Fundamentals of Combustion

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Lecture - 28

Governing Equations for Reacting Flow – Part 5

Conserved Scalars and Mixture Fraction Approach

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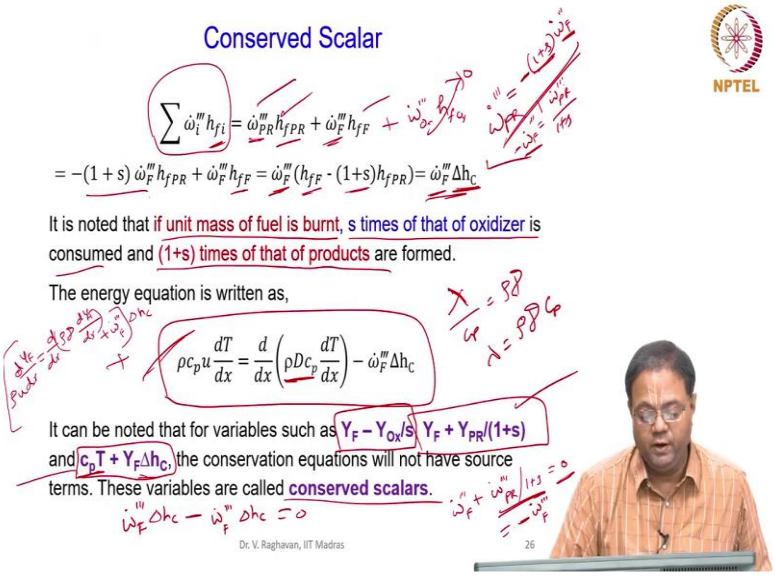

Conserved Scalar

$$\sum \dot{\omega}_i''' h_{fi} = \dot{\omega}_{PR}''' h_{fPR} + \dot{\omega}_F''' h_{fF} + \dot{\omega}_{Ox}''' h_{fOx} \rightarrow 0$$

$$= -(1+s)\,\dot{\omega}_F''' h_{fPR} + \dot{\omega}_F''' h_{fF} = \dot{\omega}_F'''(h_{fF} - (1+s)h_{fPR}) = \dot{\omega}_F''' \Delta h_C$$

$$\dot{\omega}_{PR}''' = -(1+s)\dot{\omega}_F'''$$

$$-\dot{\omega}_F''' = \frac{\dot{\omega}_{PR}'''}{1+s}$$

It is noted that if unit mass of fuel is burnt, s times of that of oxidizer is consumed and (1+s) times of that of products are formed.

The energy equation is written as,

$$\rho c_p u \frac{dT}{dx} = \frac{d}{dx}\left(\rho D c_p \frac{dT}{dx}\right) - \dot{\omega}_F''' \Delta h_C$$

$$\rho u \frac{dY_F}{dx} = \frac{d}{dx}\left(\rho D \frac{dY_F}{dx}\right) + \dot{\omega}_F''' \Delta h_c$$

$$\frac{\lambda}{c_p} = \rho D \qquad \lambda = \rho D c_p$$

It can be noted that for variables such as $Y_F - Y_{Ox}/s$, $Y_F + Y_{PR}/(1+s)$ and $c_pT + Y_F\Delta h_C$, the conservation equations will not have source terms. These variables are called conserved scalars.

$$\dot{\omega}_F''' \Delta h_c - \dot{\omega}_F''' \Delta h_c = 0$$

$$\dot{\omega}_F''' + \dot{\omega}_{PR}'''/1+s = 0$$

$$= -\dot{\omega}_F'''$$

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$$\sum \dot{\omega}_i''' h_{fi} = \dot{\omega}_{PR}''' h_{fPR} + \dot{\omega}_F''' h_{fF}$$

$$= -(1+s)\dot{\omega}_F''' h_{fPR} + \dot{\omega}_F''' h_{fF} = \dot{\omega}'''(h_{fF} - (1+s)h_{fPR}) = \dot{\omega}_F''' \Delta h_c$$

Let us do this. So, $\sum \dot{\omega}_i''' h_{fi}$ will be equal to now you expand this product $\sum \dot{\omega}_{PR}''' h_{fPR}$. So, product CO_2 and H_2O they have heat of formation so, nonzero. That into the rate at which products are produced.

Similarly, fuel has heat of formation which is nonzero that into rate at which fuel is consumed. So, that you have to add, but I should actually add $\sum \dot{\omega}_{Ox}''' h_{fOx}$, but this is 0 $h_{f,Ox}$ is 0, so, I need not add that. These are the two terms which will result from this summation.

Now, you can see that the rate at which products are produced is $\dot{\omega}_{PR}'''$. What that will be equal to? That is equal to this.

So, we can say $\dot{\omega}'''_{PR} = -(1+s)\dot{\omega}'''_F$, when 1 kg of fuel is consumed, 1 + s kg of products is formed, because 1 kg of fuel reacts with s kg of oxidizer to form 1 + s kg of products.

Now, here 1 kg of fuel is consumed. So, I have put negative sign here into 1 + s that will be the rate at which the products are formed. So, now, this $\dot{\omega}'''_{PR}$ is written as minus (1+ s) $\dot{\omega}'''_F$ + $\dot{\omega}'''_F h_{fF}$. So, taking the $\dot{\omega}'''_F$ outside, we get $h_{fF} - (1+s)h_{fPR}$, this is the heat of combustion Δh_C.

So, $\dot{\omega}'''_F \Delta h_c = \sum \dot{\omega}'''_i h_{fi}$. So, that will be this heat of combustion times the rate at which fuel is consumed.

So, that is this term. Now, if I do this then, why I am arriving at this? Because I invoke this when unit mass of fuel is burnt s times of that of oxidizer is consumed and 1 + s times of that of products is formed. That is the criteria used.

Now, write the energy equation in this way that is $\rho c_p u dT/dx$ convective term equal to $d(\rho D c_p)/dx$. So, $\lambda/c_p = \rho D$; so, $\lambda = \rho D c_p$.

$$\rho c_p u \frac{dT}{dx} = \frac{d}{dx}\left(\rho D c_p \frac{dT}{dx}\right) - \dot{\omega}'''_F \Delta h_c$$

So, that is what I have written here $\rho D c_p dT/dx$ minus this. So, this I have to minus this summation term will be equal to this term. So, I am just substituting here this. So, this is the energy equation. So, we have three equations for the species conservation, any two you can use.

