Indian Institute of Technology Madras

NPTEL

National Programme on Technology Enhanced Learning

COMBUSTION

Lecture 42
Mixture Fraction Formulation

Prof. S R Chakravarthy
Dept. of Aerospace Engineering IIT Madras

So for an aerobatic claim we have the unbound enthalpy should be equal to the burnt enthalpy

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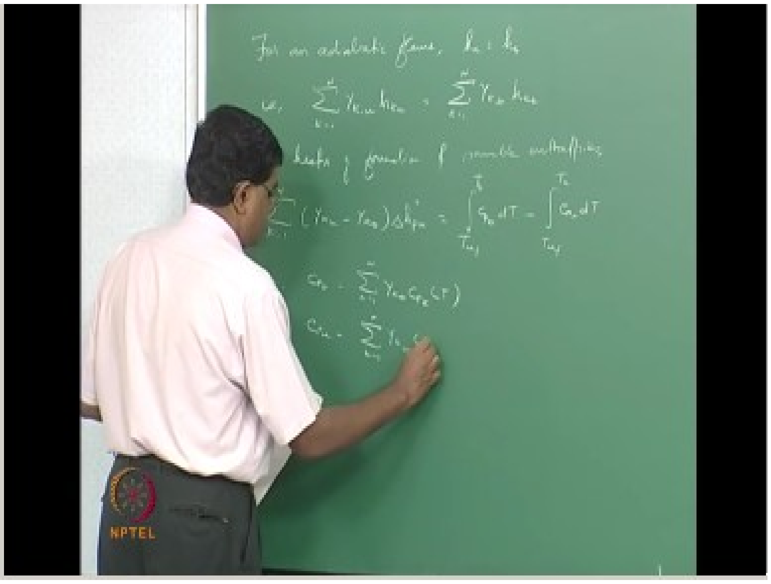

Which means we could now say σ k= 1 to n YK, u HK u =σ k = 1 to n Ykb Hkb where h kb is now the enthalpy of the bond products Ykb is something that we have seen so far so what we then do is the normal thing which is we now say enthalpies formation and tau p plus sensible enthalpy right so using heats of formation and sensible and companies without peas we can write σ k =1 to n YK u- YK b times Δ hf_0 which is the reference formation enthalpy for each species equal to now we look at the sensible enthalpy which is T graph type 2b that is cp dt - integral trf2 tu cpu right our job is to actually find out TB given t that is what you are trying to do here. So well of course a CPB =σ K=1 n YK b CP k of temperature and cpu is σk=1to n YK you CPK of T now.

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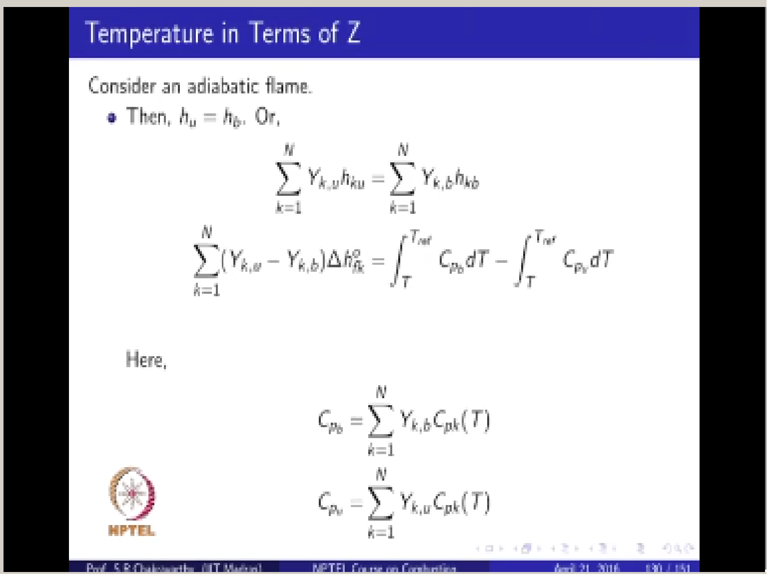

Temperature in Terms of Z

Consider an adiabatic flame.

