Fundamentals of Combustion for Propulsion

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Lecture - 25
CFD modeling aspects – Fundamentals

Let us get started. Welcome back in this session, we look at basics of CFD modeling aspects required for simulating combustion and propulsion systems.

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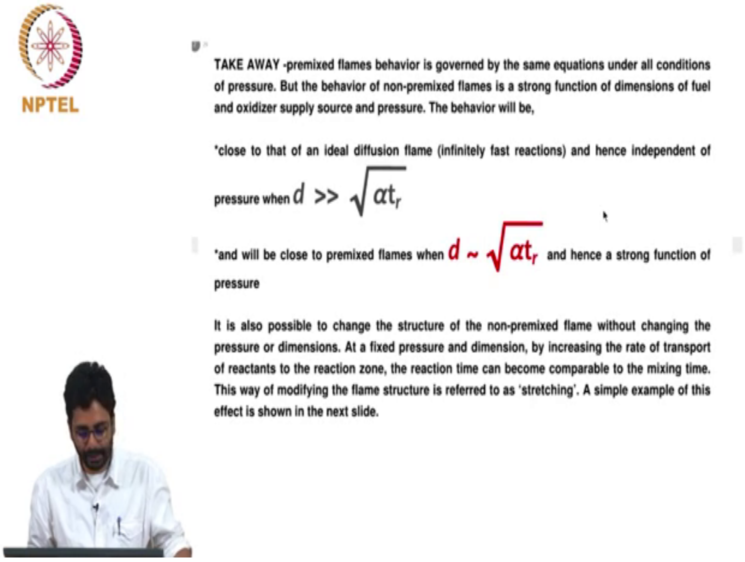

TAKE AWAY -premixed flames behavior is governed by the same equations under all conditions of pressure. But the behavior of non-premixed flames is a strong function of dimensions of fuel and oxidizer supply source and pressure. The behavior will be,

•close to that of an ideal diffusion flame (infinitely fast reactions) and hence independent of pressure when $d >> \sqrt{\alpha t_r}$

•and will be close to premixed flames when $d \sim \sqrt{\alpha t_r}$ and hence a strong function of pressure

It is also possible to change the structure of the non-premixed flame without changing the pressure or dimensions. At a fixed pressure and dimension, by increasing the rate of transport of reactants to the reaction zone, the reaction time can become comparable to the mixing time. This way of modifying the flame structure is referred to as 'stretching'. A simple example of this effect is shown in the next slide.

I just, this is a slide that we looked at yesterday just as a recap. I thought is the good slides to start with. So, from the analysis that we did yesterday the takeaway is that the premixed flame behavior is governed by the same equations under all conditions of pressure. That is reaction rate place the central role in determining premix flame behavior under all conditions, but the behavior of non-premix flames is a strong function of several parameters including dimensions of fuel and oxidizer supply source and pressure. I would like you to recall the ethylene flame case that we discussed in some detail yesterday.

So, the behavior of the flame will be close to an ideal diffusion flame; that means, controlled purely by mixing and reactions being close to being infinitely fast and therefore, the dynamics will be independent of pressure. This we formally expressed as a condition where the diameter of a fuel jet is much larger than the distance that the fuel and the oxidizer can mix in the limited reaction time that is available be much much greater than the diffusion distance.

And on the other hand, it is possible that under conditions of low pressure or the dimension of the fuel issuing orifice being very small significant premixing can happen, and this is expressed as the characteristic dimension becoming comparable to the diffusion distance. And the diffusion distance itself is limited by the reaction time, keep that in mind, t r is reaction time as we discussed yesterday.

So, the dynamics will be close to premixed flames when d is comparable to square root d t r or alpha t r. For simplicity I am assuming that Lewis number is 1, and hence the strong function of pressure, ok. These are two ways and the application of this idea to modeling of composite solid propellants is something that we discussed earlier. But there are also other ways in which the mixing time can be made similar or of the same order as the reaction time. Without changing the dimension, without changing the pressure we look at one such case which has relevance for modeling.

So, it is also possible to change the structure of the non-premix flame without changing the pressure or dimensions. It is done in the following way the fixed pressure and dimension by simply increasing the rate of transport of reactants to the reaction zone. Remember that for the ethylene flame it so turns out that the rate at which the reactants were transferred to the flame is much slower than the rate of the reaction. So, by simply increasing the rate at which you transport reactants to reaction zone you can make the mixing time and the reaction time comparable, ok.

So, by increasing the rate of transport of reactants to the reaction zone, the reaction time can become comparable to the mixing time. This way of modifying the flame structure is referred to as stretching which was also something that we looked at earlier, ok.

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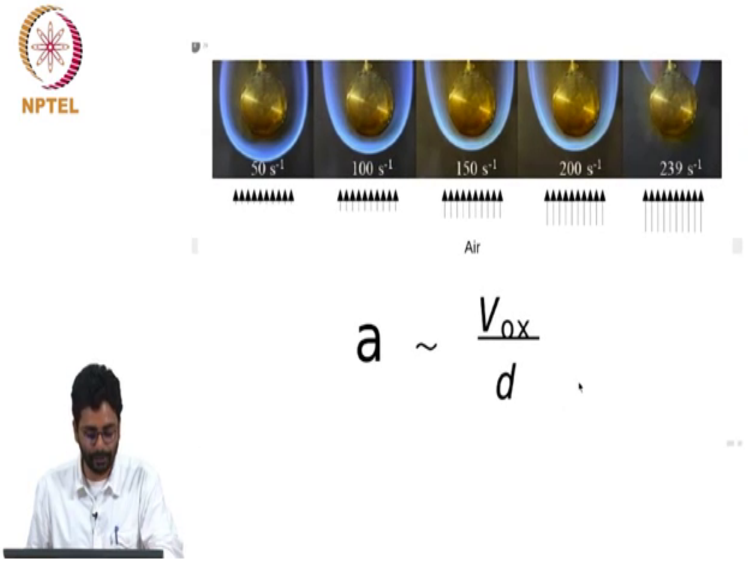

