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COMBUSTION

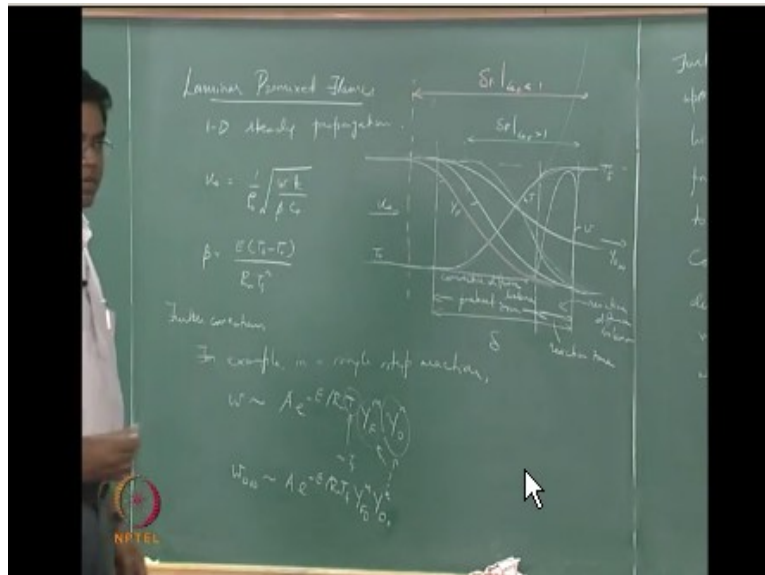
Lecture 28

Laminar Premixed Flames Corrections

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(Refer Slide Time: 00:10)



So what we were here where we found that if I now take into account the fact that the reaction zone in this flame thickness is only a fraction of the entire flame thickness and that is where the reactions are happening and therefore the heat release rate is going to actually come from a volume its corresponding to only this and I scale the reaction zone thickness over the flame thickness by a factor given by  $\beta$  which is easily with scaling factor then I can actually estimate a unit which has a  $1/\beta$  term inside.

The square root and so we now say we now notice that the flame speed is about that much smaller right because we are now factoring in that reactions are happening in only part of the flame and not in the entire flame we can now do further corrections in noting some more things the question is first of all what we had done was to assume the  $W$  is a constant across this region and now what we have said is  $W$  is actually a constant across this region approximately now that is not very difficult to imagine.

Because it is kind of rising very steeply within this region and going to a value peak value and then draw dropping steeply back in this region so it is okay but the question is what is the  $W$  so if you now think about what the  $W$  is  $w$  is the chemical reaction rate and strictly speaking the way we had to look at so for four examples in a single step reaction we should be able to write  $W$  as I mean I am just not going to say equal to but just going to say goes as because I am going to write this is  $w$  in terms of mass right.

So this is actually mass produced per unit time per unit volume and I am going to write this as something like  $E$  to the  $_{EU}$  overall  $UT$ .

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Third Approximation

- Consider a single step reaction. Then,
 
$$w \sim A \times \exp\left(\frac{-E}{RT}\right) \times Y_F^m \times Y_O^n$$
- Assume  $T \sim T_f$ . Then,
 
$$w_{\infty} \sim A \times \exp\left(\frac{-E}{RT_f}\right) \times Y_{F_0}^m \times Y_{O_0}^n$$
- The deficient reactant concentration will be very small in the reaction zone:
 
$$Y_F \sim \frac{Y_F}{\beta}$$

Thus,  $w \sim \frac{w_{\infty}}{\beta}$

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Let us say  $Y_F$  and  $Y_O$  maybe you can you can have  $Y$  of power something and  $Y_O$  power something as far as these this particular argument is concerned I am just assuming those powers to be one it is not very important what those powers are at this moment or you can keep a power you can say you know why of power  $N_F$   $y_0$  power  $N_O$  that is also fine we can go ahead with this but not very important for the kind of order of magnitude analysis that we are doing here I just this change.

So let us say that we have this right the question is this  $W$  is actually a function of  $t$   $Y_F$  and  $Y_O$  right and the  $T$  varies like this but in the reaction zone the  $T$  variation is actually very small it is going from a value that is very close to  $T_F$  a valued here and look at looking at the way the variation happens it is actually very weak variation within the reaction zone so it is it is reasonable to assume that this  $DF$   $t$  can be plugged in  $STF$  all right but what would be the values of  $Y_F$  and  $Y_O$  that we have to use as I first could estimate.