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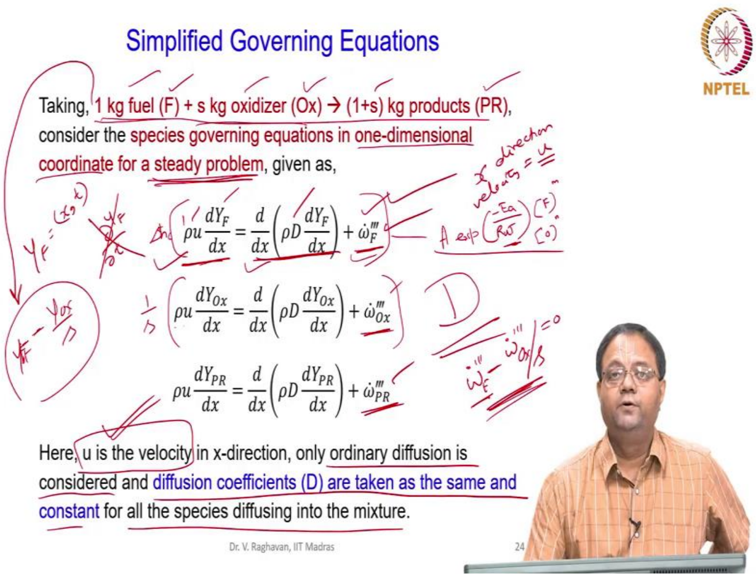

Simplified Governing Equations

Taking, 1 kg fuel (F) + s kg oxidizer (Ox) → (1+s) kg products (PR), consider the species governing equations in one-dimensional coordinate for a steady problem, given as,

$$\rho u \frac{dY_F}{dx} = \frac{d}{dx}\left(\rho D \frac{dY_F}{dx}\right) + \dot{\omega}'''_F$$

$$\rho u \frac{dY_{Ox}}{dx} = \frac{d}{dx}\left(\rho D \frac{dY_{Ox}}{dx}\right) + \dot{\omega}'''_{Ox}$$

$$\rho u \frac{dY_{PR}}{dx} = \frac{d}{dx}\left(\rho D \frac{dY_{PR}}{dx}\right) + \dot{\omega}'''_{PR}$$

Here, u is the velocity in x-direction, only ordinary diffusion is considered and diffusion coefficients (D) are taken as the same and constant for all the species diffusing into the mixture.

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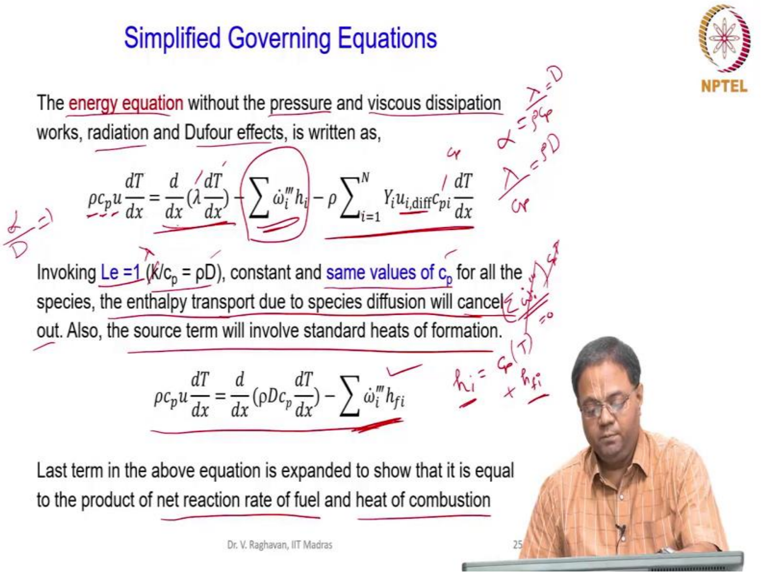

Simplified Governing Equations

The energy equation without the pressure and viscous dissipation works, radiation and Dufour effects, is written as,

$$\rho c_p u \frac{dT}{dx} = \frac{d}{dx}\left(\lambda \frac{dT}{dx}\right) - \sum \dot{\omega}_i''' h_i - \rho \sum_{i=1}^{N} Y_i u_{i,\mathrm{diff}} c_{pi} \frac{dT}{dx}$$

Invoking Le =1 ($k/c_p = \rho D$), constant and same values of c_p for all the species, the enthalpy transport due to species diffusion will cancel out. Also, the source term will involve standard heats of formation.

$$\rho c_p u \frac{dT}{dx} = \frac{d}{dx}\left(\rho D c_p \frac{dT}{dx}\right) - \sum \dot{\omega}_i''' h_{fi}$$

Last term in the above equation is expanded to show that it is equal to the product of net reaction rate of fuel and heat of combustion

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So, this three out of this any two can be used here. So, now, this plus energy conservation is this equation. Now, please understand that how will you now eliminate the source terms. How will you do that? So, if you consider variable like this Y_F - Y_{Ox}/s.

So, now what I do is I take this equation and will multiply by 1/s. The second equation I will multiply this by 1/s. First equation is Y_F this equation I will not do anything, this minus 1/s times this, then I can write the transport equation as this. The left hand side will be ρu for that combined equation, $\rho u d(Y_F - Y_{Ox}/s)/dx = d(\rho D d(Y_F - Y_{Ox}/s)/dx)/dx$.

So, these two terms no problem. So, that variable come, but now the source term will transform as $\dot{\omega}_F''' - \dot{\omega}_{Ox}''' / s$. Now, you understand that this is the equation, 1 kg of fuel + s kg of oxidizer will form 1 + s kg; that means, if 1 kg of fuel is consumed s kg of oxidizer will consume.