$$a \sim \frac{V_{ox}}{d}$$

I will show you a simple example of this in the next slide, stretched non-premix flames and extinction. What do you see here is the cylinder that you see is a porous cylinder issuing fuel. In this case diluted methane, and there is air flowing from bottom to up. The air is flowing past the porous cylinder is showing fuel and the flame is established in the boundary layer around the porous cylinder.

The rate of transport of reactant to the flame. So, under the conditions which is marked as 50 second in which I will explain in a minute what it is. Under these conditions the reactions are simply controlled by mixing rate of transport of reactants to the flame zone, and this rate is increased by increasing the air velocity. So, as you go from left to right the length of the arrow is increasing indicative of the air flow rate going, increasing air flow rate we go from low values to high values and there is a critical air flow rate at which the flame cannot remain in the stagnation point anymore. It actually gets extinct from the boundary layer and goes to the bake. This happens at a very specific value of the air flow rate.

And the quantity that is used to use to characterize this aspect of extinction is called strain rate, it is called extinction strain rate and a good measure of it is simply the velocity of the oxidizer divided by the diameter of the cylinder. Note that it has dimensions of second inverse, ok.

So, this is the inverse of this quantity is the timescale for mixing, ok. So, when the air velocity is low the strain rate is low, and therefore, the time for mixing is high, and as you progressively increase the airflow rate, there comes a point at which the rate of mixing has increased to a level which has brought down the mixing time, so that it is comparable to the reaction time. The rate of reaction is not sufficient to consume all the reactants it is being supplied to the reaction zone and therefore, the flame quenches. And it moves to a point where it can continue to burn, so it actually moves to a bake.

This is an important. So, the reason why I am showing this is this is a non-premixed situation where we have created condition under which the mixing time becomes equal to the reaction time. So, one of the one of the uses of this kind of a configuration or extinction strain rate that is measured using this configuration is at the point of extinction the rate of transport of fuel and oxidizer to the flame zone is equal to the reaction time which can be used to construct chemical kinetic mechanisms

Student: Sir.

Yeah.

Student: When you are increasing the airflow rate whether you are changing the (Refer Time: 06:31).

Ok. That is a good question. So, what can be done is that we can also increase the fuel flow rate, the strain rate will still increase, but in this case the fuel flow rate is maintained constantly. The condition that is used here is that as long as the flame is sufficiently away from the cylinder, it is not strongly interacting with the cylinder. And it is also the reason that the strain rate is mostly controlled by the oxidizer velocity as long as the flame is sufficiently away from the cylinder.

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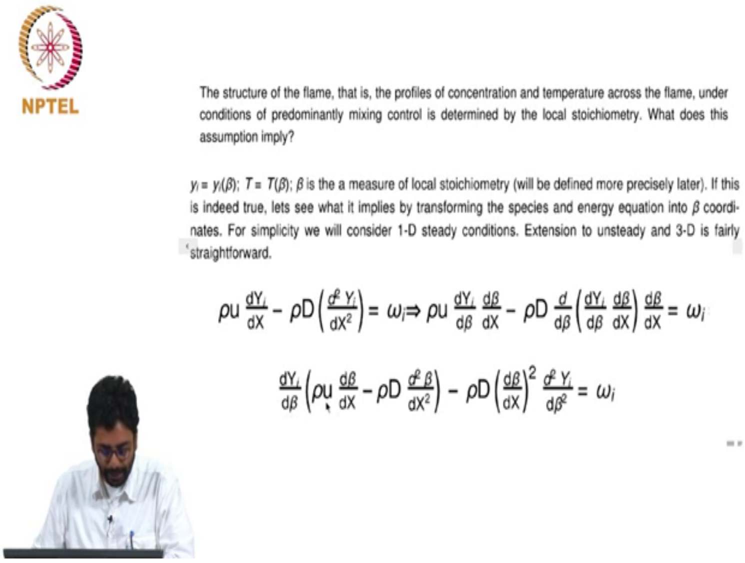

The structure of the flame, that is, the profiles of concentration and temperature across the flame, under conditions of predominantly mixing control is determined by the local stoichiometry. What does this assumption imply?

$y_i = y_i(\beta)$; $T = T(\beta)$; β is the a measure of local stoichiometry (will be defined more precisely later). If this is indeed true, lets see what it implies by transforming the species and energy equation into β coordinates. For simplicity we will consider 1-D steady conditions. Extension to unsteady and 3-D is fairly straightforward.

$$\rho u \frac{dY_i}{dX} - \rho D\left(\frac{d^2 Y_i}{dX^2}\right) = \omega_i \Rightarrow \rho u \frac{dY_i}{d\beta}\frac{d\beta}{dX} - \rho D \frac{d}{d\beta}\left(\frac{dY_i}{d\beta}\frac{d\beta}{dX}\right)\frac{d\beta}{dX} = \omega_i$$

$$\frac{dY_i}{d\beta}\left(\rho u \frac{d\beta}{dX} - \rho D \frac{d^2\beta}{dX^2}\right) - \rho D\left(\frac{d\beta}{dX}\right)^2 \frac{d^2 Y_i}{d\beta^2} = \omega_i$$

So, the structure of the flame that is what I mean by that is the profiles of concentration and temperature across the flame under conditions of predominantly mixing control dynamics is determined by local stoichiometry. Let us see what the statement means. Let us follow through the mathematics and then see what it implies in terms of the actual behaviour.