- Then, $h_u = h_b$. Or,

$$\sum_{k=1}^{N} Y_{k,u} h_{ku} = \sum_{k=1}^{N} Y_{k,b} h_{kb}$$

$$\sum_{k=1}^{N} (Y_{k,u} - Y_{k,b}) \Delta h_{fk}^{o} = \int_{T}^{T_{ref}} C_{p_b} dT - \int_{T}^{T_{ref}} C_{p_u} dT$$

Here,

$$C_{p_b} = \sum_{k=1}^{N} Y_{k,b} C_{pk}(T)$$

$$C_{p_u} = \sum_{k=1}^{N} Y_{k,u} C_{pk}(T)$$

Prof. S.R.Chakravarthy (IIT Madras) NPTEL Course on Combustion April 21, 2016 130 / 151

So what we what you want to do is we want to try to find out what, what this is right and therefore and then we have already looked at how to do the products therefore we can do the same thing so we had dyk / u K double prime -μ k single prime time’s capital W K =4 over many species up to let us say one particular speech species dy 1 /ϱ 1 double prime minus nu one single prime time’s capital W 1.

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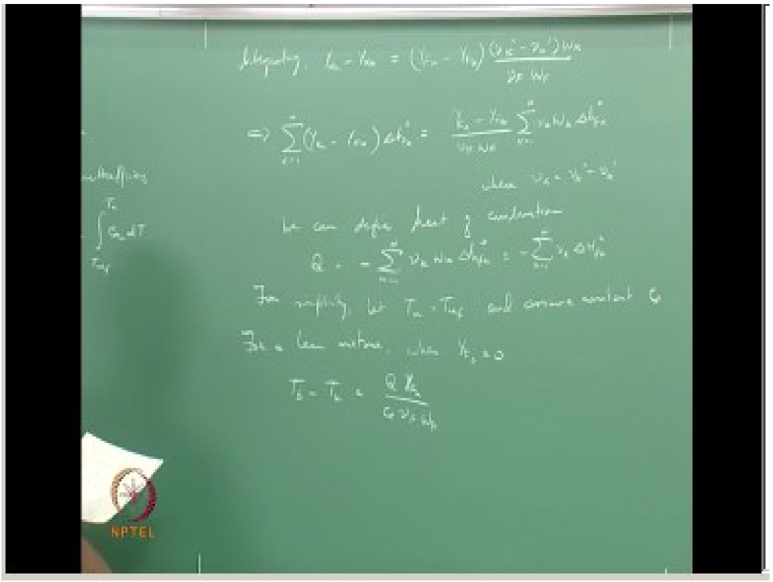

So integrating this integrating this we get r YK u- YK be equals let us suppose that you do this for the KH species in relation to the fuel so that means you take any KH species and then you take feel the left-hand side and right hand side respectively then you could you could write this as y fu minus YF be x arm new k double prime minus UK single prime W K / µ f WF now keep in mind your new F here is actually a stochiometric coefficient for the fuel and you do not have any fuel on the right-hand side there for your new k double prime minus Duke a single prime for the fuel is simply µ F right.

So you do not have to worry about that anymore because you know how the reaction looks like for this so from here if you know this difference now for the KH species multiplying by Δa hf k and something summing over all k σ k =1 to n YK u -y kv x Δhf k^0 is equal to then you see the only thing that is really getting summed over on the right-hand side is this part alright and this is all this is independent of k it is only 50 fuel therefore y YF u -YF /µ f WF x σk = 1 to NUK WK Δ hf why not where.

We now use the symbol where of course it is going to get a little bit bigger so we try to compress it by saying UK is new k double prime minus UK single Prime just to just to kind of have our bearings on we see new k = K double prime minus Duke a single Prime that is like a set that you are trying to allocate a particular symbol but we also looked at the new without a subscript which is a stoichiometric coefficient ratio mass ratio and new F is actually the stoichiometric coefficient for fuel that is already been identified which is basically this one evaluated already right so these are these are the different news that we have we are looking at so it just do not get confused about these things alright.

So if you now look at this then the , the left-hand side here is what this is effectively what it means is this essentially translates to just looking at this summation all right and therefore if you now say that summation if it is a queue let that so we can we can now define heat of combustion heat of combustion q =- K =1to n UK WK Δ Hfk not all right let us just see heat or the other way you can do is you can also say - σ K =1 to n μkΔ H of K not wear this is on a molar basis this is on a mass basis so mass basis x the molecular weight is what you are looking at so for simplicity let us now say P T u = T ref now we have already gone through this before in the context of premix flames but it does not really lose much generality here by doing this.