So, that means, if I write $\dot{\omega}_F''' - \dot{\omega}_{Ox}''' / s$, this will be equal to 0. So, that means, when I combine the variable as Y_F - Y_{Ox}/s, the source term in that equation vanishes. When you substitute for Y_F, Y_F - Y_{Ox}/s, you will get this source term $\dot{\omega}_F''' - \dot{\omega}_{Ox}''' / s = 0$; that means, the source term goes to 0.

So, Y_F is not a conserved scalar, Y_{Ox} is not conserved scalar, but combination of these two Y_F - Y_{Ox}/s defined for this equation will be a conserved scalar because the rate at which fuel is consumed will be the rate at which oxidizer is consumed divided by its mass s.

So, when you subtract these two it will become 0. Similar way we have written here in this the rate at which product is formed is nothing but the rate at which fuel is consumed multiplied by the mass of the products or we can write the this as $-\dot{\omega}_F''' = \dot{\omega}_{PR}''' / (1+s)$.

So, because of this statement, this is single step chemistry. So, we can see this is a conserved scalar now because no source term. Similarly, if you write $Y_F + Y_{PR}/(1 + s)$ as I told you $\dot{\omega}_F''' + \dot{\omega}_{PR}''' / (1+s) = 0$. Because this is the relationship here.

So, $-\dot{\omega}_{PR}''' / (1+s) = \dot{\omega}_F'''$. So, this will be equal to $-\dot{\omega}_F'''$. So, this will cancel out and become 0.

So, this is a scalar which is conserved because there is no source term. Similarly, you can combine one of the mass fraction say Y_F and multiply that equation Y_F conservation equation with Δh_C. So, here this term $\rho u Y_F \Delta h_C$. This entire equation I multiplied Δh_C and this is added to the this energy equation.

So, I have $\rho u dY_F/dx$ equal to so, totally this equation now it will be equal to $d(\rho D dY_F)/dx$ + $\dot{\omega}_F'''$. So, this I will multiply by Δh_C and add to this. I am adding these two. I will get a source term for this as $\dot{\omega}_F''' \Delta h_C$ from this equation and $-\dot{\omega}_F''' \Delta h_C$ from this equation which will equal 0. So, this $c_pT + Y_F\Delta h_C$ again becomes the conserved scalar because the source term cancels out. So, these are the way we define a conserved scalar.

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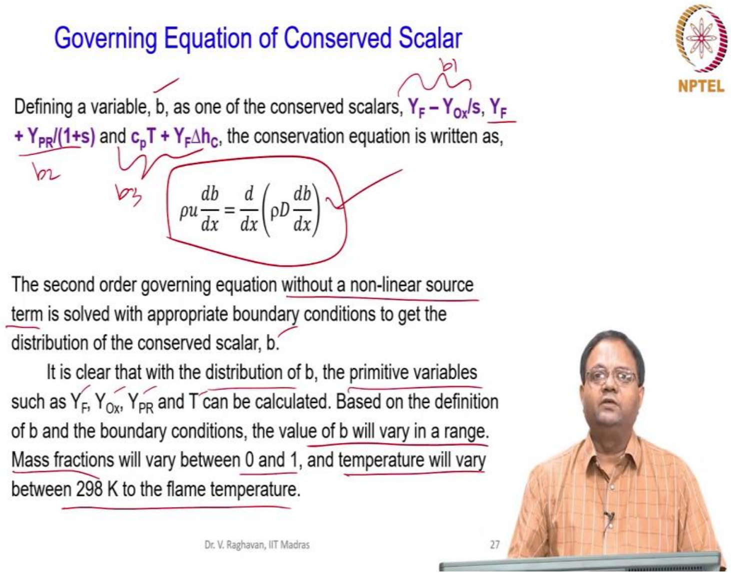

Governing Equation of Conserved Scalar

Defining a variable, b, as one of the conserved scalars, $Y_F - Y_{Ox}/s$, $Y_F + Y_{PR}/(1+s)$ and $c_pT + Y_F\Delta h_C$, the conservation equation is written as,

$$\rho u \frac{db}{dx} = \frac{d}{dx}\left(\rho D \frac{db}{dx}\right)$$

The second order governing equation without a non-linear source term is solved with appropriate boundary conditions to get the distribution of the conserved scalar, b.

It is clear that with the distribution of b, the primitive variables such as Y_F, Y_{Ox}, Y_{PR} and T can be calculated. Based on the definition of b and the boundary conditions, the value of b will vary in a range. Mass fractions will vary between 0 and 1, and temperature will vary between 298 K to the flame temperature.

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When I say I define these three variables as a b variable.

So, let us say $b = Y_F - Y_{Ox}/s$ or $b = Y_F + Y_{PR}/(1+s)$ or $b = c_pT + Y_F\Delta h_C$, then I will have the equation for b only as this without the source term $\rho u db/dx = d(\rho D db/dx)/dx$.

So, the second order governing equation without non-linear source term is solved with appropriate boundary conditions and you can get. So, define b as one of these variables calculate this and give get a reference for b.

Similarly, define b as another variable and get so, once you solve for this and this and this all the three you can retrieve back the b. So, by the distribution of b we can retrieve back the primitive variables which are Y_F, Y_{Ox}, Y_{PR} and T.

The advantage of this is we do not need to solve this using a source term, there is no source term here. So, that is the advantage of this. Even though I simplify the equations like this here the complexity has not reduced because of the presence of the source terms non-linear source terms but by defining a variable like conserved scalars I get a equation without non-linear source term I can solve it easily.

So, I can do this and solve for say let me let take this, this will be b_1 I can call so, this is b_1 and this second will be called b_2 and third will be called b_3 and I solve for b_1, b_2, b_3 then I can retrieve back these variables, but solve it by appropriate boundary conditions.

So, b_1 will have a boundary condition based upon fuel and oxidizers mass fractions; similarly, b_3 will have temperature based boundary conditions also in addition. So, based on that, you can solve this.

Now, here you can see that the b will vary in a range mass fractions normally it will vary in a range. For example, the first two if you use it will vary in range of say 0 to 1, but if you take b_3 it will vary from say 298 K to the flame temperature. So, we can see that tremendous amount of variation is there.