If the mass fractions or the concentration of the fuels let us say is a function of only a variable which we call which we will call beta which is a measure of the stoichiometry measure of the local stoichiometry. The mass fractions is a function, the mass fraction is a function of only beta and let us say the temperature, the local temperature is also only a function of beta. Beta is some measure of stoichiometry which I will define precisely later, but let us follow through the analysis and see what it means. If this assumption is true, then the species conservation and the energy equation can be transformed to a coordinate, ok, transform to a beta coordinate and for simplicity we will consider the 1-D steady conditions, instead of just working through the equations I will probably write the equations.

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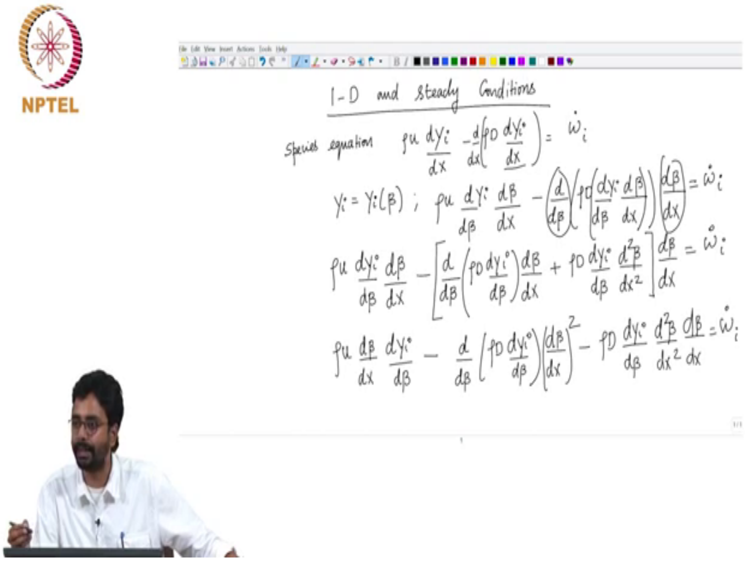

1-D and Steady Conditions

Species equation $\rho u \frac{dY_i}{dx} - \frac{d}{dx}\left(\rho D \frac{dY_i}{dx}\right) = \dot{\omega}_i$

$Y_i = Y_i(\beta)$; $\rho u \frac{dY_i}{d\beta}\frac{d\beta}{dx} - \frac{d}{d\beta}\left(\rho D\left(\frac{dY_i}{d\beta}\frac{d\beta}{dx}\right)\right)\left(\frac{d\beta}{dx}\right) = \dot{\omega}_i$

$$\rho u \frac{dY_i}{d\beta}\frac{d\beta}{dx} - \left[\frac{d}{d\beta}\left(\rho D \frac{dY_i}{d\beta}\right)\frac{d\beta}{dx} + \rho D \frac{dY_i}{d\beta}\frac{d^2\beta}{dx^2}\right]\frac{d\beta}{dx} = \dot{\omega}_i$$

$$\rho u \frac{d\beta}{dx}\frac{dY_i}{d\beta} - \frac{d}{d\beta}\left(\rho D \frac{dY_i}{d\beta}\right)\left(\frac{d\beta}{dx}\right)^2 - \rho D \frac{dY_i}{d\beta}\frac{d^2\beta}{dx^2}\frac{d\beta}{dx} = \dot{\omega}_i$$

We will consider 1-D and steady. So, the species equation, it is rho mu, this is species equation. This is 1-D and steady, steady, so rho u is constant. What we are trying to do is we are trying to see what if this is true what it implies, ok. So, we will convert from the coordinates of space to beta coordinates. So, we will have rho u d by d beta of Y i, ok. Let us follow through rho u dX minus ok. I think now we have; we will leave it as such. So, this is the form of the equation that I have in the slide.

Student: (Refer Time: 11:58).

Sorry.

Student: (Refer Time: 12:01).

In the second line, yeah.

Student: Second term.

Second term, yeah.

Student: (Refer Time: 12:10).

This term, this term.

Student: Yeah.

I have a d by d beta and the d beta by dX at the end. Is that ok? It is ok. Is the algebra, ok? I think, I think it is ok. So, I have a b by d beta here and d beta dX here and the dY dX is written as dY i d beta d beta dX, ok. So, this is the form in which I have the equation written here with some rearrangement. What we see here is dY i by d beta multiplied by this term minus rho D d beta dX square d square Y by d beta square equals omega dot i. That is if you rearrange the equation that I have written in the final expression you will get this.