And also zoom constant CP constant CP therefore now for a lean mixture for a lean mixture when y of b=0 right it means you are running out of the burnt fuel because you do not have any of it as in excess as for a lean mixture then all you do is you now say here why just plug in y f be =0 here right that is what you would actually do for the left-hand side on the right-hand side there's a simply CP times CP times TB minus T you effectively right so that means the CP can come to the other side in the denominator and then you will get a TB minus T u = q YF u /CP new f WF ok now it is not for nothing that we chose to actually look at fuel as one of the sides of this equation.

So in this equation we chose one of them to be fuel with the other one being any KH species on the left-hand side because we are looking at the lean mixture where you are going to substitute Y =0 but, for a rich mixture you would want to actually substitute y 0 = 0 right which means we need to have a place in which we can substitute 0 = 0 for which we should have started out having oxidizer integrated rather than fuel right so that is what we would do for a risk for a rich mixture we go back.

And integrate again as yku-ykb trying to redo is again with oxidizer on the right hand side is to the fuel so YK b minus what you U=Y y so this must be yu/μoμo2wo2 to x times μ k WK / that is it I will read out this so new key of course is again new k double prime -μk single time which I had not done before so if you do this and of course you know can take this step where you x Δ hfk and some over and then you now recognize this is q and plug this back in here and write your TB-TU you at that stage you now plug your wire were 2b= 0 right for the rich mixture.

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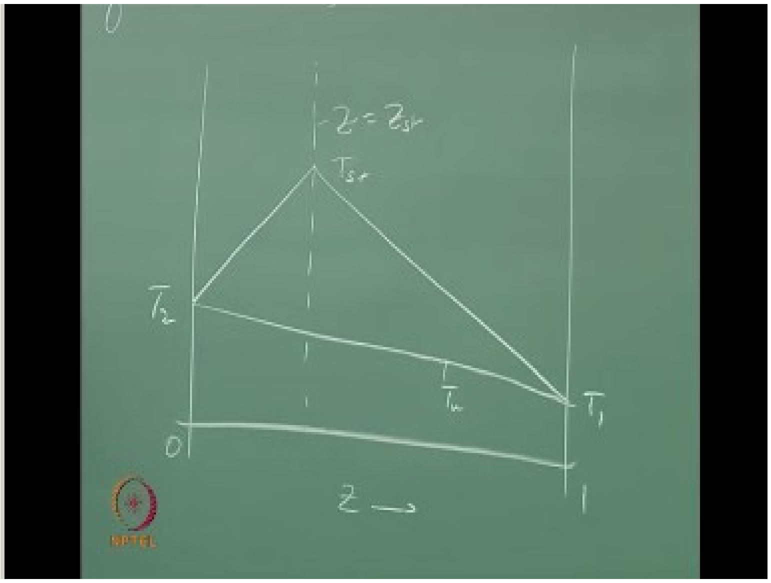

And plug y = 0 for rich mixture right T V - T U = Q / CP u 0 2 wo2now what we are really looking for is the bond temperature in terms of the mixed fractions are because mixed refraction is kind of like our basic function now so we want to now represent this in terms of sorry YF u in terms of z and y 0 to you in terms of Z which is not very difficult okay so you can say that this is basically z x y y f, 1and this is 1-z times y 0 2,2 right so we know how to do that so we now right YF u and you to you in above expressions in terms of Z mixed refraction.

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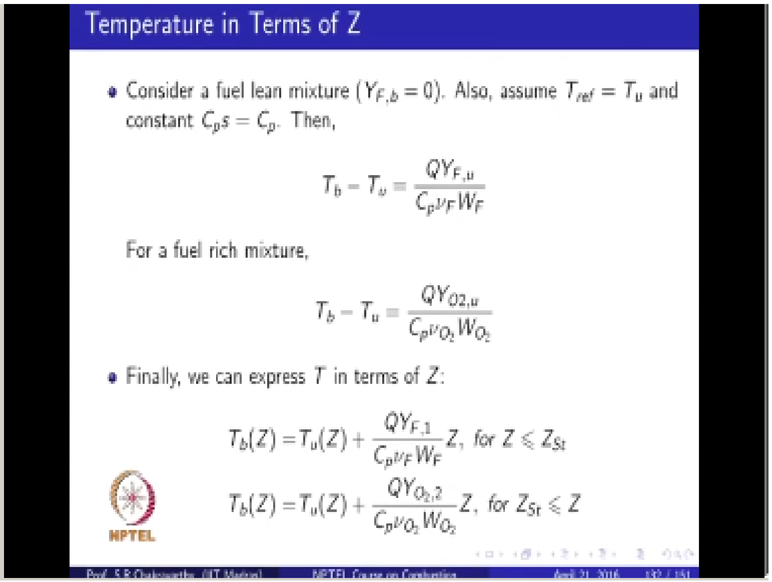