What we would immediately think about is these are actually the mass fractions of the reactants  $k$  this  $F$  is the fuel oxidizer  $O$  is oxidizer and therefore these are the mass flow rate mass fractions of the reactants in the incoming stream and therefore we should actually if you have a premix big stir you have a certain mixed mixture ratio in which they are they are mixed right so There should be a certain mass fraction for the  $Y_F$  and certain mass fraction for the  $Y_O$  and that is what we need to use right.

So that would be given by some value some are here let us suppose that this is  $Y_F$  and  $Y_O$  which are far upstream ahead of the flame and for us the flame is starting here with if pre-heat zone right and what we are talking about is to actually estimated  $W$  that is going to be evaluated here we find that the  $W$  is actually lying dormant and nearly very low values up until here because of the temperature sensitivity do  $E$  right.

But that is not because  $Y_F$  and  $Y_O$  or  $0$  that happens only here you are going to have either  $Y_F$  or  $y_0$  or both going to  $0$  over here so what does that mean for  $Y_F$  and  $y_0$  how are they going to

vary can I can I just plug this up to this value and then now say where it is supposed to go to 0 at that I think since I said TF is not going to vary a whole lot I should not expect why after very a whole lot and then he suddenly goes to 0 is that the way it is going to behave if this is the way it is going to behave then.

I would rather take the far upstream value like with subscript 0s so you mean the Rankine-Hugoniot formulation we had subscript 0 for the upstream conditions and  $\infty$  for the round stream conditions TF corresponds to a corresponds to an  $\infty$  condition and if I were to plug in  $y_f$  as  $Y$  of 0 and  $y_0$  as  $y_{OU}$  not then this would actually mean that  $W_0 \rightarrow \infty$  then goes as  $e$  to the  $-\frac{E_Y}{T_F}$ ,  $Y_F$  not and  $Y_0$  right now this is actually a gross overestimate of what the  $w$  is so previously we said whatever is the  $w$  constant across.

The entire thing that was a gross overestimate then we said you know constraint this to a smaller region and got this factor and now we find how do you actually find out the  $W$  and if you now use the flame temperature in the Iranian expression and the far upstream reactant concentrations for the law of mass action then that is an overestimate as well because we cannot expect the mass fractions to drop so steeply in this region what I have what happen show would the mass fractions change fractions of the reactants vary across the flame that is essentially.

The question that we have to worry about so the question that we have to ask is okay, so we had reactants come in getting heated they get heated up and then they react to do what so what happens when the reactions happen they produce products right so the products are supposed to go that way right so this is the direction in which we are having the flow so the products are supposed to go that way but would they just do that would they just do that that is really the question right.

So if you now say that you have a product concentration that sort of is the opposite of what we anticipate without thinking about a particular thing that I am coming to then I would expect the product concentrations you probably rise like this right and then go all the way up to a maximum value let us say  $Y_p \rightarrow \infty$  all right, but if that was that if that were the case then you can

see that overall of the products are supposed to be get formed and then flow out but they now sense that you have a huge concentration gradient of the products.

Over here so what happens when you have a concentration gradient you will have diffusion anytime you have a concentration gradient you are expecting to have a diffusion and the diffusion flux is in the direction of a region of high concentration to a region of lower concentration so as the products are actually getting formed you have the fresh reactants coming and pushing them towards the other side but as they are getting form they are looking around and finding.

I am not there so let me try to go there it is only that the reactant flow is trying to push them here but they have a tendency to mix up there right so you now have a competition between convection of the flow of the mixture on the whole and typically you are always thinking about convection for a mixture okay, and upstream diffusion of the products so sure enough in this place where you do not have reactants happening you have a lot of products.

That are produced here you know or witnessing a incursion of products because of an upstream diffusion against the convection and there must be a balance between these two which is exactly the same as what we talked about for the energy balance which is a convective diffusive balance for the product species mass right, so effectively we should now begin to expect a product concentration profile that is similar to the temperature profile.