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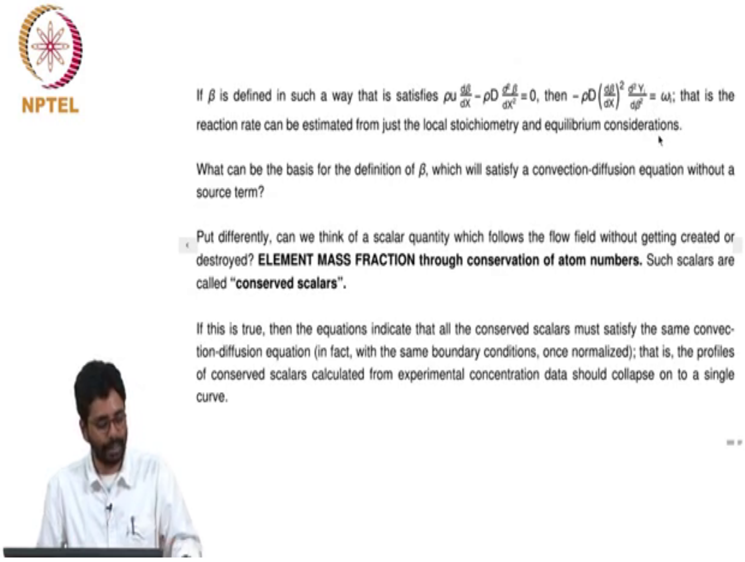

If β is defined in such a way that is satisfies $\rho u \frac{d\beta}{dX} - \rho D \frac{d^2\beta}{dX^2} = 0$, then $-\rho D \left(\frac{d\beta}{dX}\right)^2 \frac{d^2 Y_i}{d\beta^2} = \omega_i$; that is the reaction rate can be estimated from just the local stoichiometry and equilibrium considerations.

What can be the basis for the definition of β, which will satisfy a convection-diffusion equation without a source term?

Put differently, can we think of a scalar quantity which follows the flow field without getting created or destroyed? **ELEMENT MASS FRACTION through conservation of atom numbers.** Such scalars are called "**conserved scalars**".

If this is true, then the equations indicate that all the conserved scalars must satisfy the same convection-diffusion equation (in fact, with the same boundary conditions, once normalized); that is, the profiles of conserved scalars calculated from experimental concentration data should collapse on to a single curve.

So, if beta is defined in such a way that it satisfies convection diffusion equation exactly like the one that is satisfied by species conservation, species concentration, but without the reaction term on the right hand side, then the previous equation the previous page will suggest that the reaction rate can be written in this form, ok. That is the reaction rate can be estimated from just the local stoichiometry and equilibrium considerations, ok.

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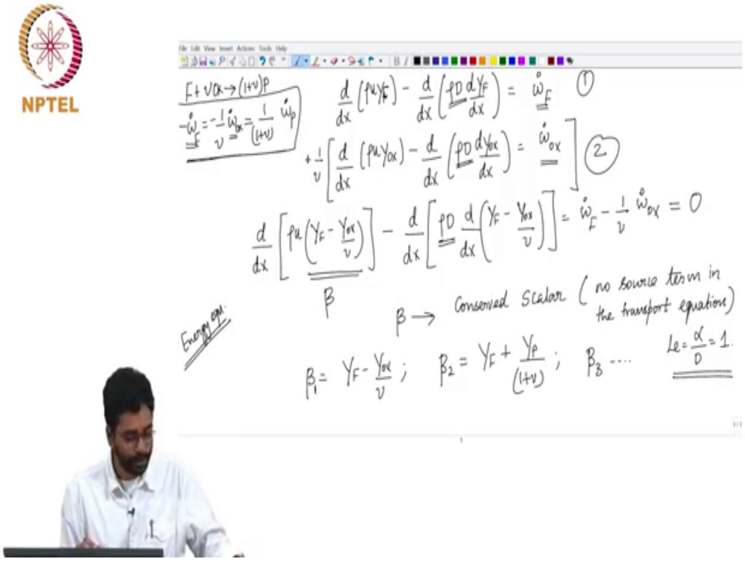

$F + \nu Ox \rightarrow (1+\nu)P$

$-\dot{\omega}_F = -\frac{1}{\nu}\dot{\omega}_{Ox} = \frac{1}{(1+\nu)}\dot{\omega}_P$

$$\frac{d}{dx}(\rho u Y_F) - \frac{d}{dx}\left(\rho D \frac{dY_F}{dx}\right) = \dot{\omega}_F \quad ①$$

$$+\frac{1}{\nu}\left[\frac{d}{dx}(\rho u Y_{Ox}) - \frac{d}{dx}\left(\rho D \frac{dY_{Ox}}{dx}\right) = \dot{\omega}_{Ox}\right] \quad ②$$

$$\frac{d}{dx}\Bigg[\rho u \underbrace{\left(Y_F - \frac{Y_{Ox}}{\nu}\right)}_{\beta}\Bigg] - \frac{d}{dx}\left[\rho D \frac{d}{dx}\left(Y_F - \frac{Y_{Ox}}{\nu}\right)\right] = \dot{\omega}_F - \frac{1}{\nu}\dot{\omega}_{Ox} = 0$$

$\beta \rightarrow$ Conserved Scalar (no source term in the transport equation)

Energy eqn.

$\beta_1 = Y_F - \frac{Y_{Ox}}{\nu}$; $\beta_2 = Y_F + \frac{Y_P}{(1+\nu)}$; $\beta_3 \ldots$

$Le = \frac{\alpha}{D} = 1$

So, one simple way that we can define beta, in a general situation it is different, but the simplest way to define beta is like this. I am again starting from the species conservation equation and I am writing it for the fuel mass fraction the omega dot F.

Now, I am reading same equation for the oxidizer, ok. Remember, yesterday we looked at this example we have 1 gram of fuel reacting with nu grams of oxidizer producing 1 plus nu grams of products. And if this is the only reaction that is allowed and this is a irreversible reaction, if you assume that this is an irreversible reaction then the rate at which the fuel is consumed must be 1 by nu times the rate at which the oxidizer is consumed that should be equal to 1 plus 1 over nu times the rate at which the products are formed, ok. So, if 1 gram of fuel disappears nu grams of oxidizer must disappear the smelting in the formation of one plus nu grams of products, ok.