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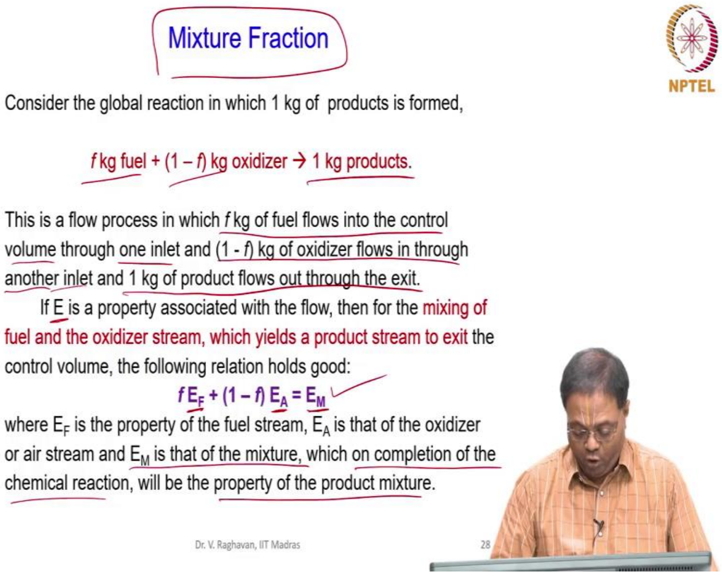

Mixture Fraction

Consider the global reaction in which 1 kg of products is formed,

f kg fuel + (1 – f) kg oxidizer → 1 kg products.

This is a flow process in which f kg of fuel flows into the control volume through one inlet and (1 - f) kg of oxidizer flows in through another inlet and 1 kg of product flows out through the exit.

If E is a property associated with the flow, then for the mixing of fuel and the oxidizer stream, which yields a product stream to exit the control volume, the following relation holds good:

$$f E_F + (1 - f) E_A = E_M$$

where E_F is the property of the fuel stream, E_A is that of the oxidizer or air stream and E_M is that of the mixture, which on completion of the chemical reaction, will be the property of the product mixture.

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So, is there any way to normalize this that is what we are trying to do here by defining what is called a mixture fraction? When I define a mixture fraction what I assume is let us see this. So, I want 1 kg of products. So, some fraction of fuel, fraction of 1 kg I burnt, f kg of fuel, then 1 - f is the stoichiometric air required for this.

So, 1 - f kg of oxidizer you know, 1 kg of product. So, that is the equation I consider for example, but we can see that there is a flow process where f kg of fuel flows into the control volume through one of the inlet then 1 - f kg of oxidizer flows in through another inlet and finally, 1 kg of products are formed and they exit through another exit port.

So, now any extensive property, E, I will take or it may be a specific property also. So, I take any property associated with the flow and what I do is I can write this.

$$f\, E_F + (1 – f)\, E_A = E_M$$

f times $E_F + (1 – f)\, E_A = E_M$. What is this? This is the property's value E_F is the property value at the fuel stream. Similarly, E_A is the property value at the air side or the oxidizer side.

Similarly, I say mixture which is the product finally. So, E_M is the property of the mixture or when complete reaction is finished it will be the property of the product. So, this equation holds good.

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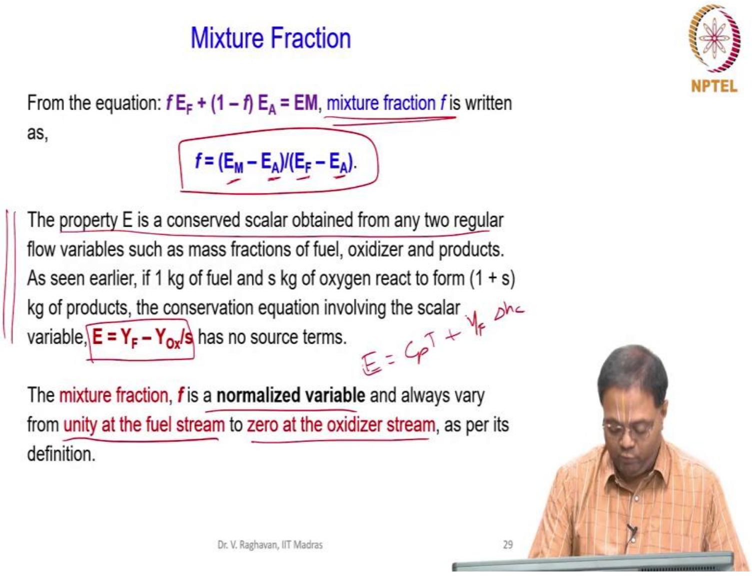

Mixture Fraction

From the equation: $f\, E_F + (1 – f)\, E_A = EM$, mixture fraction f is written as,

$$\boxed{f = (E_M – E_A)/(E_F – E_A).}$$

The property E is a conserved scalar obtained from any two regular flow variables such as mass fractions of fuel, oxidizer and products. As seen earlier, if 1 kg of fuel and s kg of oxygen react to form (1 + s) kg of products, the conservation equation involving the scalar variable, $\boxed{E = Y_F – Y_{Ox}/s}$ has no source terms.

$E = C_pT + Y_F\, \Delta h_c$

The mixture fraction, f is a **normalized variable** and always vary from unity at the fuel stream to zero at the oxidizer stream, as per its definition.

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Now, based upon this equation I define f as property at the mixture stream minus property at the air side or the oxidizer side divided by property at the fuel side minus property at the oxidizer side. When I do this, this I call mixture fraction do you understand?

$$f = (E_M – E_A)/(E_F – E_A).$$

So, now the property can be anything as I told you I can have property, the property is a conserved scalar. So, that is what I have already defined, conserved scalar. So, let us take property as Y_F - Y_{Ox}/s, one of the conserved scalar I have and I can write also C_p. So, E can be also $C_pT + Y_F\Delta h_C$. So, this can also be called. So, here what we defined in this here. So, this can also be one of the E values, property values.

So, when you use this then you can see that f is a normalized variable that will vary from one at the fuel stream and it goes to 0 at the oxidizer stream. So, that is the definition of mixture fraction. Now, based upon this any variable we can take.