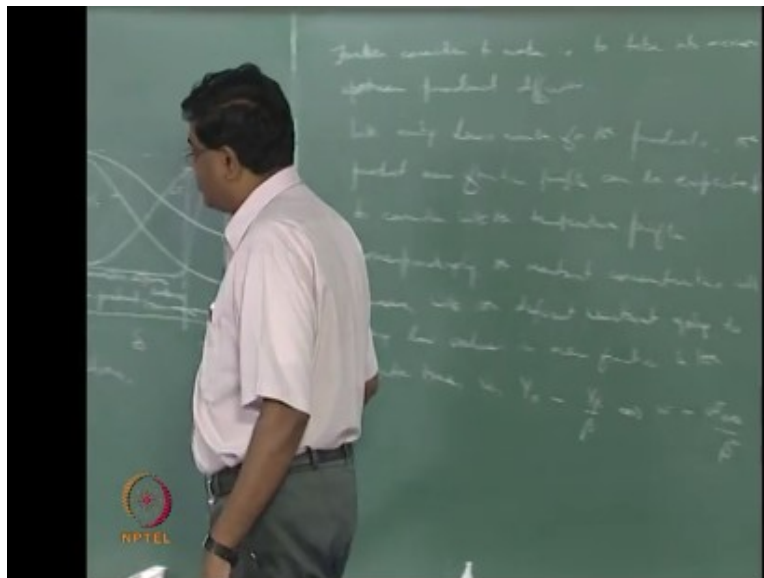
Itself because the way it happened was you now had a lot of temperature here that was produced temperature being produced that is essentially heat is being produced so the temperature is locally getting raised and then it gets conducted that is not very different from species mass getting produced and getting diffused upstream right even in the case of energy balance enthalpy flux that was trying to wash this hot region way from here.

And this heat conduction was like a convective diffusive balance it is trying to conduct heat upstream despite the flow wanting to go to ground downstream right exactly the same thing is happening for product mass right so this convective reviews the balance is happening for the

product species mass as well and if you were to actually now invoke a unity Lewis number for the products right so the lowest number is the one that is actually trying to tell you how well a species can diffuse versus how well it can conduct heat right.

So if you had a unity lowest number for the products then what it means is it is going to go through the same extent of convective diffusive balance in the preheat zone for it is species mass balance as the mixture went through for the energy balance therefore we should expect that the product concentration will be having pretty much the same profile as the temperature profile for a unity lowest number assumption on the products okay. Very So the further correction that we have to make is to take.

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An account upstream product diffusion upstream product diffusion and with unity Lewis number for the products the product mass fraction profile can be expected to coincide the temperature profile what has been why coincide how can you actually have mass fraction that is going from 0 to 1 coincide with the temperature profile that is going from let us say something like 300 Kelvin to about twenty-five hundred Kelvin the answer is of course we normalize okay, so you take the maximum in the minimum.

And then try to fit them from 0 to 1 ok 44 both cases then you should actually expect that the profiles will coincide well if that means you had a product upstream diffusion what is that thing as far as the reactant concentrations is concerned concentration really means concentration how much of what you have is there in relationship with what else is there right mass fractions are all about the density of this species divided by the density of the mixture right so that means if you now have products over here.

You have other things that are coming in and contaminating your reactants so the reactant concentrations are going to depth right so effectively then you do not have either this profile for the products that you would anticipate naively without taking the count of streamer product diffusion and correspondingly we have to know we have now to alter what the anticipated reactant concentrations are going to be so what you could expect is the reactant concentrations should now be the inverse of the product concentrations.

So if you now start with something like a normalized value with respect to the initial concentrations as here then you should expect your reactant concentrations should go like this now this is obviously for the deficient the efficient reaction let us suppose that we are considering a few lean situation okay, if you now consider a few lean situation then that species concentration mass fraction is going to go all the way to zero and that is the reason why your  $W$  is also going to zero at the end of the reaction zone right.

So now look at what happens to the species a mass fraction variation within the reaction zone instead of actually having a value that is about that high you are now looking at a value that is about so high okay there is hardly any variation of this away from 0 so we are now talking about fairly small values so correspondingly you should anticipate that if your  $W$  were to be calculated with  $GST f$  which is all right you should probably actually now have a factor  $\beta$  thrown in on your  $YF$  okay.

We have to now decrease the amount of a  $YF$  relative to the initial or the upstream far upstream value and therefore we have to bring that in right so in fact we could be good just for the sake of

completeness go back and then say let us suppose that this is M and N and we want to say mm m and n so correspondingly the reactant concentrations will decrease with the deficient reactant with the deficient reactant going to very low values in mass fraction in the reaction zone right now if you think about.

So that means we should basically say that is Y F for example should now actually be move like Y F divided by  $\beta$  so correspondingly our W should be going as what you would call us w not  $\infty$  divided by  $\beta$  power m right.