So, now that the omega dot F and omega dot o are connected by this equation and we have omega dot F and omega dot oxidizer on the right hand side. Calling it oxidizer, so let me also call it here oxidizer, ok. So, the equation itself suggests simple way to get a scalar for which the right hand side will be 0. So, all we need to do is multiply the second equation by 1 by nu, multiply this is the first equation and the second equation. Multiply the second equation by 1 by nu and subtract it from the first equation, the right hand side will become omega dot F minus omega dot ox divided by nu which is 0 from this condition, ok.

So, we will have the resulting equation will be, from here you can clearly see that omega dot F is equal to 1 by nu omega dot ox and therefore, this is equal to 0, ok. Just by the simple rearrangement we have in in fact, we have been able to identify a scalar like beta which can satisfy a convection diffusion equation without a source term, ok. And beta is also, so beta is what is called a conserved scalar, something is called a conserved scalar if it is governed by a convection diffusion equation without a source term, in the transport equation.

Now, we can immediately see that we can define several betas. For example, instead of using the transport equation for oxidizer, I could have used the transport equation for products and divided that equation by negative 1 by 1 plus nu and added subtracted from the first equation I would have got another beta. So, I have 1 beta which is Y F minus Y ox by nu, let us called beta 1. I could have also gotten another beta which is Y F plus Y P 1 plus nu, ok.

We can do one more thing which is you can also have the energy equation which we saw yesterday and combine it with linearly combined with either the fuel equation oxidizer equation or reproduct equation and get another beta which is a linear function of mass fraction of the fuel and temperature. The only thing that you need to keep in mind is that when I am subtracting these equations I am assuming that the D, rho D for all these species are the same, ok. And when we subtract one of these equations from the energy equation, we also have to assume that the Lewis number is 1, ok. These assumptions may look restrictive, but they are not an identifying a scalar and using it in the analysis of non-premix flames is a powerful tool that is available for both laminar diffusion flames and turbulent diffusion flames.

So, what we have done so far is that we started with the assumption that a scalar of this sort exists. And what it means? It means that the reaction rate can be written as negative rho D d beta dX squared d squared Y i by d beta squared you have done that and we have also shown that starting from the species conservation equation and the energy conservation equation. We can actually identify such scalars, ok.

In a more general situation where Lewis number is not 1 and the system is not adiabatic a good definition for a conserved scalar is the element mass fraction of one of the species that is involved in question. There is rearrangement of molecules that happened, but the total number of elements of carbon hydrogen oxygen and nitrogen are conserved. So, the element mass fraction is a conserved scalar, it is a general conserved scalar, So, element mass fraction through the conservation of atom numbers is a good conserved scalar to work with in general situations.

If this is true, then the equations indicate that the all indicate that all the conserved scalars must satisfy the same convection diffusion equation. Of course, I have not explained what it means, but I will. In fact, at the same boundary conditions once normalized that is the profiles of conserved scalars calculated from experimental concentration should collapse onto a single curve.

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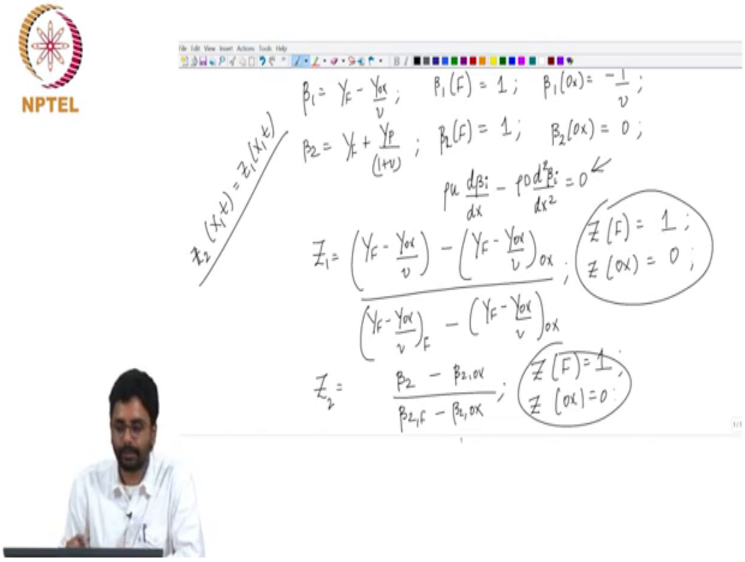

$$\beta_1 = Y_F - \frac{Y_{ox}}{\nu}; \quad \beta_1(F) = 1; \quad \beta_1(ox) = -\frac{1}{\nu};$$

$$\beta_2 = Y_F + \frac{Y_P}{(1+\nu)}; \quad \beta_2(F) = 1; \quad \beta_2(ox) = 0;$$

$$\rho u \frac{d\beta_i}{dx} - \rho D \frac{d^2\beta_i}{dx^2} = 0 \leftarrow$$

$$Z_1 = \frac{\left(Y_F - \frac{Y_{ox}}{\nu}\right) - \left(Y_F - \frac{Y_{ox}}{\nu}\right)_{ox}}{\left(Y_F - \frac{Y_{ox}}{\nu}\right)_F - \left(Y_F - \frac{Y_{ox}}{\nu}\right)_{ox}}; \quad \boxed{\begin{matrix} Z(F) = 1; \\ Z(ox) = 0; \end{matrix}}$$

$$Z_2 = \frac{\beta_2 - \beta_{2,ox}}{\beta_{2,F} - \beta_{2,ox}}; \quad \boxed{\begin{matrix} Z(F) = 1; \\ Z(ox) = 0; \end{matrix}}$$

$$Z_2(x,t) = Z_1(x,t)$$

So, what is meant by that is that if your beta 1 is Y F minus Y ox by nu. So, beta 1 in the fuel boundary will be let us say there is pure fuel entering from the fuel boundary, then beta F will be 1, beta 1 of F will be 1 and beta 1 in the oxidizer boundary will be minus 1 by nu, ok.