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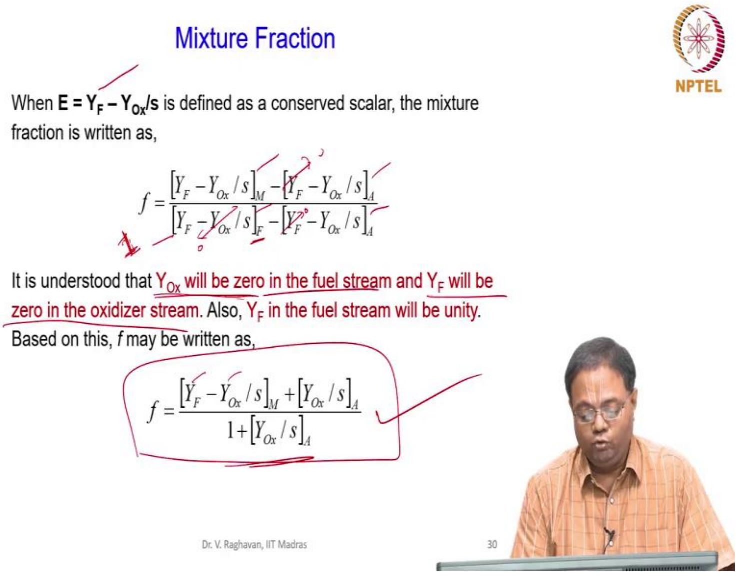

Mixture Fraction

When **E = $Y_F - Y_{Ox}/s$** is defined as a conserved scalar, the mixture fraction is written as,

$$f = \frac{[Y_F - Y_{Ox}/s]_M - [Y_F - Y_{Ox}/s]_A}{[Y_F - Y_{Ox}/s]_F - [Y_F - Y_{Ox}/s]_A}$$

It is understood that Y_{Ox} will be zero in the fuel stream and Y_F will be zero in the oxidizer stream. Also, Y_F in the fuel stream will be unity.

Based on this, *f* may be written as,

$$f = \frac{[Y_F - Y_{Ox}/s]_M + [Y_{Ox}/s]_A}{1 + [Y_{Ox}/s]_A}$$

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Now, I can write, let us take this for example, Y_F - Y_{Ox}/s then f can be defined as what Y_F - Y_{Ox}/s at the mixture stream minus the same quantity at the oxidizer stream divided by the difference between Y_F - Y_{Ox}/s at the fuel stream minus that of the oxidizer stream. So, this will be the mixture fraction.

$$f = \frac{[Y_F - Y_{Ox}/s]_M - [Y_F - Y_{Ox}/s]_A}{[Y_F - Y_{Ox}/s]_F - [Y_F - Y_{Ox}/s]_A}$$

But, you know that at fuel stream let us take fuel stream, $Y_{Ox} = 0$ at the fuel stream. So, if complete combustion takes place Y_F and Y_{Ox} will be consumed, but let us just take this. Similarly, since fuel is supplied through a particular inlet and oxidizer is supplied through a separate inlet. So, $Y_{Ox} = 0$ at the fuel stream; similarly, $Y_F = 0$ in the oxidizer stream that is for sure.

So, when you say the oxidizer stream, this will be zero, here this also will be 0. But, in the fuel stream this will be zero, that is it. Now, what will be the value of Y_F in the fuel stream? This will be equal to 1 only fuel is coming out of this. So, this will be equal to 1.

So, I can write this as 1 + Y_{Ox}/s in the denominator and in the numerator Y_F I am eliminating and in the mixture I have both Y_F and Y_{Ox}. That means that in the mixture until the complete combustion takes place there will be some amount of fuel and oxidizer. So, this will be the mixture fraction in the mixture and this is the definition of mixture fraction.

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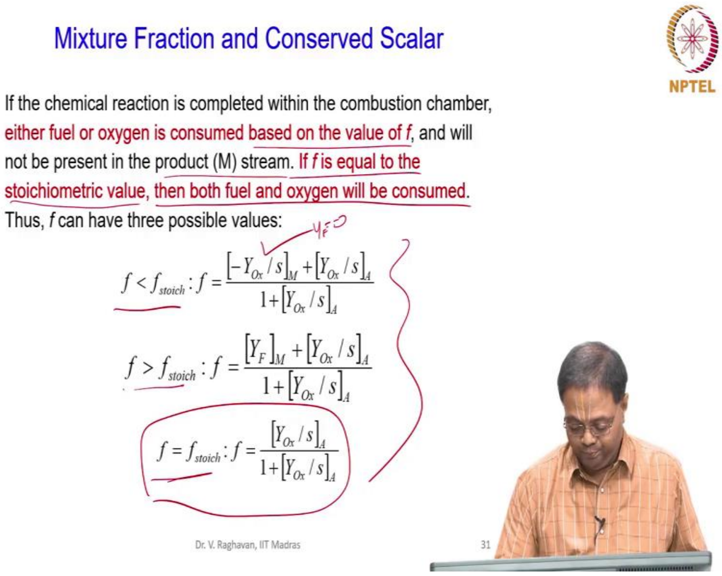

Mixture Fraction and Conserved Scalar

If the chemical reaction is completed within the combustion chamber, either fuel or oxygen is consumed based on the value of *f*, and will not be present in the product (M) stream. If *f* is equal to the stoichiometric value, then both fuel and oxygen will be consumed.

Thus, *f* can have three possible values:

$Y_F = 0$

$$f < f_{stoich} : f = \frac{\left[-Y_{Ox}/s\right]_M + \left[Y_{Ox}/s\right]_A}{1+\left[Y_{Ox}/s\right]_A}$$

$$f > f_{stoich} : f = \frac{\left[Y_F\right]_M + \left[Y_{Ox}/s\right]_A}{1+\left[Y_{Ox}/s\right]_A}$$

$$f = f_{stoich} : f = \frac{\left[Y_{Ox}/s\right]_A}{1+\left[Y_{Ox}/s\right]_A}$$

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Now, if chemical reaction is completed either fuel or oxygen is consumed based upon the value of s, f and will not be present in the mixture. So, for example, chemical reaction is incomplete; that means, if insufficient oxygen is there and that is consumed. Excess fuel will be there in the product. If excess oxygen is supplied and fuel is consumed, then oxygen excess oxygen will be there in the product.