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Third Approximation

- Consider a single step reaction. Then,
 
$$w \sim A \times \exp\left(\frac{-E}{RT}\right) \times Y_F^m \times Y_O^n$$
- Assume  $T \sim T_f$ . Then,
 
$$w_{\infty} \sim A \times \exp\left(\frac{-E}{RT_f}\right) \times Y_{F_0}^m \times Y_{O_0}^n$$
- The deficient reactant concentration will be very small in the reaction zone:
 
$$Y_F \sim \frac{Y_F}{\beta}$$

Thus,  $w \sim \frac{w_{\infty}}{\beta^m}$

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So you would now say YF is 0 divided by  $\beta$  so  $\beta$  power amp should show up for your denominator with W not  $\infty$  in the numerator to give you W so question then is what happens to the X species okay, so the X spices work could actually come out like that to whatever value let us say y 0  $\infty$  all right.

Now that is an appreciable fraction of the original value and so if you from an order of magnitude basis it is probably a factor of about two or three that is not a factor of ten so it is not really an order of magnitude different right so without worrying about the non deficient or excess



species a mass concentration reduction we are still within an order of magnitude okay, within the order of magnitude in our estimate so that that is reasonable so you do not have to worry about this that that is essentially.

How we should go on to look at on the other hand if you are thinking about like a mixture then both of them are going to be equally deficient right so you have to make this correction so keep that in mind so that that is an additional correction that we want to do we want to go back and say this  $w$  is not going to be just  $w_{\infty}$  right this  $\beta$  here was to make sure that this  $w$ -whatever it is  $w_{\infty}$  or not is going to be confined to a small region when compared to the flame thickness but on top of it.

If you now say  $W$  is actually  $W_{\infty}$  then that correction basically says no it is not it is  $w_{\infty}$  divided by  $\beta$  power amp this what did he have to plug in there alright can we do more right can we anticipate something more than this or are we really pushing our luck trying to get insights into how things are supposed to happen right without doing the mathematics give you hardly doing much mathematics here we are just doing mostly order of magnitude anticipating things how they are supposed to happen and so on right.

So in fact I specifically say expected to coincide that is the crux there to get you this and this is not robust to say that this is going to be like this is not robust they are just an order of magnitude estimate good then what else can we do what are we made an assumption here on we have made the assumption about unity Lewis numbers right we made a unity Lewis number assumption on the product to say that it is going to coincide with the temperature profile all right.

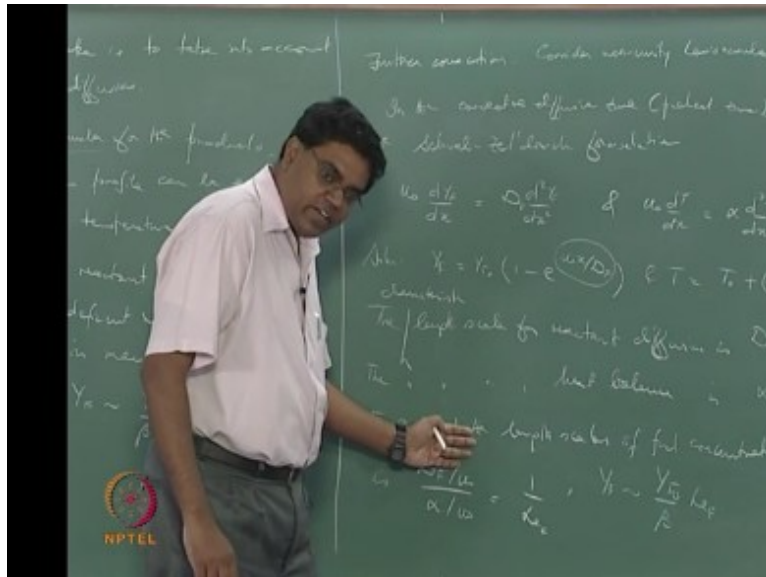
And correspondingly we if you now say that if the product concentration profile is like this the reactant concentration profile should follow like this is how we have actually built up our argument now that implicitly then assumes that the rare concoction goes number is also on right because effectively whatever we talked about for the product happens for the reactant species mass balance as well that means as far as the reactant species mass is concerned.