Temperature in Terms of Z

- Consider a fuel lean mixture ($Y_{F,b} = 0$). Also, assume $T_{ref} = T_u$ and constant $C_ps = C_p$. Then,

$$T_b - T_u = \frac{QY_{F,u}}{C_p \nu_F W_F}$$

For a fuel rich mixture,

$$T_b - T_u = \frac{QY_{O2,u}}{C_p \nu_{O_2} W_{O_2}}$$

- Finally, we can express T in terms of Z:

$$T_b(Z) = T_u(Z) + \frac{QY_{F,1}}{C_p \nu_F W_F} Z, \text{ for } Z \leqslant Z_{St}$$

$$T_b(Z) = T_u(Z) + \frac{QY_{O_2,2}}{C_p \nu_{O_2} W_{O_2}} Z, \text{ for } Z_{St} \leqslant Z$$

Then right also the unbound temperature, temperature in terms of mixed of fact how does that work out you have k= t2 - Z times t2- t1 right how do I know that this is right t2 is the oxidized or stream temperature and t1 is the fuel stream temperature right so if you are now plug to z=0 then it is all oxidizer then I get the unbound temperature for the oxidizers team to bet 2 that is what this is if z =1 then it is a fuel stream right then the Tito gets cancelled and you get T 1for burnt temperature so that is the temperature of the fuel stream so this is basically like a linear relation relationship between the two temperatures for the burnt temperature of a mixture of any given mixed refraction in between right.

So if we with that being the case you now go back and plug that and in terms of Z and then plug your Y of you in terms of that and y 0 2 in terms of Zod right so all of them put in put in terms of z will be then TV of z= t you observed q yf ,1/ CP µ f WF x z ah but that much mean less than or equal to z stoichiometric or TV of Z =z + Q2,2/cp new o2 wo 2 times 1- z 4 z >=0 0 as T right now the maximum temperature you can calculate the maximum temperature so that keeps on increasing you see TV will keep on increasing up to and when you now cross you now have to use this expression where as dessert keeps on increasing ttb keeps on decreasing right.

And adds equalizer you should actually get the same expression from both that means you should have like one temperature at which the stoichiometric mixture as a burn temperature. So the maximum temperature and that will be the maximum temperature the max temperature TST is calculated forestry from either expression either exhibition about so how does this look like now we have been drawing these pictures at every now and then as and as and when we get a bunch of expressions are into in terms of Z we try to plot them.

So here you see if that is plotted along the horizontal axis and let us say go from 0 to 1 all oxidizers stream here and all fuels stream there and let us say they oxidize the temperature is t 2 and the fuel temperature let us say is t1 the unburned temperature is not going to depend on whether you had a stoichiometric surface. And so on okay whatever it may be you just get a straight line that connects the two which is basically following this expression that is a linear expression in Z as well okay and you just get a straight line that connects these two this is to as far as bond temperature is concerned you have to not worry about whether you are a fuel rich of you lean right.

And that means you have to look at where your zesty will be so if you are thirsty is going to be here then the PST is going to be the peak and on the one side when you are now having won lee oxidizer you do not have any reactions you're simply not having any fear at all so you go back to t2 right and similarly on the other side you just have to look at in linear variation from TS t to t 1 so it just becomes that that simple all right so in some sense what this really means is we can now put the whole picture together in what we are doing in a bigger, bigger graph let us just try to do that now need more space so let us now say we had a unburned situation.

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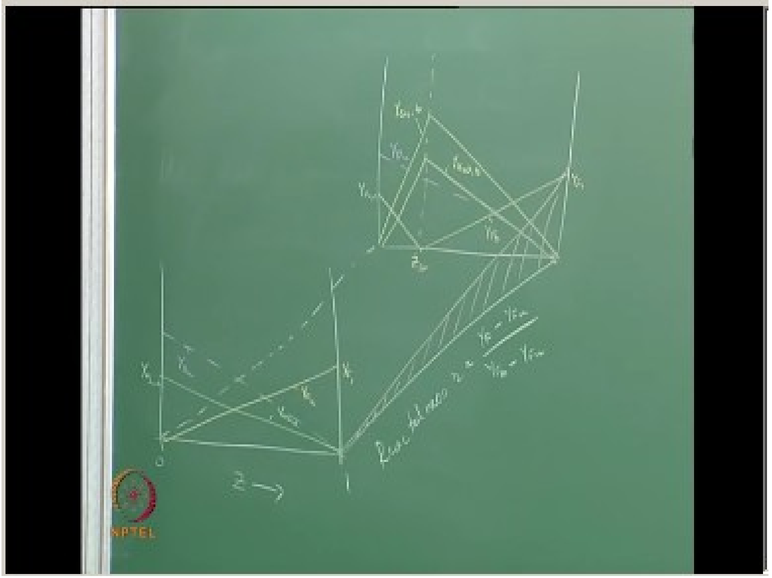

