

Indian Institute of Technology Madras

NPTEL

National Programme on Technology Enhanced Learning

COMBUSTION

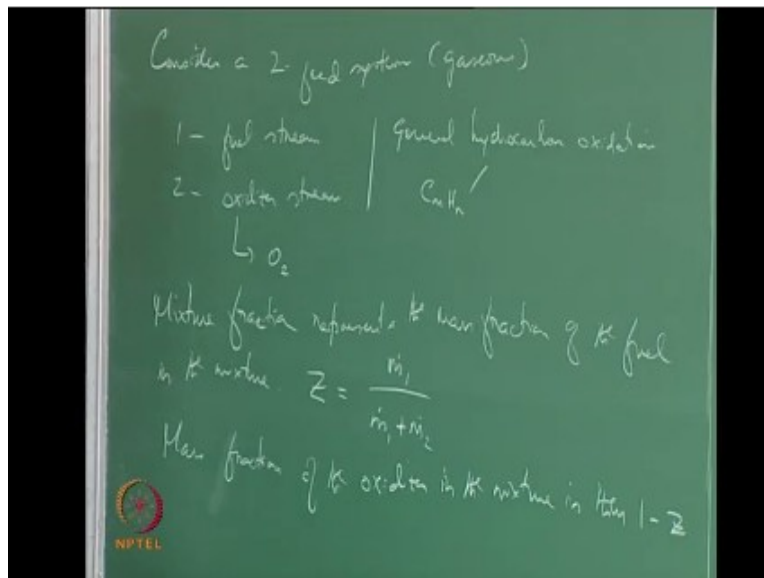
Lecture 41

Mixture Fraction Formulation

Prof. S R Chakravarthy

Dept. of Aerospace Engineering IIT Madras

(Refer Slide Time: 00:09)



We will adopt what is called as the mixed refraction formulation in trying to describe diffusion flames this is actually a powerful idea for combustion in general and with particular context of diffusion flames and partially pre-mixed flame. So the idea basically is we now try to define this variable called the mixed refraction mixed refraction, extremely useful then in diffusion flames and partially pre-mixed flames. So what we will do is let us consider a to feed system that means we have 2 inlets that are allowing gases to come, so we are looking at a homogeneous gaseous system.

And let us say that 1 represents fuel stream and 2 represents oxidizer stream, in fact we will try to adopt this for a general hydrocarbon, fuel hydrocarbon oxidation that means from now say oxidizer we will mainly be thinking about Houghton and for the fuel we might mainly be thinking about a C_n H_n kind of hydrocarbon right.

(Refer Slide Time: 02:24)

Mixture Fraction Formulation

Mixture fraction variable Z is extremely helpful in diffusion flames and partially premixed flames. Consider two stream: 1 - fuel stream, 2 - oxidizer stream

- Z represents mass fraction of fuel in the mixture: $Z = \frac{\dot{m}_f}{\dot{m}_f + \dot{m}_o}$. Then mass fraction of oxidizer = $1 - Z$.
- The mass fraction of unburned fuel in the mixture with other diluents would be: $Y_{F,u} = ZY_{F,1}$. Here, $Y_{F,1}$ is the mass fraction of fuel in stream 1. Similarly, for oxidizer, $Y_{O_2,u} = (1 - Z)Y_{O_2,2}$, where, $Y_{O_2,2}$ is the mass fraction of oxidizer in stream 2.
- Consider a single component general hydrocarbon fuel reaction:

