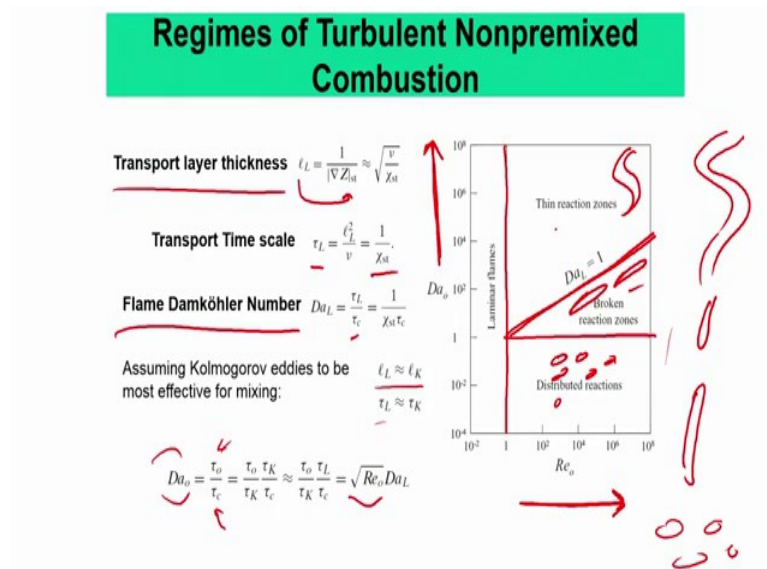
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And you see that how to do this how to get this pdf is that because of high dimensionality of pdf transport equation, this finite volume and finite difference methods are not suitable they were very high cost when you apply these things.

And. So, the montecarlo techniques are employed and for this the Lagrangian particle tracking algorithms are used to overcome the difficulty of montecarlo methods and for that you have to basically insert particles which falls the dx^j/dt over the j particle is equal to u^j and this is the reactive scalar essentially changes. So, this is just the basic very brief claims of these two advanced techniques of conditional moment closures and pdf methods.

So, will close this discussion on the non premix flames by just looking at to the regime diagrams of course, the regime diagrams will be much more useful in the premix flames, but in non premix flames you can also use that. So, in this regime diagrams you have basically two coordinates one on the Reynolds number large scale Reynolds number on the x axis and the Damkohler number on the y axis ok.

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Now we define our transport layer thickness whereas, which is of course, you do not have a flame thickness as such here and either you have a velocity scale. So, we have to construct this transport layer thickness based on this on the gradient of Z at the stoichiometry location, which is defined like this and which can be shown to scale like this viscosity divided by the scalar dissipation rate at ψ_{st} and then you define a transport time scale.

And the transfer time scale of course, is the inverse of this scalar dissipation rate at the stoichiometric location, and from that we can define a flame damkohler number which is essentially the ratio of the transport time scale to the chemical timescale and this is given by $1/\psi_{st} \tau_c$ and now assuming Kolmogorov eddies to be most effective for mixing.

We can have this kind of thing and we can define a revised Damkohler number which is the ratio of the flow timescale at large scales to the chemical timescale and that can be

shown to be essentially the square root of the hydro dynamic scale Reynolds number to the n times the flame Damkohler number ok.

So, this is my y axis and this is my x axis of course, you see when the Reynolds number is small then of course, all flames will be laminar of course, when the Damkohler number is large then you will only have distributed then when the Damkohler number is large essentially you have thin reaction zones. So, you only have essentially the regions which are we only have flames which are essentially wrinkled and folded by the turbulence.

So, this is the essentially the thing reaction zones and then you have as you reduce the Damkohler number you have broken reaction zones when you cross this Damkohler number equal to flame Damkohler number equal to one line you have broken reaction zones, when the reactions get detached and then you have distributed reaction zone when you have the reactions happening in different spots happening in different spots in these things.

So, this is the and you have ignition happening at different points in the in the flow. So, this is typically a very basic regime diagram which we have shown you and of course, this regime diagram should become much more useful in the premixed combustion. So, in this class what we have learnt is that we have learnt that to analyze turbulent combustion one very important concept that can be introduced is a mixture fraction concept.

And the introduction of the mixture fraction concept what you can do is essentially of course, you solve for the you essentially as soon as you have the mixture fraction concept we essentially can construct, go back to the 1D chamber flame and construct the solutions of the reactive scalars in terms of mass fraction and temperature exclusive of any function of the mixture fraction ok and store that solution.

Then for turbulent flames we essentially have to solve the average momentum equation averaged kinetic energy turbulent kinetic energy equation scalar dissipation mean turbulent kinetic energy dissipation rate equation that is key epsilon model is essentially, then the density for our radiations of course, have to take care by solving the other equations.

We have to couple it with somehow and that coupling for that you essentially has to obtain this reactive scalar field how you do that? You also then solve for the average mixture fraction and the variance of the mixture fraction equation and as soon as you do that you know the average mixture fraction and average the variance of mixture fraction at each point in your combustor ok.

Then at each point in the combustor is you basically construct a pdf when the pdf of Z which tells you the what how much this mixture fraction can vary, and this pdf is essentially controlled by your Z average your mean mixture fraction and the variance of mixture fraction which you already know at that point because you solve the governing equations; after you do that you obtain. So, you have a know that what is can be the distribution around this rate and Z primes.

And then you essentially map your reactive scalars temperature enthalpy and reactive scalars on to the mixture fraction by using the 1D chamber flames solution, and then immediately you know the all possible values of the temperature and reactive scalars that can that can happen at that point, and then by using that pdf of Z you can immediately solve for the find out the average of this reactive scalars that can happen at this particular points, and then once again from those densities you can again couple back to the continuity and the momentum equations.

So, this is how you can have a complete solution of course, you may this one may not like the idea that we use the one d chamber flame or this partial flame or an equilibrium solution at each point in the flow. So, for that one can basically define one can go from the physical space to a mixture fraction space and basically attach a coordinate system which is where the mixture fraction varies normal to the to the flame surface.

Which is considered to be the mean mixture fraction which is considered to this stoichiometric iso contour of the mixture fraction, and then you basically transform your reactive scalar equation from the physical space to the mixture fraction space and then you basically can obtain ψ_i this reactive scalar as a function of the mixture fraction.

So, once again then going back you can one can find out the given or steady or unsteady situation would and appropriate choice of the scalar dissipation rate one can find out the pdf or the or the mean ψ_i or the mean reactive scalar at a particular point. And then of course, we have seen that in this approach the one big takeaway is that the scalar

dissipation rate emerges as the characteristic diffusivity of the reactive scalar in the mixture fraction space.

And then of course, we introduced just came through just glance through the two modern approaches, with this conditional moment closure and pdf approach and then we closed it with the turbulent non premixed combustion diagram. So, this is so much for the turbulent non premixed combustion and then in the next class we will take up turbulent premix combustion, and then later we will take up appropriate will take up the practical aero engine combustors at the towards the end of the course. So, till then goodbye friend's bye.