You have a convective diffusive balance in this region for the reactant species mass right and if you now assume that the length scale of this particular balance is the same as the temperature

profile then we are implicitly assuming that the Lewis number for the reactant species is also equal to one right that means the species the reactant species can diffuse just as well as it can conduct heat is what we are basically assuming that need not be the case and that is why are we talking specifically about the reactant Lewis number and just forgetting about or abandoning the product Lewis number that you originally constructed argument based.

On is because the reactant concentrations the ones that are showing up in the law of mass action that is what we are beginning to correct and we want to now see if a reactant Lewis's number is not going to be one is it going to be this way or that way right is this is this a profile going to actually change right so how do you how do you take this into account there are there is a quick way of doing this.

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So further correction consider so considered non-energy Lewis number of deficient reactant right so how do you expect the reactants profile to behave and how do you expect the temperature to behave so in the convective diffusive zone which is the preheat zone right we could apply the Schwab's elevated formulations and what would you have let us suppose that you

had a velocity  $u_0$  which did not change significantly then you have a convection balanced by the species diffusion.

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**Fourth Approximation**

- Apply Schvab-Zeldovich formulation in the convective-diffusive zone (preheat zone):
 
$$u_0 \frac{dY_F}{dx} = D_F \frac{d^2 Y_F}{dx^2}$$
- and
 
$$u_0 \frac{dT}{dx} = \alpha \frac{d^2 T}{dx^2}$$
- Solutions are:
 
$$Y_F = Y_{F_0} \left( 1 - \exp\left(-\frac{u_0 x}{D_F}\right) \right)$$
- and
 
$$T = T_0 + (T_f - T_0) \times \exp\left(-\frac{u_0 x}{\alpha}\right)$$
- The length scale for reactant diffusion is  $D_F/u_0$  and for heat diffusion is  $\alpha/u_0$ . Thus the ratio of length scales is  $D_F/\alpha = Le_F^{-1} \Rightarrow Y_F \sim \frac{Y_{F_0} Le_F}{\beta} \Rightarrow w \sim w_{\infty} \left(\frac{Le_F}{\beta}\right)^m$ .

You can write it assuming a fixed off formerly fixed law kind of diffusion going on and a you not dt over DX equal  $\alpha d^2 t / DX^2$  now what you are going to do is this just focused only on this particular region and as far as this region is concerned you are going to simply say let me not worry about the difference between this in this okay let me not worry about the difference between this in zero right.

So it is as if like it started from this value and went 2-0 here you start from this value and went to TF there within this region okay and so with these kinds of boundary conditions that you want to apply in fact you should you should be able to also fix your coordinate system and say that these values are actually in at negative  $\infty$  so if you now apply these kinds of boundary conditions you can get solutions I am not rigorously solving this step by step for you just going to write the solution here and trying to explain.

The adoption of these boundary conditions intuitively some very important for us to go through the steps of the stage let us go back and write  $DF$  to be taking into account the diffusivity should be if the fuel particularly which is not necessarily the same as the other diffusivities of species and here you are going to have three equals  $T_0 + TF - T_0$  times  $E$  to the  $U_0 u_0 X$  divided by  $\alpha$  so let us see what is going on it is easier to see this first is what we have been considering.

First we take the thermal profile you see what is going on we have a temperature that is now going to actually increase in excess of  $T_0$  by a difference of  $TF - T_0$  times a exponential factor right which obviously is going to actually increase exponentially beyond the preheat zone so the temperature as far as this profile is concerned is going to give you something that keeps going like that okay, disregard that that is not part of our domain as far as this equation is concerned this equation is valid and only in this domain.

Okay so once you understand that then this profile is quite reasonable for you to think about right and correspondingly you will now have your  $YF$  starting from  $Y F_0$  and decreasing by this factor okay, why are we doing this we want to be able to see this in both the cases right so as  $x$  increases within the preheat zone you are now actually looking at a exponential of  $x$  divided by  $D F$  divided by you not right so the length scale for reactant diffusion is or should say characteristic length scale right characteristic length scale for species diffusion is  $DF_0$  you not are we okay.

This is like meter square per second this is meters per second so meter square per second divided by meter per second should give you meters right so is how to wherever you come across these kinds of things you have to quickly check your dimensions right then the characteristic length scale for heat balance right this is this is in the preheat zone for the conductive refuse of balance right is  $\alpha$  mobile resolved that is a characteristic length scale so the ratio of the characteristic of the length scales of full concentration.

