Combustion in Air Breathing Aero Engines Dr. Swetaprovo Chaudhuri Department of Aerospace Engineering Indian Institute of Science, Bangalore

> **Lecture - 17 Governing Equations V**

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Now, coupling function formulation is the topic, and now we will consider a general reaction and general reaction, but a 1 step reaction because it is though it can be applied to multistep reaction it is easy to understand in terms of a overall 1 step reaction.

So, general 1 step overall reaction overall one step reaction is nothing but this 1 i is equal to 1 to n if you remember our formulation from the kinetics class M i goes to summation i is equal to 1 to n nu i double dashed times M i. And then the species independent reaction rate which was omega is given by the species consumption rate W i divided by capital W i which is a molecular weight of this species nu i double dash minus nu i dashed.

If you have any confusion with this formulation you can just go back to the kinetics theory the chemical kinetics class and just take a look and get refreshed, whereas this guy is nothing but B T to the power of alpha exponential of minus e a by R 0 T this part is the reaction rate constant K times the law of mass action it is depends on the continued product of the species concentration raised to the a stoichiometric exponent C j nu j

dashed. Now if we consider the distinct specific formulation and which was and got get the species conservation equation that was this is C p i and the distinct specificate whereas, D i j is equal to D that was the statement of the species specificate distinct specificate formulation.

So, this was this species conservation equation was dou rho Y dou T plus divergence of rho v vector species consumption production rate and that becomes when you apply sorry when you apply this onto here is a left hand side. So, this is once again convection term this is the species diffusion term this is the characteristic diffusive becomes rho D is equal to the molecular weight of the species i times nu i double dash minus nu i dashed times a species independent reaction rate omega.

Now, now what we can do is that we can define a stoichiometrically weighted mass fraction now we will use some non dimensional parameters because these non dimensional parameters as you see will be make our life much simpler in terms of the analysis it will immediately. Immediately it will look little complicated and it will not be clear why you are actually doing this kind of non dimensionalisation, but later we will see that when you do this kind of a non dimensional the equations become very simple and solution just will involve 1 or 2 3 1 or 2 steps.

So, equations become much much simpler to solve and of course, it becomes much more insightful. So, Y i tilde we define as the non dimensional stoichio or stoichiometrically weighted mass fraction is given by one by sigma i n Y i divided by Y n at boundary what is Y n B i will define sigma immediately, but before that Y n B is the species mass fraction of an nth species which is the reference species at a boundary of my domain what I will come to this when we will consider a specific example which is at the domain boundary where this thing is essentially known and fixed.

So, that is why we define it at the boundaries of course, you need to know the boundary conditions to solve it. So, it must be known at the boundaries. So, whereas, sigma i n is equal to molecular weight times S, this stoichiometric coefficient difference divided by the same for the nth species which is the reference species this is the thing.

So, now, when you put this into this what we get is nothing but we get we can write in terms of an operator D rho D T, this is the operator actually not the full thing rho v there is a convection term plus operating on a quantity any quantities and this can be actually operating on Y i tilde and that is equal to W n, whereas so this is what we have obtained from the species conservation equation.

We took the species conservation equation and the distinct specificate formulation we applied this non dimensionalisation of Y i tilde is nothing but Y i by Y n at the boundaries which is known divided by one by sigma i n sigma i n is nothing but W i divided by nu i double dash minus nu i dashed divided by W n nu n double dash minus nu n dashed. And then if you apply this these 2 things in the distinct specificate formulation in the species conservation equation we arrive at this thing.

So, this is an operated form which we can write it as this L D Y i tilde is nothing but W n of course, because of the coefficients in the front now W n changes and W n is nothing but this thing. Now this was the species independent reaction and all these things arises, because of the non dimensionalisation you should I mean it does not look at all complicated you should just take the equation and just do these things yourself and then it will become as clear as possible it will become very very clear.

But then you see that now we can write this full thing the thing is that whereas, this is our operator L D this bracket whatever is in the bracket which is operating on essentially this guy this Y i tilde and that is equal to W n so that we can write this form essentially. Now, we can because it is true for any species W i now the advantage that you see here is that, but we have written this operator this dou rho dou partial rho dou T operating on Y i plus divergence of rho v vector minus rho D divergence authorating on Y i is equal to W n.

Now, the advantage is that on the right hand side you do not have a species this species specific the species specific reaction rate in the sense that you have a W n which is only written in terms of the reference species it is not in terms of the i-th species. So, this on the Y line the L; L Y on the left hand side you have an L D Y i it is on the right hand side you have a basically a source term which is not dependent on Y i i i-th species or such it will it is dependent implicitly. So, this think that not explicitly, but. So, what I can do is that I can write another equation L D Y j tilde and that is also equal to W n and then we can just subtract. Now because all these differential that we see are commutative with respect to linear operations that is addition subtraction I can write L D Y i tilde minus Y j tilde is equal to 0 because these are just when you subtract them this becomes equal to 0.