And a mixing field in which you have the submarine along the horizontal axis going from 0 to 1 all oxidizer to all fuel right and we now want to look at how those proceeds in a third axis where we are interested in constructing the same kind of picture for the bunt process so let us suppose that that is what it is right and along, along the third axis we now have a variable called reactive what is the level of reaction that is going on how do you monitor this by looking at Y F -YFu / y FB minus y fu so when you start it out alright when you started out you have Y F = Y of you so r = 0 okay when you end YF becomes Y of be there for our becomes 1 alright .

So you can we can plot this along this axis maybe let us say along this axis maybe we just plot along this right that is that is a way the reaction is going alright and, and y YFYF is turning into turning on turning from YFB but y fu two YFB initially we are having your YFU actually starting, starting from let us say why of one here 20 on this side and therefore you are going to have a straight line that looks like this so this is your Y a few all right and somewhere in here you are going to have your right and your YFB is going to be.

So maybe you can look at you do not have to worry about at all here you just to just to get a perspective on how this kind of a linearly increasing why a few actually turns out to start increasing up to y of1 over here right and similarly you could think about a y 02u which stands from y 0 to 2 and goes all the way to 0 when Z goes to one that is the unburned oxidizer right and that now is going to go all the way to so this is also why 0 to 2 and of course I should have mocked YF one there right and then we could do a couple of things one let us assume that you have diluents only the oxidizer like an air right.

So more the air more the oxygen and correspondingly more diluents if you do not have any air you do not have any oxygen you do not have any del u and either right so you could now think about a W and concentration that is going to grow with more and more o2 as we go along backwards in this axis starting from zero so, so this is like yd you where d 4 D is for diluents right and this picture is not going to change at the end of the reaction it is about the same so you are now going to get this picture to look like yd you right and of course there is a value here that corresponds to how much de Leon's you have for how much oxygen.

So this could be for example point 2 3 that could be like point 7, 7 and this could be now point 77 all right yeah and so on then we talked about temperatures oh no I think we talked about products so we talked about products you do not have any products here to talk about all right we are talking about products only here and the way we talked about it is you now said you are going to have your y0 to be go like that and why h2o be go like that all right and finally we talked about temperature so the temperature we can plot two things the unborn temperature.

And the burn temperature right so the unborn temperature let us suppose would be we now pick a scale like that this is your T 2 and this is your T 1 it is as if like the fuel stream is colder than the oxidizer screen right it could be and then you can mark these two points into here and t1 there may be t1 is somewhere there according to this and now going to go on the way to TST and go back here so if you think about it this is like what we were saying for the vicinity of the berks Schumann flame so in the work room inflamed if you have a diffusion flame sheet in the z axis it is going to be located at z = 0 right and from Zurich colas RSV the temperature is going to fall on either side on the field its side one way.

And they oxidize a regicide the other way right but in the lame we are looking at how it is behaving in space rather than in the spaces in the physical space about the burner rather than looking at it in what is called as the mixed refraction space so in this picture everything looks very nice straight lines gay all linear dependences in the mixed diffraction space but that is not how the curves were looking, looking like in the physical space and that is one of the reasons why the mix tape fraction space is quite valuable so question basically now is how do we transform this into or how to utilize this in the physical space system that is what we are worried about like for example if somebody is giving you a burner.

And asking you to find out how the flame is going to look like and how the species concentrations and the temperatures are going to vary and all the things you cannot give them a picture back like this which is in the mixed refraction space you have to now translate this into the physical space so you now look at how the mixture fraction for example can be utilized in looking at the spatial variation that means we need to have a governing equation for how the mixed refraction varies in space that means we have to have an evolution equation for this what I am going to now write is basically the steady state counterpart but there is nothing that really stops you from doing an unsteady counterpart just like how you would do an unsteady Schwab's Ella which formulation which we did not go through but we said it is possible to do so.