Now, if at some location say for example, if there is excess oxygen supplied, some location there will be stoichiometric combustion. If f is equal to stoichiometric value; that means, at that location there will be no fuel or oxygen, then both fuel and oxygen will be consumed. So, based upon that we have scenarios like this.

$$f = f_{stoich} : f = \frac{\left[Y_{Ox} / s\right]_A}{1+\left[Y_{Ox} / s\right]_A}$$

So, let us say the value is stoichiometric. For example, here also see here this is the stoichiometric value. Let us take that first. When I say f equal to, for this definition of f when I say f = f_{stoich}; that means, I should not have any fuel or oxidizer in the mixture. So, that means, see here $Y_F = 0$, $Y_O = 0$.

So, this term will go out and stoichiometric value of f will be the oxidizer side Y_{Ox}/s at the oxidizer stream divided by 1 that is the fuel mass fraction at the fuel stream + Y_{Ox}/s at the oxidizer stream. This will be the stoichiometric f value, by this definition what we have done here.

So, this is the stoichiometric, but if there are two conditions now: if f is less than stoichiometric what will be the mixture. This f is less than stoichiometric, then what happens? Fuel will not be there in the mixture.

$$f < f_{stoich} : f = \frac{\left[-Y_{Ox} / s\right]_M + \left[Y_{Ox} / s\right]_A}{1 + \left[Y_{Ox} / s\right]_A}$$

So, other terms will be the same, the fuel will be consumed here. So, fuel $Y_F = 0$, you can note that $Y_F = 0$ here. So, you have to put $Y_F = 0$ in this and write that situation. So, $f < f_{stoich}$. So, f will be defined as putting $Y_F = 0$ in the product mixture.

Similarly, when f is greater than f stoichiometric, then oxygen will not be there, fuel rich mixture.

$$f > f_{stoich} : f = \frac{\left[Y_F\right]_M + \left[Y_{Ox} / s\right]_A}{1 + \left[Y_{Ox} / s\right]_A}$$

So, Y_F will be there, oxygen will go to 0 in the product. So, this will be the definition. Now I only trace the mixture fraction values and get these values. We can retrieve the value of Y_F, Y_{Ox} etcetera just by solving the mixture fraction alone that is the advantage of defining the mixture fraction.

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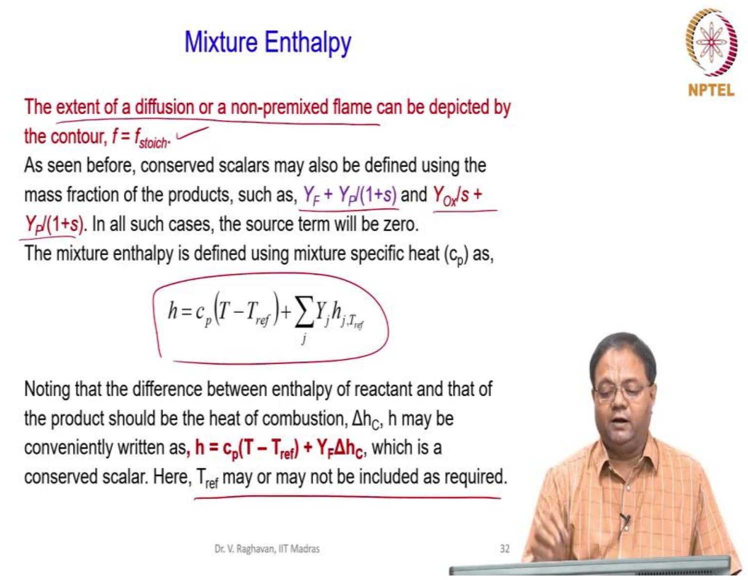

Mixture Enthalpy

The extent of a diffusion or a non-premixed flame can be depicted by the contour, $f = f_{stoich}$.

As seen before, conserved scalars may also be defined using the mass fraction of the products, such as, $Y_F + Y_P/(1+s)$ and $Y_{Ox}/s + Y_P/(1+s)$. In all such cases, the source term will be zero.

The mixture enthalpy is defined using mixture specific heat (c_p) as,

$$h = c_p\left(T - T_{ref}\right) + \sum_j Y_j h_{j,T_{ref}}$$

Noting that the difference between enthalpy of reactant and that of the product should be the heat of combustion, Δh_C, h may be conveniently written as, $h = c_p(T - T_{ref}) + Y_F \Delta h_C$, which is a conserved scalar. Here, T_{ref} may or may not be included as required.

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Now, once I know, I do not need chemical kinetics as I told. So, the extent of diffusion or non-premixed flame is depicted by the contour of $f = f_{stoich}$. When I note the points where f = f_{stoich} and connect them then I get the flame shape. So, that is the location at which the reaction takes place.

So, several conserved scalars like $Y_F + Y_{PR}/(1 + s)$ or $Y_{Ox}/s + Y_{PR}/(1 + s)$ anything can be used here. Similarly, this h also defined like this, say I can either use T_{ref}. T_{ref} may or may not be used here. I can say just $c_pT + Y_F\Delta h_C$ or if you want you can add reference temperature $T - T_{ref}$ plus this anything can be done.

$$h = c_p\left(T - T_{ref}\right) + \sum_j Y_j h_{j,T}$$

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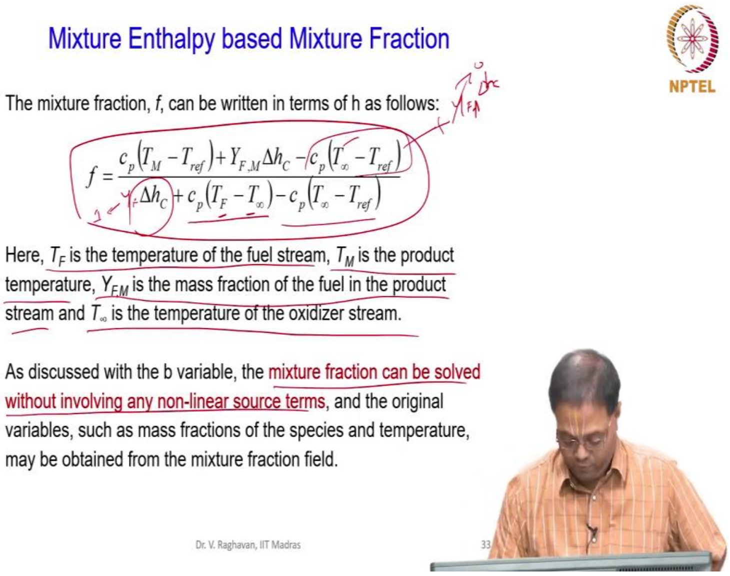