Similarly, beta 2 which is Y F plus Y P by 1 plus nu will be beta 1 of F will be again 1. There are no, there is no oxidizer or product in the fuel inlet, sorry this is beta 2, beta 2 in the oxidizer boundary will also will be 0, ok.

So, one problem that this is both beta 1 and beta 2 satisfy the same equation which is actually this, both the betas satisfy this equation, but the solutions need not be the same because the boundary conditions are different, ok. So, one way to take care of this problem is to normalize. So, the normalization is done in the following way.

Student: (Refer Time: 22:09) oxidizer (Refer Time: 22:10).

There is no fuel, there is no oxidizer in the oxidizer boundary. There is no fuel, there is no product in the oxidizer boundary, yeah.

Let me see if this normalization is correct. We will just check. If I define a scalar like this then the value of Z at the fuel boundary would be 1, a definition, ok. And the value of Z in the oxidizer boundary will be 0, ok; is that clear. Say I put fuel here the numerator and the denominator are the same if I put oxidizer here the numerator is 0 denominator is the same, ok.

Similarly, I can define Z like this with the other scalar instead of writing the whole thing. I will write beta 2 minus beta 2 in the oxidizer boundary divided by beta 2 in the fuel boundary minus beta 2 in the oxidizer boundary. If I define it like this then Z defined using beta 2 in the fuel boundary will be 1 and in the oxidizer boundary will be 0, ok. Just by this normalization, we have not only shown that these scalars are governed by the same transport equations, but the transport equations also have the same boundary conditions and therefore, beta 1 or Z 1 and Z 2 will have the same solution, ok.

So, this is the reason, this is the this is what is summarized in the last paragraph in this slide. If this is true then the equations indicate that all conserved scalars must must satisfy the same convection diffusion equation, in fact, when normalized with the same boundary conditions, ok. That is the profiles of conserved scalars calculated from experimental concentration data should collapse onto a single curve because they are all the same solutions to the same equation with a same boundary condition. That is what is I shown here this is from a paper by Bilger, ok.

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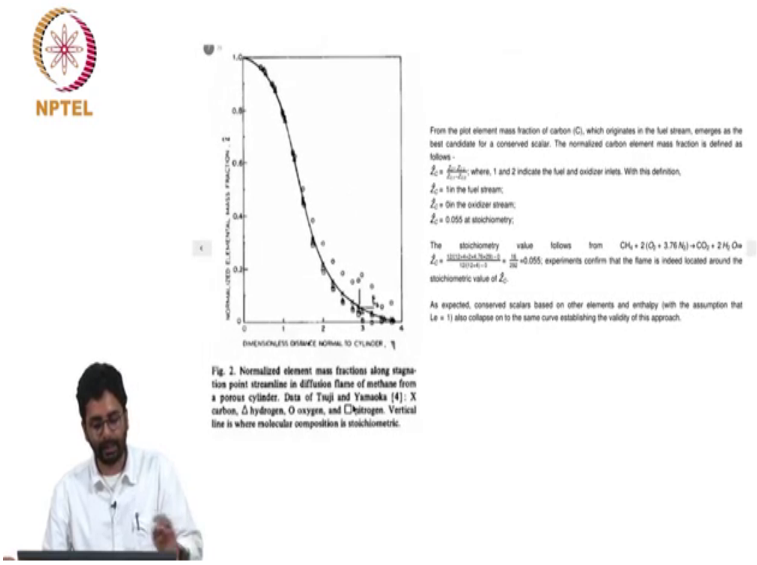

Fig. 2. Normalized element mass fractions along stagnation point streamline in diffusion flame of methane from a porous cylinder. Data of Tsuji and Yamaoka [4]: X carbon, △ hydrogen, O oxygen, and □ nitrogen. Vertical line is where molecular composition is stoichiometric.

From the plot element mass fraction of carbon (C), which originates in the fuel stream, emerges as the best candidate for a conserved scalar. The normalized carbon element mass fraction is defined as follows -

$\hat{Z}_C = \frac{Z_C - Z_{C,2}}{Z_{C,1} - Z_{C,2}}$; where, 1 and 2 indicate the fuel and oxidizer inlets. With this definition,

$\hat{Z}_C = 1$ in the fuel stream;

$\hat{Z}_C = 0$ in the oxidizer stream;

$\hat{Z}_C = 0.055$ at stoichiometry;

The stoichiometry value follows from $CH_4 + 2(O_2 + 3.76 N_2) \rightarrow CO_2 + 2 H_2 O +$ $\hat{Z}_C = \frac{12/(12+4+2\times 4.76\times 28)-0}{12/(12+4)-0} = \frac{15}{272} = 0.055$; experiments confirm that the flame is indeed located around the stoichiometric value of $\hat{Z}_C$.

As expected, conserved scalars based on other elements and enthalpy (with the assumption that Le = 1) also collapse on to the same curve establishing the validity of this approach.

What is shown here is plot of data of measurements of species concentration and temperature from a flame of this kind made along the radial direction intersecting the stagnation point, ok. That is what is shown here. So, the dimensional dimensionless distance normal to the cylinder which is just the distance from the cylinder normalized by the radius of the cylinder and on the Y axis what is shown is a normalized element mass fraction which we just saw is a conserved scalar, ok.