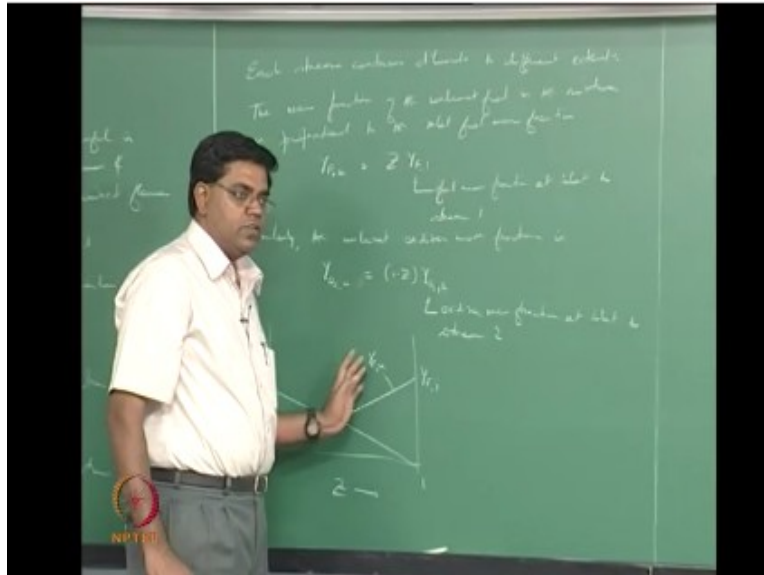
$$\nu'_F C_m H_n + \nu'_{O_2} O_2 \rightarrow \nu''_{CO_2} CO_2 + \nu''_{H_2O} H_2O$$
- At stoichiometric surface,

$$\left. \frac{n_{O_2,u}}{n_{F,u}} \right|_{St} = \frac{\nu'_{O_2}}{\nu'_F} \quad \text{or} \quad \left. \frac{Y_{O_2,u}}{Y_{F,u}} \right|_{St} = \frac{\nu'_{O_2} W_{O_2}}{\nu'_F W_F} = \nu$$

So then the way the mixed refraction is defined is essentially like a mass fraction okay, so the mixed refraction next refraction, represents the mass fraction mass fraction of the fuel in the mixture fuel in the mixture right. That means let us say Z is the symbol given to a mixer fraction then this is basically $m.1 / m.1 + m. 2$ where $m.1$ is the mass flux of or the mass flow rate of the fuel stream $m.1$ is $1\lambda 2$ is the mass flow rate of the oxidizer screen and of course what this means is the mass fraction of the oxidizer then is oxidizer in the mixture is then when it alright.

It would be defined as $m2. / m1. + m2$ that therefore is $1 - Z$, now each stream contains diluents it's not as if like the fuel stream is fully fuel it could have some nitrogen, you could also have the oxidizer stream is like a let us say air and most of it is nitrogen.

(Refer Slide Time: 04:33)



So you have only part of it as oxygen so contains diluents different extents right then what you are looking at is the mass fraction of the unburned fuel in the mixture, what we expect is it should be proportional to the inlet mass fraction of the fuel in the fuel stream times the mixed fraction. So the mixed refraction is a fraction of fuel when compared to the total, so the mass fraction of the unburned fuel in the mixture is proportional to the inlet fuel mass fraction, so that is to say $Y_{f,u}$ that is the unburned fuel mass fraction anywhere in the mixture can then be written as $Z Y_{f,1}$.

So why I have come up 1 is essentially the mass fraction film mass fraction at in at the inlet to stream 1 right, now previously we were using the symbol Y if not for this purpose the corresponding oxidizer would be Y_{O} not well this allows for us to actually think about a $Y_{f,2}$ which means you could also dope some fuel into the oxidizer stream and vice versa alright. So this notation somewhat is a little bit more general of course it is not too general it is still confining ourselves to 2 streams alright.

But we could say $Y_{f,1}$ $Y_{f,2}$ $Y_{f,3}$ and so on so this is a little bit more general notation then and similarly the unburnt the oxidizer mass fraction the unburned oxidizer mass fraction is $Y_{O,u}$

is $= 1 - Z$ times c_{O_2} right. So Y_{O_2} is actually the oxidizer mass fraction at inlet to stream 2, so for example if it were air this number would be like point 2 three or so right with this if you now think about it what happens is you unburnt fuel mass fraction or the unburned oxidizer mass fraction both vary with the mix 2 fractions are linearly okay.

Ron Awards if thought were more your y if you would be more than a place proportional to Y of 1 right if there were more Y_{O_2} unburned will be less correspondingly proportional to Y or 2, so if this is represented in a graph that could go like this, so if you now plot Z along the horizontal axis it goes from 0 to 1 so if your mixer fraction is going all the way from 0 to 1, 0 would correspond to no fuel and 1 would correspond to all fuel all right, no oxidizer.