Mixture Enthalpy based Mixture Fraction

The mixture fraction, *f*, can be written in terms of h as follows:

$$f = \frac{c_p\left(T_M - T_{ref}\right) + Y_{F,M}\Delta h_C - c_p\left(T_\infty - T_{ref}\right)}{\Delta h_C + c_p\left(T_F - T_\infty\right) - c_p\left(T_\infty - T_{ref}\right)}$$

Here, T_F is the temperature of the fuel stream, T_M is the product temperature, $Y_{F,M}$ is the mass fraction of the fuel in the product stream and T_∞ is the temperature of the oxidizer stream.

As discussed with the b variable, the mixture fraction can be solved without involving any non-linear source terms, and the original variables, such as mass fractions of the species and temperature, may be obtained from the mixture fraction field.

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So, now if you use this then you will get another equation based upon the f. So, for example, when I write the enthalpy $c_p\Delta T + Y_F\Delta h_c$. Now, we can say that T_{ref} can be 0 also. Reference number can be 0 also 0 K.

So, in that case I write the f like this. So, we can see this when I say M this is the mixture.

$$f = \frac{c_p\left(T_M - T_{ref}\right) + Y_{F,M}\Delta h_C - c_p\left(T_\infty - T_{ref}\right)}{\Delta h_C + c_p\left(T_F - T_\infty\right) - c_p\left(T_\infty - T_{ref}\right)}$$

So, mixture temperature $c_p(T_M - T_{ref}) + Y_{F,M}\Delta h_C - c_p(T_\infty - T_{ref})$, there $Y_F = 0$ and this is air side. So, $Y_F = 0$ here. So, we can actually write $Y_F\Delta h_C$ at the oxygen side which is equal to 0 or this is air side, but this is equal to 0. So, I do not include that.

Similarly, in this term you can see the c_pT_F T of fuel here this capital F is fuel $T_F - T_\infty + Y_F\Delta h_c$, this $Y_F = 1$ here in the fuel stream and in the oxidizer stream again the same term appears here because $Y_F = 0$ there. So, this will be the definition of mixture fraction.

So, this conservation, I have same conservation like b variable I can write a variable and solve for mixture fraction which will not have any source term. So, as I wrote the equation here for b, instead of b you substitute f here. So, that will be the conservation equation for the mixture fraction, solve that.

Once you solve that, then you can retrieve the original variables. So, you can see that this T_∞ is the air temperature, I have given everything. So, T_M is the product temperature, Y_{FM} is the mass fraction of the fuel in the product stream and T_∞ is the temperature of the oxidizer stream and T_F is the temperature of the fuel stream.

So, we have separate fuel stream, oxidizer stream etcetera. So, that will allow us and until the combustion is complete we will note all the values as the function of x for this one-dimensional problem the value of f and we can note exactly where the fuel and oxidizer are consumed and there we can say the flame zone is formed.

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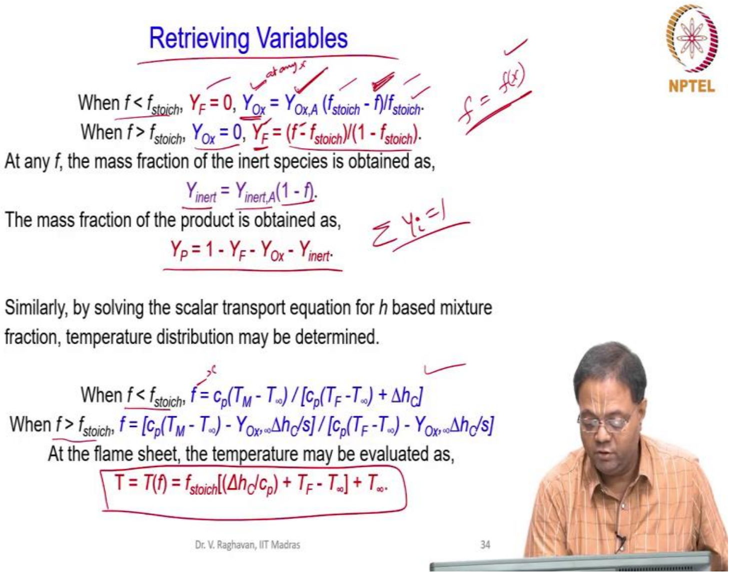

Retrieving Variables

at any x

When $f < f_{stoich}$, $Y_F = 0$, $Y_{Ox} = Y_{Ox,A}\,(f_{stoich} - f)/f_{stoich}$.

When $f > f_{stoich}$, $Y_{Ox} = 0$, $Y_F = (f - f_{stoich})/(1 - f_{stoich})$.

$f = f(x)$

At any f, the mass fraction of the inert species is obtained as,

$$Y_{inert} = Y_{inert,A}(1 - f).$$

The mass fraction of the product is obtained as,

$$Y_P = 1 - Y_F - Y_{Ox} - Y_{inert}.$$

$\Sigma Y_i = 1$

Similarly, by solving the scalar transport equation for h based mixture fraction, temperature distribution may be determined.