So, data for all the elements are shown, the X is for carbon the triangles are showing hydrogen, the O is for oxygen, and the squares are nitrogen, ok. And it is clear that for most of the zones all the element mass fractions collapse onto the same curve and therefore, the approximation that mixing and local stoichiometry controls the structure of the flame is a very good approximation. Another important thing to note here is that right at the point where the flame is located the value of the conserved scalar, is 0.055, ok.

How did we get this 0.055? Z C is the element concentration of carbon, which is according to the normalized formula will be defined by this equation, ok. So, Z C is 1 in the fuel stream because all the carbon elements are in fuel form. Z C equals 0 in the oxidizer stream because it is there are no carbon elements in the oxidizer stream and Z C at stoichiometry is nothing but Z C minus Z C 2 minus divided by Z C 1 minus Z C 2 which you can calculate from the stoichiometric expression for methane which we saw yesterday.

This will simply be the element mass fraction in the fuel stream minus element mass fraction in the oxidizer stream divided by; I am sorry the element mass fraction for the stoichiometric mixture minus the element mass fraction for the oxidizer stream, divided by the element mass fraction for the fuel minus the element mass fraction for the oxidizer. So, it will be you can work this out for this stoichiometric equation and it will turn out to be 16 over 292 which is 0.005.

So, this confirms that the flame is indeed located around the stoichiometric value of Z C. This is an experimental verification or the statement that was made earlier that the diffusion flame always locates itself at a point where the fuel and oxidizer are mixed in stoichiometric proportion.

So, as expected conserved scalars based on other elements and enthalpy with the assumption that the Lewis number is 1, also collapse onto the same curve establishing the validity of this approach. So, what it means is that this also means that the reactions are much much faster than mixing and therefore, the flame is thin, ok.

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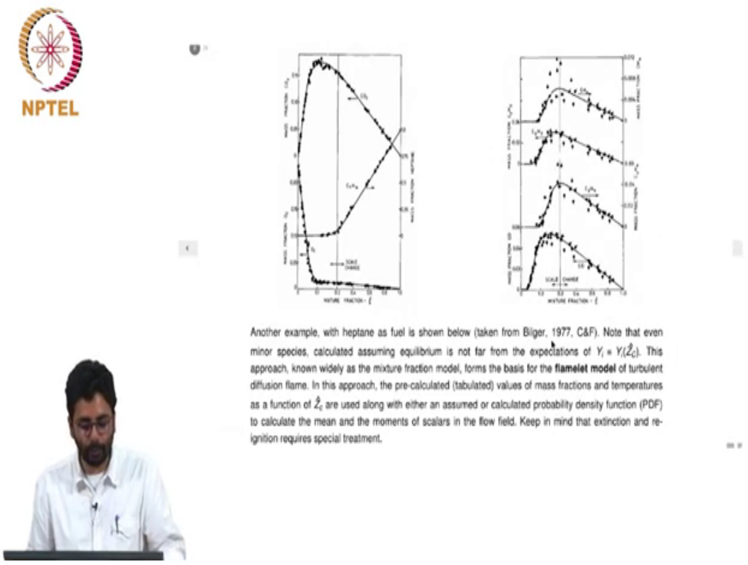


Another example, with heptane as fuel is shown below (taken from Bilger, 1977, C&F). Note that even minor species, calculated assuming equilibrium is not far from the expectations of $Y_i = Y_i(\hat{Z}_C)$. This approach, known widely as the mixture fraction model, forms the basis for the **flamelet model** of turbulent diffusion flame. In this approach, the pre-calculated (tabulated) values of mass fractions and temperatures as a function of $\hat{Z}_c$ are used along with either an assumed or calculated probability density function (PDF) to calculate the mean and the moments of scalars in the flow field. Keep in mind that extinction and re-ignition requires special treatment.

Again, more comparison are shown for other variables, I just want to emphasize the following that the lines indicate the calculations made we assuming that everything is mixing controlled and equilibrium is achieved and the dots show the data points. It is not just that this is correctly predicting the major species. As you can see on the right hand side it also predicts some of minor species fairly accurately, ok. So, this is with heptane as fuel taken from Bilger 1977.

Note that even minus species calculated assume assuming equilibrium, is not far from the expectation of the mass fraction being a function of only the conserved scalar, ok. So, this the reason why I am describing this in some detail is that the this forms the basis for the important model that is used for simulating turbulent diffusion flames.

So, this approach known widely as the mixture fraction model forms the basis for the flamelet model of turbulent diffusion flames. The advantage is that in this approach the pre calculated or pre tabulated values of mass fractions and temperature as a function of the conserved scalar can be calculated a priori and tabulated, and during the calculation you solve only for the flow and look up this table to get the species concentration and temperature which is a result of the chemical reaction, ok.