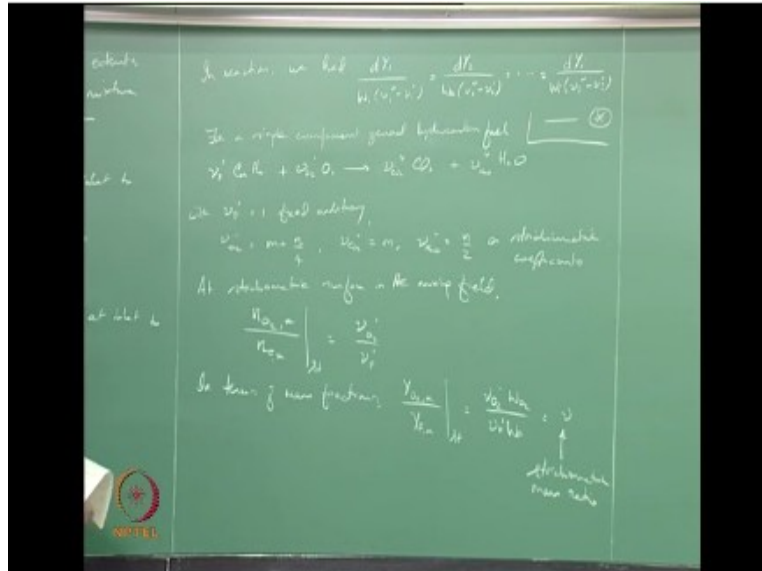
Therefore as that keeps on increasing then you have a straight line that keeps on increasing from 0 all the way to Y of 1, this is to say in the mixing field at the inlet you would have only oxidizer in the oxidizer stream and you will have no fuel at all in the you would have Y of 1 in the fuel stream and you would have no fuel in the oxidizer stream and anywhere else in the mixing field you would now have a mixed refraction which is having different values and corresponding to that the fuel mass fraction would lie on this line essentially all right.

Similarly if you want to think about how D so just this is this is the plot of Y_F , u similarly if you want to look at the plot of you to come on you that is another straight line that starts with the value of u to come on you, let us say at the oxidizer steam Inlet why you do not have any fuel and goes all the way to 0 and the fuel Inlet where you do not have any oxidizer anywhere in the mixing field your mass fraction of the oxidizer lies on this line corresponding to whatever is the mixed refraction locally right.

So this is regarding how the unburned fuel and unburned oxidizer mass fractions work out what we want to now do is to further proceed and see if we can actually get mass fractions of burnt products right and where you have burned where you are in non stoichiometric proportions you will have excess fuel and excess or excess oxidizer, depending upon which is in excess whether you're in fuel rich of your lean conditions and we would like to also find out what is the burnt fuel concentration and they burnt oxidizer concentration depending upon whether it is excess or

not. So for which we need now have to actually go through what happens when you have a reaction.

(Refer Slide Time: 11:46)



So in a reaction we had this is long ago maybe came up with this ν_1' / W_1 times $1 - \nu_1'$ single prime etc the you could also write of course $1 - \nu_1'$ more dy_2 / W_2 times μ_2 double prime - μ_2 single prime etc and the general species you could say dy_i / w_i times μ_i double prime - μ_i single prime I am sure you re call this, so let us suppose that you can call this set of equations star we will pick at least 2 of these in order to integrated at different times therein the near future.

So for a single component general hydrocarbon that is to say you do not have different mixtures of hydrocarbons for example if you take liquid petroleum gas it is actually a mixture of hydrocarbons butane and propane, so instead of that if that is supposed to be our considering only 1 hydrocarbon at a time hydrocarbon fuel and let us suppose that we write this equation as C_mH_n for the generalized hydrocarbon the P considered + μ_2 single trying o to gives $\mu_2 \text{CO}_2$ double prime, $\text{CO}_2 + \mu_2 \text{H}_2\text{O}$ double prime H_2O right.

With new $F_{single\ prime} = 1$ fixed arbitrarily let us suppose that we just say we are interested in 1 mole of this hydrocarbon right we could get new single trying $=M + n / 4$ new CO_2 double prime $=M$ and μ_{H_2O} double prime $= n / 2$ as psychometric coefficients, that means these values correspond to the reaction happening stoichiometrically right the means you do not have any of the fuel or oxidized the leftover as part of the products.