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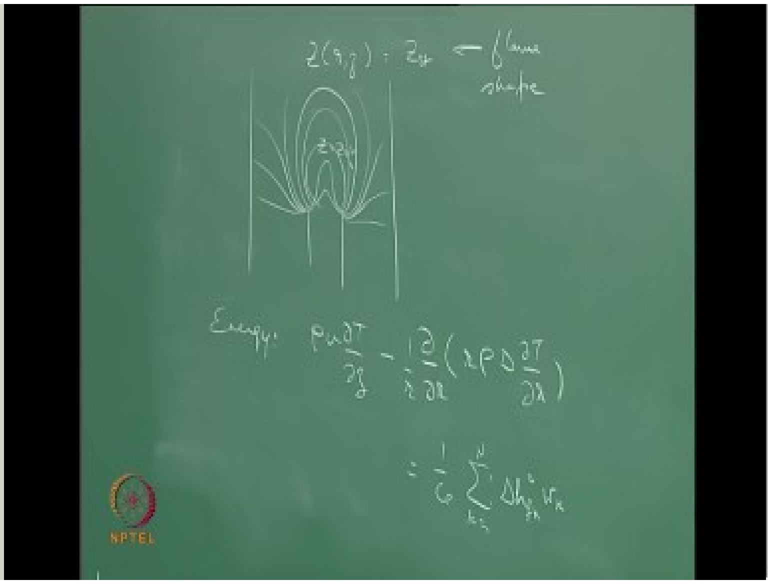

So similarly we can now write for example a evolution equation for the mix diffraction right so the mix diffraction essentially is like a conserved scalar and it is now being evolved by convective and diffusive processes okay now that is the physics behind how, how this goes you can actually derive this mathematically in two different ways one go back to the definition of mixed refraction mixed refraction is nothing but a fuel mass fraction kind of notion right so you can now find that you have like a new Y F -y 02 / something plus some plus new arm wa-wa' 22 /something.

So the all the things that are getting added up and / or constants which depend on the inlet concentrations but what's really happening is you are now performing this coupling function like new F- y Y F- y 0 to write if you now use the evolution equations for species concentration YF and y 0 2 and you are now x news subtracted one from the other added something else / something some other constant and so on you should now be able to get this and while you do that you can also find out that the right hand side being the reaction rate term is now going to go to is not going to get subtracted out pretty much like the way we did in the burgh human problem so the work shipment problem we started looking at the Schwab's el de Wit species equation with the reaction rate on the right-hand side.

And we now try to normalize things and subtract and form the coupling function such that you get the same expression on the right-hand side you saw that when you subtract you get to get a zero so we get you get zero here similarly the other way of looking at it is while we were looking at the mixed refraction we also notice that we could form element mass fractions like for example sub c z h z 0 and so on and we could form mixed refraction based on the element mass fractions so long as the mixed refraction is essentially defined based on the element mass fractions and in a combustion process the chemical reaction that we are going through conserves elements it does not really destroy the elements.

So no matter whether carbon is present in her inner Hindi in the hydrocarbon or carbon dioxide no matter whether hydrogen is present in the hydrocarbon or water no matter whether oxygen is present as itself as part of our or as part of carbon dioxide or water right the mixture fraction gets conserved because it is based on element mass fractions and therefore the reaction rate term will not show up and you now try to write, write a evolution equation for this so we just write this out as it is and then the other thing that we need to do in order to actually look at the structure of difference.

So this is okay as far as the infinite chemistry kind of approach is concerned so what we what we talked about in the book Sherman problem was that this is like a sheet that corresponds to ∞ chemistry and on either side you have these things dropping and varying correspondingly but if you want to now think about finite rate chemistry okay so if you are to think about finite rate chemistry you have to have the reaction rate show up somewhere and typically the problem with finite rate chemistry is define it kind of finite chemical reaction depends on species concentrations as well as temperature right and the Schwab's which formulation what we have noticed is we have to keep the reaction rate at least in one equation even while you are subtracting a lot of other things therefore if you now say let us.

Now we have to consider the energy equation where the reaction rate depends on the temperature as well as react concentrations on the concentration is governed by reactions sort of equations that have been subtracted from each other to get this okay so this represents a pair of species reactions let us be species equations and then we have the energy equation so if you now write this as so this is course before, before we do that we can we can say this for a simple case of let us say the buck shoo-in kind of problem if you now say ϱ u du z / ϱX minus right or if you want to do it in cylindrical polar this would be our like this and one over R and so on that is okay equal to zero now you could go ahead.