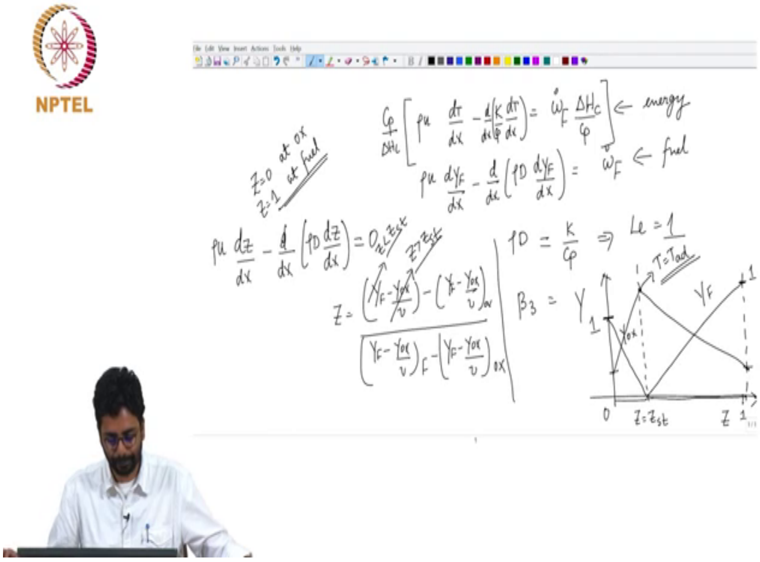
So, the flow and the reaction problem can be separated simplifying the calculation significantly, ok. Just want to emphasize this that that extinction and reignition requires special treatment. These are cases where everything is not mixing control there is chemistry role also. Of course, methods have been developed to deal with this in within the flamelet framework.

So, another example with heptane as fuel is shown in these two plots. What I would like to I would like to draw your attention to the fact that it is not just the major species that seem to agree well with the predictions of this model, the minus species also a reasonably good agreement, ok.

And this approach called the mixture fraction approach forms the basis for the flamelet model of turbulent diffusion flame and then this approach the pre calculated or pre tabulated values of mass fractions and temperatures is a function of a conserved scalars are used along with either an assumed or calculated probability density function. We will see what it means later.

The implication is that the flow and the reaction problem can be separately dealt with and that offers a lot of simplification in simulating flows and reacting flows, in complex geometries.

(Refer Slide Time: 30:48)



$$\frac{C_p}{\Delta H_c}\left[\rho u \frac{dT}{dx} - \frac{d}{dx}\left(\frac{K}{C_p}\frac{dT}{dx}\right) = \dot{\omega}_F \frac{\Delta H_c}{C_p}\right] \leftarrow \text{energy}$$

$$\rho u \frac{dY_F}{dx} - \frac{d}{dx}\left(\rho D \frac{dY_F}{dx}\right) = \dot{\omega}_F \leftarrow \text{fuel}$$

$Z=0$ at ox
$Z=1$ at fuel

$$\rho u \frac{dZ}{dx} - \frac{d}{dx}\left(\rho D \frac{dZ}{dx}\right) = 0 \quad Z<Z_{st} \quad Z>Z_{st}$$

$$Z = \frac{\left(Y_F - \frac{Y_{ox}}{\nu}\right) - \left(Y_F - \frac{Y_{ox}}{\nu}\right)_{ox}}{\left(Y_F - \frac{Y_{ox}}{\nu}\right)_F - \left(Y_F - \frac{Y_{ox}}{\nu}\right)_{ox}}$$

$$\rho D = \frac{K}{C_p} \Rightarrow Le = 1$$

$$\beta_3 = Y$$

Questions. So, one question was about the assumption of unity Lewis number. So, that assumption is required when we are combining the transport equations to get a scalar that has both the mass fraction and temperature. So, this is the energy equation and the mass fraction equation for fuel is this, ok. This is the fuel equation I do not need the negative sign here it will be automatically taken care of.

Now, if I need to combine these two equations. I need to assume that rho D and K by Cp are equal. If I have to subtract one equation from the other, I need to assume that rho D and K by Cp are equal which implies that Lewis number is 1, ok.

Student: (Refer Time: 31:50).

Yeah, it will be if you normalize the scalar like we did for the other cases the it will be 0 at one boundary and 1 at the other boundary, ok. That will happen for this combination of scalars also. So, let us call this beta 3 this will be I think I need to multiply or divide this equation by C p by delta H c and subtract from the other equation. If you normalize it one boundary it will be 0 the other boundary to be 1. Any other questions? Yeah.

Student: (Refer Time: 32:27) from the (Refer Time: 32:29) beta.

See, I will show you in just a minute. Anyway, we are discussing that in some detail, but I will quickly tell you. So, you have one equation for the conserved scalar. This is the equation that you will solve for getting the conserved scalar as a function of space, Z equals 1, Z equals 0 at oxidizer boundary, Z equals 1 at the fuel boundary, ok. And the definition of Z is. As you can see from this equation that Z and Y F are linearly related, right.

So, this will how this is how the solution for Z versus F will look Z is 0, Z is 1, ok. And this is a fuel boundary, so the mass fraction of the fuel here will be 1, ok. This is the oxidizer boundary, here the mass fraction for the oxidizer will be 1, ok. And the flame will sit exactly at the point where the value of Z is equal to the stoichiometry which we saw for methane here is 0.055. And now between these two limits Z is linearly related to F, Y F, ok.

And also remember that we are assuming that the reactions are infinitely fast; that means, there is no oxidizer on the right side of Z equals Z st. There is no fuel on the left side of Z equals Z st. So, the oxidizer mass fraction here is 0. The fuel mass fraction here is 0 and then the rest of the domain it should change linearly with Z. So, this is how Y F will change with Z. This is how Y ox will change with Z, ok.

On the right side of Z equals Z st there is no oxidizer, ok. So, all this term will drop out and there is no fuel on the other side. Using this fact you can deduce that this will be a linear function of, ok. Temperature will look like this. By manipulating the scalar you can also show that this temperature is equal to the adiabatic fuel, ok. And this is how you calculate the mass fractions and temperature from the conserved scalars, ok.

We will see this again when we discuss the turbulent diffusion fuel, ok.