Now at the stoichiometric surface in the mixing field, we then have the number of moles of oxygen unburnt / the number of moles of fuel unburnt at stoichiometric $= \mu_{O_2\ single\ prime} / \nu_f$ single prime right as given above. So in terms of mass fractions so this is this is mole fractions so in terms of mass fractions whether bars in terms of moles not moles fractions I am sorry but of course you can divide by the total number of moles and get the mole fractions as well so here we are going to be looking at the mass fractions $Y_{O_2\ unburned} / Y_{f\ unburned}$ at stoichiometric is $\nu_{O_2\ prime} \mu_{O_2\ prime} / \nu_f \mu_{fuel\ prime} \times WF$.

Which lets us say we call as ν which is the stoichiometric mass ratio, so what we want to do is we want to see if we can integrate this equation for a situation where you have a stoichiometric reaction, so that we can we can make use of the fact that you are not going to have any of the reactants left over alright. So for a stoichiometric reaction for a stoichiometric reaction both filled and oxidized that are completely consumed right.

Therefore we use this to integrate the this equation here star at any mixture condition relative to the unburned mixture because you are not going to have any of the reactants leftover, so you can you can you can now say we integrate.

(Refer Slide Time: 18:49)

in new, we get

$$Z = \frac{vY_f - Y_{O_2} + Y_{O_{2,z}}}{vY_{f,1} + Y_{O_{2,z}}}$$

For stoichiometric mixture, $vY_f = Y_{O_2}$

⇒ the stoichiometric mass fraction is

$$Z_{st} = \left[1 + \frac{vY_{f,1}}{Y_{O_{2,z}}} \right]^{-1}$$

Start at any mixture condition that means giving a look at any intermediate mixture condition mixed condition relative to the unburnt condition right the piece the limits of integration go from unburnt values to any value, so during the reaction has $Y_{O_2} - Y_{O_2,u} / \mu - \mu_0$ right you strategic and you can just pick let us say oxidizer and fuel then you would get $Y_f / Y_{f,u}$ a few developed by new prime W_f or rearranging this all this means is new $Y_f - y \mu_2$ equals new $Y_f Y_{O_2} - u$.

So what this tells us is this is sort of a preserved quantity right you started out with unburnt values Y_{fu} and Y_{O_2} will do you at a point in the mixture mixing filled in a proportion with a new here right, where should I should I have yes new that is right he caught this μ so and that is the same even during the reaction between the 2 that is essentially the idea okay. So whatever are the unburnt values that difference is what is preserved, so what you can then do is we are interested in writing everything in terms of the mix diffraction.

So we had the Y_{fu} in terms of mixed refraction and the inlet mass fraction, so here I will do you in terms of mixed refraction and the inlet mass fraction of the oxidizer, so substituting the expressions for expressions for Y_{fu} and Y to you in terms of Z in here we get and then of course

rearrange, so you say that $= \mu \times Y_F - Y_{O_2} + y_{O_2}$, $2 / \mu Y_F$, $1 + y_{O_2}$, so you can see that you to come out to these things are showing up from the inlet mass concentrations mass fractions of the oxidizer and fuel in the respective streams.

So for stoichiometric mixture for stoichiometric mixture μF new wire I am sorry should be $= Y_{O_2}$ in fact this is what we had also got for the Berkshire moon solution where we said γ is $= 0$ means β is $= 0$ that means $\alpha F - \alpha O$ is $= 0$ right and that amounted to exactly this, we say Y_F / y_{O_2} is more rather why yeah should be $= \mu$ and that should be the same as Y_F / y_{O_2} would Y_F you right the unburnt mass fractions should be in stoichiometric proportions just as well as whatever is in the reaction.

So from this what we can do is this will actually, now tell us what should be the stoichiometric mass fraction right. So the stoichiometric mass fraction stoichiometric mass fraction is $0 C = 1 + \mu Y_{F,1} / Y_{O_2,2} - 1$.