And solve this as it is and then finally look at the solution and find out wherever that is equal to 0 as T is where the flame shape is in terms of so you are now going to get finally Z of our commas are equal to Z is a flame shape right so you could go ahead and do it your solution that way and once you do this on either side in DY in the burner let us say you have your flame like this is your Z equals EST you can now get the solution to give others are values and so on that lecture looks very good is not it right that is how it actually turns out to be you can solve the show up Pelvic formulation and get this kind of picture.

And so these will correspond to different values of Z with Z = 0 being where it is to correspond to where the flame is and then you can now look at four different values of Z what should be your YFB what should be your wife why would you be what should be your TB and so on all right so you could do this but that is actually the infinite rate chemistry approach now for the final fate chemistry approach as I said you need to have at least one equation which, which contains the reaction rate that means you have to have the energy equation let us say minus one over ∂u=∂t/∂z-1/r∂/∂r=1 C p σ k =nΔ hf k not WK this is directly coming from our Schwab Zeldovich energy equation right now what we have to do next and I am not going to do this in great detail you just going to point two directions that that will take you there because this is just getting a bit too involved and I think the idea is essentially made and we could leave it there.

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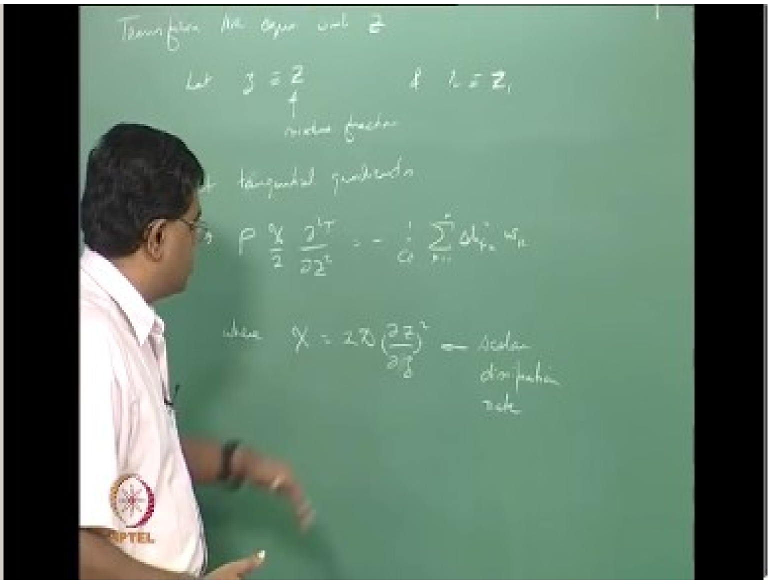

So what you now do is transform the equations with respect to Z the pains we could say let one of the variables let us say X = Z which is the mixed refraction and let us say r = z1 so no big change they are just changing symbols BU there we are actually changing meanings okay and this is kind of like what is called the transformation where you are replacing one of the independent variables by a dependent variable upon which you want other dependent variables to depend so involved that we have seen so far all the dependent variables that we are talking about or depending upon Zed Anson itself is governed by this given that it is depending on X.

And sorry certain are right so once you know Hauser depends on the spatial variables we now transform our equation in terms of capitals are being the independent variable and now try to obtain the energy equation in terms of capitalism get your solution in terms of capital sir if you know how Z varies you know how your temperature varies right so this is not this is not so trivial you will actually end up with lots of so essentially what you have to go through is like if you do not want to say ∂/∂z then that is like that that is actually ∂/∂z+∂Z+∂Z by and so on so you change your apply chain rule across and you have to bring in the deepens on Capital Z everywhere by chain rule.

And then you plug this in these equations and this actually becomes a fairly huge term because of this and you will have lots of cross derivatives and so on and then you could make know an approximation you can make an approximation you say gradients that are perpendicular to the flame are important gradients that are tangential to the flame or unimportant this is typically valid whenever you have aflame sheet kind of situation right and you can now throw away a lot of jumps and two leading order you can even throwaway terms that are there in other derivatives accept these and finally what you will get is so neglect tangential greens, greens.