To temperature profile temperature profiles temperature profiles is then  $DF$  over  $u_0$  divided by  $\alpha$  over  $u_0 t$  which is equal to one over  $lef$  because  $lef$  is  $\alpha$  over  $DF$  okay so we have if your these number of the fuel is greater than one all right then the fuel concentration length scale is going to

be less than the temperature profile length scale that means if I go back and use a different color chalk piece and say forget about that that say that say X species so what you are talking about is we are saying that this length scale for the species is now going.

To be  $\Delta f$  NE  $f$  greater than 1 if I had a space number for the fuel greater than one then whenever something greater than 1 is less than 1 therefore  $DF$  over  $u_0$  is less than  $F$  over you not and therefore this distance should actually be less than that distance so instead of just talking about a single  $\Delta$  we will now talk about a thermal flame thickness and then we will now talk about a mass flame thickness right so what then happens is how do you now think about the concentration profiles the concentration profile is now going to actually begin to drop only here nor there right and considering that it is continuing to be a deficient react reactant let us say for the fuel is what you are talking about you have to get back to this as you come down.

So you are now going to drop a line that goes like this well let us try to make this a little bit better so what has happened here what we find is instead of having a variation that was like only so small within this region right you know having a larger variation within the thermal region right so that means your concentrations have to be taken to be higher than what we did here so this  $\Delta$  was to take into account the reaction zone based on the thermal flame thickness rights calling the thermal flame thickness.

For the reaction zone thickness but we found that as a Lewis number is greater than 1 the concentrations in the reaction zone based in the terms flame thickness will be higher than this so correspondingly we have to say are right  $YF$  then will become  $YF$  not divided by  $\Delta$  times  $lef$  because  $lef$  is greater than one and we need to now  $x$  this axis  $LEF$  than unity to factor in that your concentration is going to be more.

Now of course we hope that this factor of multiplying  $LEF$  should now be the same when you knocked think about a  $LEF$  that is less than one right so how would that work so when we take a different color chalk piece let us try pink when you now say that  $lef$  is less than 1 then the mass if  $d, d, d, d$  the species mass balance length scale is going to be greater than the thermal balance length scale right.

So the pins we should now be thinking about a, a flame thickness based in this to  $b \Delta F_{lef}$  less than 1 and how would you draw your profiles you would start from here but you would start dropping your concentration right here and then reach up to this point right so that would be something like this what you then find is the concentrations are even lower than the situation corresponding to unity lowest number so the Rays number was actually less than one for you so you just multiply by that factor to get a concentration that is less than that so sure enough so you need to have this kind of a multiplication going on therefore then your  $w$  should go as  $W \propto \infty$  times LEF divided by  $\beta$  power  $m$  right so this is what we could actually plug in back here too now not only take in the count of stream diffusion of products and correspondingly downstream diffusion of reactants in addition to downstream convection of the reactant.

So that the concentrations of the reactants are actually coming down in the reaction zone we could also now look for preferential diffusion that means you now say we only have a non unity Lewis number the reactants actually diffuse preferentially depending upon their Lewis number relative to the thermal balance right and then we find that the concentrations of the deficient reactant which is no critical in the reaction zone can vary with the lowest number.

Itself in a way that we can see so this is amazing in my opinion because we just think about what is going on okay and then start expecting how these variations should be and the interesting thing is if you have to do the rigorous analysis as we will momentarily comments to do number one we will be constrained to make assumptions particularly about unity Lewis number like for example the Schwab's earlier which formulation essentially assumes one other one of the assumptions is the unity loose number.

So if you now adopt the Schwab Zeldovich formulation to solve the problem of a one-dimensional laminar flow pre-mixed flame propagation then we will be constrained to do this for a unity lowest number and then we will have to relax the assumption of unity Lewis number and then expand the scope of the analysis and then take the take the burden of nonentity Lewis number upon ourselves and do a fresh analysis for that what you will find at every stage of doing the mathematically rigorous analysis with a unity lowest number.

Assumption that is up to the stage right or taking into account a non-integer lowest number and reaching up to this stage you will find that the mathematical analysis is different from this only by a factor of square root of two right otherwise you get all the all the factors that you want in there in the way we have done this square root of two is like one point four and four so you are X Y or your order of magnitude estimate is actually okay, within about forty one percent right that is essentially the power of daughter of Magnus's the additional bonus is we started actually using some of our gray cells instead of just now plugging and chugging equations and so on which we will now do you.

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