(Refer Slide Time: 24:49)

Mixture Fraction Formulation


- From chemical kinetics we have: $\frac{dY_i}{W_i(\nu_i' - \nu_i'')} = \text{constant}$. Applying this for the reactants and integrating them we get:

$$\frac{Y_{O_2} - Y_{O_2,u}}{\nu_{O_2,u}} = \frac{Y_F - Y_{F,u}}{\nu_{F,u}}$$
- Or,

$$\nu Y_F - Y_{O_2} = \nu Y_{F,u} - Y_{O_2,u}$$
- On substituting for $Y_{F,u}$ or $Y_{O_2,u}$, we get:

$$Z = \frac{\nu Y_F - Y_{O_2} + Y_{O_2,2}}{\nu Y_{F,1} + Y_{O_2,2}}$$

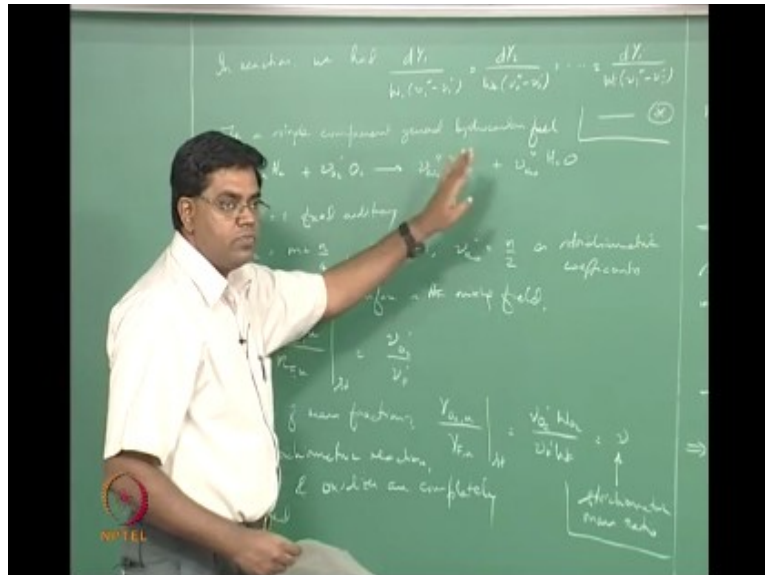
Hence, on the stoichiometric surface, where, $\nu Y_F = Y_{O_2}$, we have:

$$Z_{St} = \left[1 + \frac{\nu Y_{F,1}}{Y_{O_2,2}} \right]^{-1}$$


I should be able to show that right if you, now say this is going to go away right then you rearranged what this tells us is there is a particular value of Z which is the stoichiometric mixture

fraction naturally and it is related to how the inlet stream mass fractions of fuel and oxidizer work out right.

(Refer Slide Time: 25:24)



So if Z is less than Z_{st} right we are less than fuel, so as that keeps on increasing you have more and more fuel that is essentially the idea, so if Z is less than Z_{st} we know clearly that it is fuel deficient right deficient or fuel lean whichever way you want to write then Y_{fb} burnt is going to be 0 this is this is, now the mass fraction of fuel in the burnt products. So you are not going to have any excess fuel in the in the product therefore you can now substitute $Y_{fb} = 0$ which terminates a combustion right.

So the combustion essentially does not proceed simply because your grant ran out of fuel you do not have any more fuels plug in plug this in third exhibition right and use definition of Z_{st} you should now get if we now plug in the expression for Z $Y_{fb} = 0$ then from there you now rewrite you should get why would Z be $= Y_{ho} - \text{come on } 2 \text{ times } 1 - Z / 0$ for that less than or $= 0 - 3$ similarly for fuel rich mixture right combustion terminates when why would to be $= 0$, so you not plug this in the expression for Z and rewrite for Y_{fb} .

You now get an expression $Y_{F,b} = Y_{F,1} \frac{Z - Z_{st}}{1 - Z_{st}}$ - the dusty / 1 - and this is this is valid for sub greater than or = 0-3.

(Refer Slide Time: 28:50)

Mixture Fraction Formulation

- Consider a fuel lean situation. Then on the products side, $Y_{F,b} = 0$. Using the Z & Z_{st} equations, we can get $Y_{O_2,b}$:

$$Y_{O_2,b} = \left(1 - \frac{Z}{Z_{st}}\right) Y_{O_2,2}, \quad Z \leq Z_{st}$$

For a fuel rich situation, we would have excess fuel:

$$Y_{F,b} = \left(\frac{Z - Z_{st}}{1 - Z_{st}}\right) Y_{F,1}, \quad Z \geq Z_{st}$$