When $f < f_{stoich}$, $f = c_p(T_M - T_\infty) / [c_p(T_F - T_\infty) + \Delta h_C]$

When $f > f_{stoich}$, $f = [c_p(T_M - T_\infty) - Y_{Ox,\infty}\Delta h_C/s] / [c_p(T_F - T_\infty) - Y_{Ox,\infty}\Delta h_C/s]$

At the flame sheet, the temperature may be evaluated as,

$$\boxed{T = T(f) = f_{stoich}[(\Delta h_C/c_p) + T_F - T_\infty] + T_\infty.}$$

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Now, retrieving the variables. Once f is known as I told you when $f < f_{stoich}$, $Y_F = 0$, $Y_{Ox} = Y_{OA}$ (that is the oxidizer mass fraction at the oxidizer stream) × $f_{stoich} – f/f_{stoich}$.

So, you know the value of f as a function of x. So, that is this f. That you substitute at any location, I want value of Y_{Ox} this is at any x location I want value of Y_{Ox}. I can retrieve it by knowing the value of f at that location f(x) that f_{stoich} is known to me.

So, that Y_{Ox} at the oxidizer stream is known to me this is known f_{stoich} is known. So, when I know f(x) I will calculate $Y_{Ox}(x)$. Similarly, when $f > f_{stoich}$ then I know that $Y_{Ox} = 0$ at that location and it is the fuel side.

Y_F can be calculated as the function of x at any x as with this relationship where f is calculated as a function of x. So, once f is known as a function of x, then Y_F is calculated as a function of x, using this I will retrieve the variables.

For inert species, Y_{inert} will be equal to Y_{inert} at the oxidizer stream × (1 – f). I am assuming nitrogen for example. So, nitrogen mass fraction at the oxidizer stream × (1 – f). Similarly, products can be retrieved once you know inert then use this identity to get the product mass fractions, that is it. So, that is the way you retrieve.

Similarly, temperature, when $f < f_{stoich}$, then you see that f can be written like this. f as a function of x can be written in terms of this and you get this. Similarly, $f > f_{stoich}$ you can write this equation and get the values of T. Similarly, the flame temperature can be calculated with this equation.

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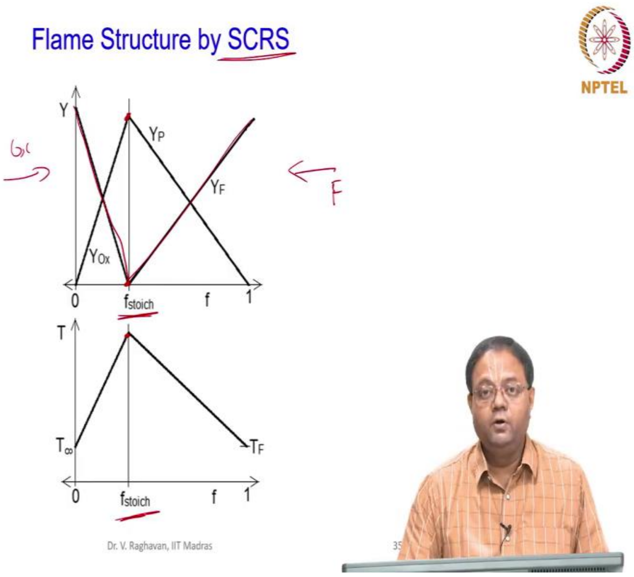

Flame Structure by SCRS

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So, now once you retrieve this, I can plot the structure. So, you can remember this I will go back to this and show this.

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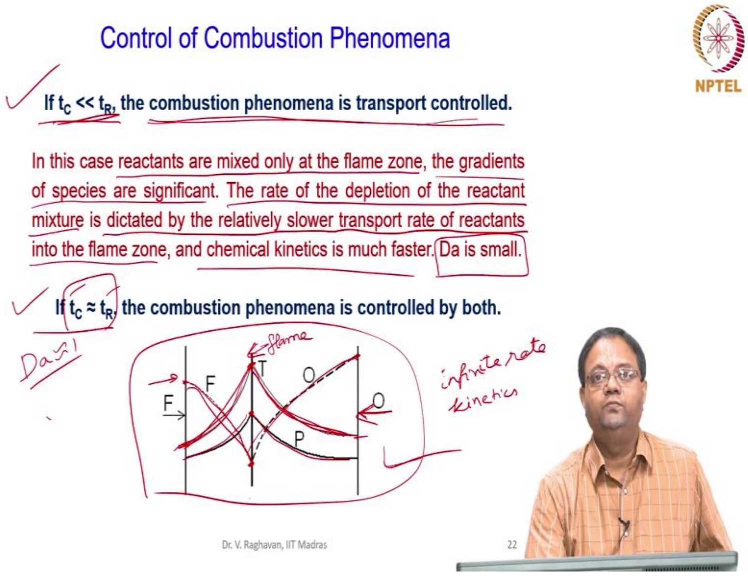

Control of Combustion Phenomena

If $t_C << t_R$, the combustion phenomena is transport controlled.

In this case reactants are mixed only at the flame zone, the gradients of species are significant. The rate of the depletion of the reactant mixture is dictated by the relatively slower transport rate of reactants into the flame zone, and chemical kinetics is much faster. Da is small.

If $t_C \approx t_R$, the combustion phenomena is controlled by both.

You can see the gradient. So, the temperature varies like this. This is the flame sheet, this is fuel side, oxidizer side and flame is formed and you can see the depletion of fuel, depletion of oxidizer, maximum temperature formed at the flame zone and decreases towards the fuel side and the oxidizer side.

So, this is the structure of the diffusion flame which we get in the final slide you can see here. Now, fuel is depleted, the oxidizer this is the oxidizer side and this is the fuel side. So, fuel is depleted here to 0, where the flame is formed or the maximum products are formed. Similarly, oxidizer is depleted from the oxidizer side to 0 and they react to form the products; products go to both the sides.

Similarly, temperature reaches maximum at the stoichiometric value F stoichiometric. You get a linear variation only here because already we have linearized the problem. We have removed the sources. In practice, actually I will get some non-linear variation as I have shown here. Schematically I have shown here, non-linear variation will be seen.

But, it is fine. Actually it is not so non-linear. So, here at least we get the location of flame properly and the distribution of the species mass fractions and temperature. So, this simple chemically reacting system will be very useful to analyze the diffusion flame. So, from this I will stop the equations, governing equations for the reactive flow.