And you will now get something like ϱδ/ 2 ∂√t by ∂ R^2=-1 c p σ =1 to nΔ hf not k WK where 2d goes that by ∂ duals up the whole square okay in general in 3d you could actually have this is a gradient squared good r squared and this would basically call be call this business basically what is called as a scalar dissipation rate and this is essentially looking like a diffusion term in fact the scalar dissipation rate has dimensions of 1over time and essentially it gives a gives the characteristic diffusion time scale right and basically it tells us how the diffusion happens sub mixed czardas mixed refraction keep that in mind.

And you now have the gradient coming in picture that means assertion essentially represents a transport phenomenon of mixing how the how the mixed refraction variable is now going to decay because of diffusion right while the mixing happens between fear and oxidizer and this is actually quite important in turbulent diffusion wherever you are looking at for example scalar transport by turbulence then you have the turbulent diffusion more mass diffusion coming into picture and the scalar dissipation rate in the turbulent conditions would be would be quite important quantity there where the moment.

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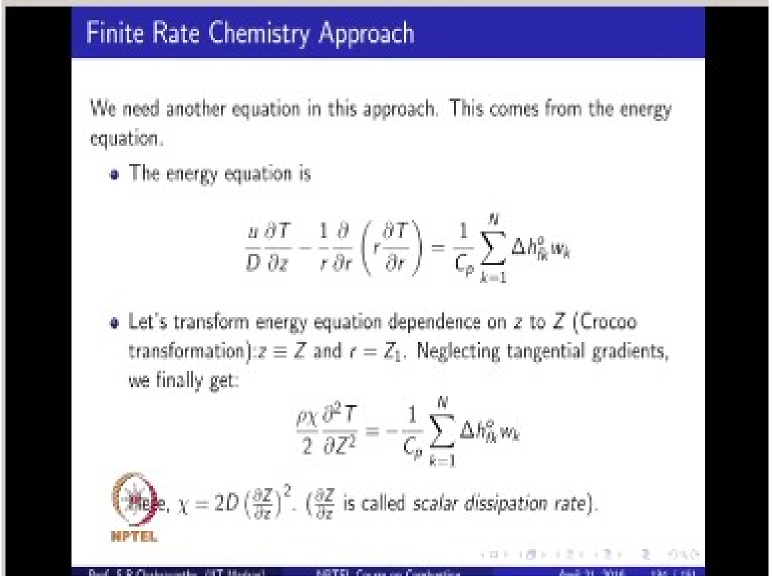

Finite Rate Chemistry Approach

We need another equation in this approach. This comes from the energy equation.

- The energy equation is

$$\frac{u}{D}\frac{\partial T}{\partial z} - \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right) = \frac{1}{C_p}\sum_{k=1}^{N}\Delta h_{fk}^{o} w_k$$

- Let's transform energy equation dependence on z to Z (Crocoo transformation):$z \equiv Z$ and $r = Z_1$. Neglecting tangential gradients, we finally get:

$$\frac{\rho\chi}{2}\frac{\partial^2 T}{\partial Z^2} = -\frac{1}{C_p}\sum_{k=1}^{N}\Delta h_{fk}^{o} w_k$$

Here, $\chi = 2D\left(\frac{\partial Z}{\partial z}\right)^2$. ($\frac{\partial Z}{\partial z}$ is called *scalar dissipation rate*).

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Let us not worry about all those things at the point I wanted to make is it looks like you have a diffusion term and reactive term and the effect of this would be to try to find out what goes on in between in a very narrow region in this in desert space where things are varying did a finite rate chemistry and that is the effect of this okay and what you will find is in reality you do not really have the oxidizer concentration come all the way down to zero it could leak across the reaction zone if you now take finite fit chemistry into account because it is not able to consume all the oxygen right it is not really infinite rate reaction now.

And then it will look like this is like a essentially a diffusive reactive valance that we saw for the reaction zone the pre premix flame and I also pointed out that this region is going to be like the reaction zone in the premix flame and whatever is outside of this in the near vicinity is going to be like the preheat zone in terms of transport processes dominating except it is going to be radial transport versus axial convection and so on in the book Sherman problem or any Co flow diffusion flame problem like get diffusion flames and so on except this is not really a diffusion term alone you have it actually as a function of as a second derivative of capital Z which is the mixed refraction so this is a derivative in the mixed fraction space.

So it is a transformation that contains within it convection as well as diffusion but by making this transformation in terms of the mix diffraction we have essentially enabled it to look like a reactive diffusive balance all right but the transformation contains in it the convective and the diffusive effects so we would like to stop here and then we can pick up on let us say droplet combustion from next class.

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