NPTL

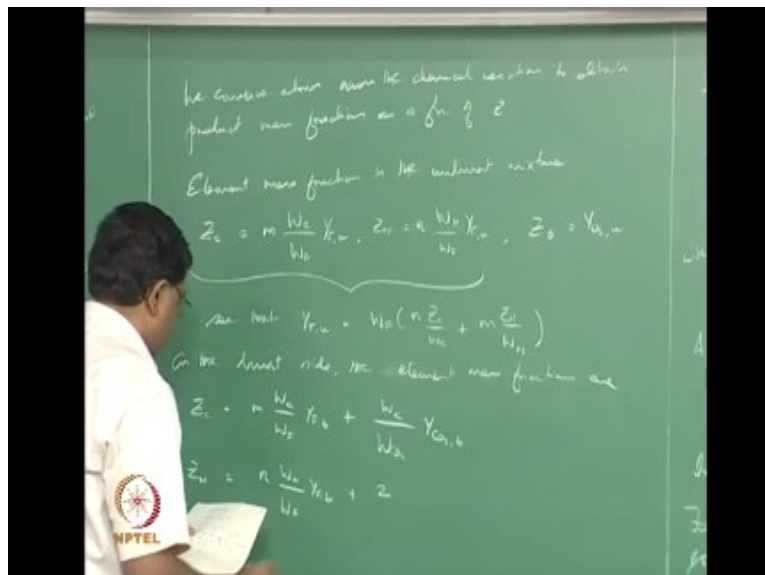
That means we can now draw a picture similar to this is for the unburnt fuel that unburnt oxidizer in the mixing field but we can now anticipate how the unburned, sorry the burnt fuel and burned oxidizer should look like if you now halves up going in the horizontal axis from 0 to 1 somewhere and there you should now be able to locate $Z = Z_{st}$ now that that become that becomes an important thing but there are we on this side of Z_{st} or that side of zealously because this is going to correspond to a fuel rich situation that is going to correspond to an oxidizer lean situation.

Therefore you are $Y_{F,b}$ is valid only for greater than right on this side B is =0 therefore you come and this is also linear enzyme okay, so this goes so your Y_{FB} is going to go all the way to from 0 to $Y_{F,1}$ right as a matter of fact when you go to this corner when Z is =1 your Y_F is = $Y_{F,1}$ you know and so this or $Y_{O_2,b}$ goes to 1 so $Y_{F,b}$ goes to $Y_{F,1}$ alright and this is what we were looking at the last class were at the flame, you now have the fuel concentration go all the way to 0 and then stay flat on the other side okay.

So here the fuel is going to go all the way from the fuel Inlet screen all the way down to 0 at the stoichiometric surface and then lie flat on the oxidizer regicide right and similarly you now, have a straight line that goes from 0 here backwards to Y_{O_2} in the mixing feed, so essentially if it is possible for us to now go back and redo the Berkshire 'men problem in terms of Z instead of β which is not very different if you think about it alright and it is also possible then you can actually look at contours of Z several contours of Z and dependent upon the contours of values of Z.

You now try to actually look at what the values of Y_{FB} and Y_2 be should be you now can map how the fuel concentration and oxidizer concentration should show up, this is still for the excess field a side to the products and excess oxidizer the products or fuel rich side and fuel inside. So have not talked about the actual products of combustion right like CO_2 and H_2O so for getting the product concentrations we should do something similar to what we have here in order to obtain your new CO_2 double Prime and new H_2O or double Prime all we have d1 by saying we are balancing this reaction is to basically conservatives week. We compared carbon atoms hydrogen atoms oxygen atoms and then came up with these things.

(Refer Slide Time: 32:39)



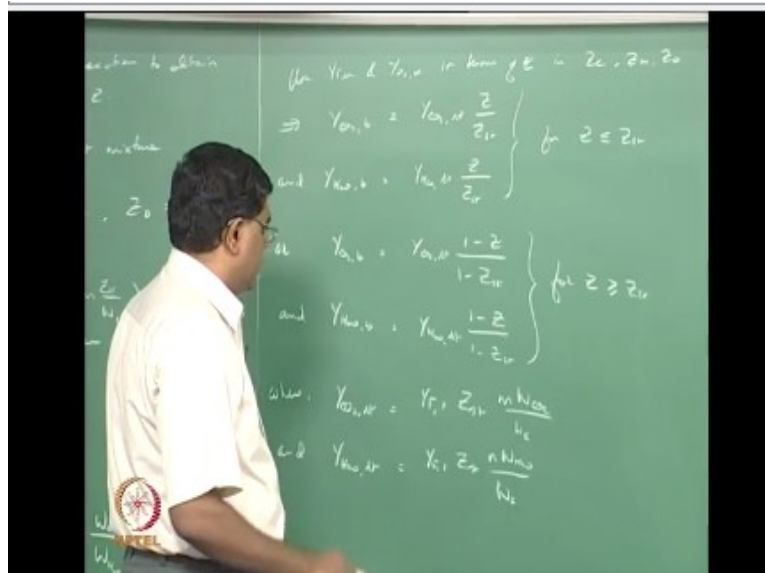
So we conserve atoms across the chemical reaction to obtain product mass fractions as a function of Z still we are interested in what happens at the function of the mixture fractions are and that is a hero for the day it makes the fraction so we keep on looking at everything as a function of Z, so element mass fractions so look at what happens in the unburned mixture element mass fraction in the unburned mixture, so look at the fracture of carbon atoms so you had m carbon atoms in the hydrocarbon right.

So this is M times molecular weight of carbon atom / the molecular weight of the fuel right times why I have come on you, so this is the mass fraction of the unburned fuel times this fraction is what is going to give you the carbon fraction. Similarly if you now look at H that is going to be n times W_h / W_{fuel} times y_{fu} for the oxygen it is mainly coming from the oxidizer stream so you might as well just write $0 = Y$ or to you.

Whatever is the mass fraction of the oxygen in the oxidizer stream unburned right is easy to 0 of course from here we should now be able to also write C see that Y of U is $=W_F \text{ times } n \cdot C / W_{C+M}$ or did I make a m0h by wh all right on the bond side on the bond side for the products are the element mass fraction or for the carbon we have $c = m_w c / w_f Y_F$, b that is actually for if you have excess burnt fuel right + if carbon is also there in carbon dioxide that is what we are more interested in WC were 2 times c were too burnt and this is what we are trying to find out in terms of Z okay.

And hydrogen is going to be like n times $W_h / w_f Y_F$, b + twice because water contains 2 hydrogen atoms so $W_h / w_{H_2O} \times y_{H_2O}$, b there is also the next thing that we are trying to find out in terms of that currently, so and finally we have to conserve oxygen atoms so that o from the products would be twice $W_o / W_{O_2} \times y_{O_2}$, b + twice W_o / W_{CO_2} because there are 2 oxygen atoms in carbon dioxide Weiss you were to come a week + 1 $W_o / w_{H_2O} Y_{H_2O}$, B right, So now if you know equate these,

(Refer Slide Time: 38:01)



So use Y_{O_2} and Y_{H_2O} in terms of Z in that C. H. O and rewrite okay, so you then get y_{CO_2} B would be y_{O_2} stoichiometric times Z / Z_0 + y_{H_2O} , $b = y_{H_2O}$ or stoichiometric times Z / Z_0 stoichiometric.

(Refer Slide Time: 38:55)

Mixture Fraction Formulation

- Further, we can obtain element mass fraction in both unburned and burned sides:
 - On the unburned side:

$$Z_C = \frac{mW_C}{W_F} Y_{F,u}$$


$$Z_H = \frac{nW_H}{W_F} Y_{F,u}$$

$$Z_O = Y_{O_2,u}$$
 - On the burned side:

$$Z_C = \frac{mW_C}{W_F} Y_{F,b} + \frac{W_C}{W_{CO_2}} Y_{CO_2}$$

$$Z_H = \frac{nW_H}{W_F} Y_{F,b} + \frac{2W_H}{W_{H_2O}} Y_{H_2O,b}$$

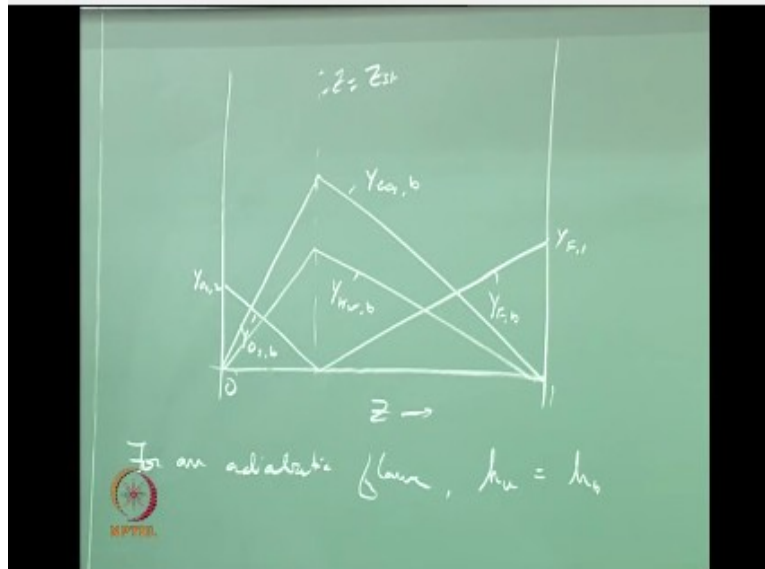
$$Z_O = \frac{2W_O}{W_{O_2}} Y_{O_2,b} + \frac{2W_O}{W_{CO_2}} Y_{CO_2,b} + \frac{W_O}{W_{H_2O}} Y_{H_2O,b}$$



This is for Z less than or $= Z_0$ C or why see what to, be $= Y_C$ were to strike geometric times $1 - Z / 1 - Z$ stoichiometric and h_2o , be $= Y_{h_2o}$ stoichiometric times $1 - Z / 1 - Z$ this is for Z greater than or $= Z$ of T, where we have to say what is y_{co_2} stoichiometric and Y_{h_2o} stoichiometric so why co_2 stoichiometric is why F, times $M W_0 / W_F$ and why h_2o , striker metric is why F, $10 Y_{200} / W_F$ alright.

So what do you what do you expect we can still see that why co_2 is still going linearly as dud Y_{h_2} is going linearly Z , so long as zealous lessons are s t white sea water is still going linearly but decreasing with Z Y_{h_2o} is decreasing linearly with Z as Z is greater than right. So let us think about plotting this.

(Refer Slide Time: 41:10)



There is no half third along the horizontal axis going from 0 to 1 and we know locate it is like a metric surface at somewhere in between and we noticed earlier from that picture just to reproduce your $Y_{F, B}$ goes from 0 at these are equal is that stoichiometric to $Y_{F, 1}$ when Z is =1 this is the excess burnt fuel and you now have $Y_{O_2, B}$ going all the way up to $Y_{,2}$ – that is not =0 but what we are looking for now is how this varies Y_{CO_2} goes to a peak value ads are equal as a discrete and then comes all the way down to 0.

So this is your $Y_{CO_2, B}$ and similarly of course depending upon the numbers they should now get a similar set of lines for $Y_{H_2O, B}$ so it reaches a peak value you get the same expression same numbers I should say from both the expressions at $Z = 0$. So you can plug that and then let us see what I got right, now we are still interested in the temperature so for temperature all these things are essentially like looking at an equilibrium you see. So for the temperature where we now say for an adiabatic flame right for an adiabatic flame we have the unburned enthalpy = the bond enthalpy and it is probably a good time to stop just stop.

Production and Post Production

M V Ramchandran

G Ramesh

K R Mahendra Babu

Soju Francis

S Subash

R Selvam

S Pradeepa

Ram Kumar

Ram Ganesh

Udaya Sankar

Robert Joseph

Karthi

Studio Assistants

Krishnakumar

Linuselvan

Saranraj

NPTEL Web & Faculty

Assistance Team

Allen Jacob Dinesh

P Banu

K M Dinesh Babu

G Manikandansivam

G Prasanna Kumar

G Pradeep Valan

C Rekha

J Salomi

P Santosh Kumar Singh

Sridharan

P Saravana Kumar
S Shobana
R Soundhar Raja Pandian
K R Vijaya

Administrative Assistant
K S Janakrishman

Principal Project Officer
Usha Nagarajan

Video Producers
K R Ravindranath
Kannan Krishnaµrthy

IIT MADRAS PRODUCTION

Funded by
Department of higher Education
Ministry of Human Resources Development
Government of India
www.nptel.iitm.ac.in

Copyrights Reserved