So, now we can basically we arrive at a conserved scalar which is nothing but this quantity beta I can say it is beta i_j which is Y i tilde minus Y j tilde and this operator L D is equal to 0. So, by this you know basically you got rid of the reaction rate term right. So, that is the advantage here. So, you just summarise what we have done is that we have basically arrived at this we took this was a species conservation equation for constant D that is specific heat constant specific heat.

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And then it consider this one step reaction and this was our species independent reaction rate and what we saw here is that that when we write it in terms of this we can write this in terms of omega. And then of course, this is you know slightly different form. And then similarly for j we can write it as like also in omega. And then you must subtract these 2 things it becomes 0 of course, this here we have not done non dimensionalisation, but if you look at non dimensionalisation is actually the same thing.

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So, by this we have actually obtained that this B i j is becomes essentially a conserved scalar and for the reacting flow. So, L this conserved scale with this operator L B $\rm i$ j is equal to 0. Now consequently the fundamental variable is not Y i, but a stoichiometrically weighted variable this. So, that is the trick essentially here which we have done it was the same thing you know when we have did it in the non dimensionalisation and which you can also do without this non dimensionalisation, but it has to be weighted with the stoichiometric variable and that is what causes.

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This removes this right hand side and this one also as I said that we can also define a non dimensional function like and also we can define a beta i j be like Y i tilde minus Y i j tilde that is what we just shown here. So, this store essentially the same things and we can do it in both way now the thing is that this we got rid for the for the species essentially.

Now, for the energy conservation you can actually do a similar thing of course, the energy equation is little more complex this is a sensible energy equation where we have a 2 source time one from D p D T and from this thing. And now we can again define rather ash a non dimensional quantity that is h s tilde which is equal to h s divided by Y n B divided by q C n or T tilde is equal to C p T divided by this thing now Y n B. Once again the species mass fraction for a reference specie known at the boundaries and what is q C n q C n is essentially a stoichiometrically weighted heat release rate. So, this is what this

thing is and then if you one dimensional as p tilde. So, as rho one T tilde then we can define another operator operating on a non dimensional h s tilde and that is given by this.

So, if you add the results of A and D that is the previous thing that we have obtained that is this; this contents once again and W n. So, the if you if you see that this L that is that is L D of Y i tilde is equal to W n and here from this we get this of h s tilde is equal to this transient term 1 minus 1 by gamma D p tilde D T minus W n now if you add these 2 things what you find is that this these 2 actually are essentially the same thing. So, we can write it as the capital l. So, Y i plus n and if it is a steady state which is said that D p is equal to 0. So, then we have this I think becomes is equal to 0 and then you have can define this we can define this whole thing as beta i and then you have L of beta i is equal to 0.

So, this is another when you couple we can using this coupling functions you can essentially couple between your stoichiometrically weighted or non dimensionalised enthalpy sensible enthalpy and your non dimensionalised species mass fraction the stoichiometrically weighted species mass fraction of course, species mass fraction itself is a non dimensional quantity, but with this you can when you stoichiometrically weighted you can essentially sum these 2 to get rid of the W n term that is the source term.

And so you have seen that this is what we did you know coming this and chemically reacting flows and diffusive system governed by n plus 1 equations you have L of Y i tilde is equal to W n L of h s tilde is equal to minus of W n is D p D T is equal to 0 and this can be alternatively described as L of beta i that is if we sum these 2 things Y i plus h s tilde is equal to 0 and or L h s tilde is equal to W n.

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So, this of course, the thing to note here is that if we have n species of course, you have n governing equations and you have one h s tilde, right. So, you have n plus 1 equation actually. So, you can combine between all of these with each species you can sum up this h s and then can rid of this species reaction rate term, but then you will still be left with this one that is L of h s is equal to minus W n and it should be there because you cannot really if you something for a combustion system you cannot really get rid of the reaction rate is not physically not possible.

So, you still keep it there and this will be used to basically obtain the h s tilde. So, with this you can simplify the equation by we can get rid of essentially the source term and this coupled. So, each of this beta is can be solved independently and then after you have solved you have solved for this and then you get the complete information about the Y is and h s tildes.

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So, this is what we want to say that n equations can be solved for conserved scalars say beta i, but the chemical information is essentially then contains in the n plus oneth equation and then LHS is equal to is equal to minus n which is solved last now of course, the key assumption is that we have to include that that diffusivity is equal for all the species that is the this was the distinct specificate thing. Specificate assumption which means the diffusivities are equal and if the diffusivities are not equal you could not have solved in this manner.

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So, that is very important though other formulations when you those are the problem is that as we you see that this coupling function formulation requires equal diffusitivity or equal unutilised number or essentially unity Lewis number and there is a local coupling function formulation which we will essentially which means that the local coupling formulation which will show which holds in a very local region in space which can basically work for a different diffusivities and non unity Lewis number.

So, we will do that and we will do that analysis and because that is a revealing in terms of how basically species diffusion affects this coupling function now that is also important because in combustion systems this unity Lewis number assumption is another very good assumption. And there are various key processes like instabilities in flames with this you not the thermo (Refer Time: 17:57), but other instabilities like diffusion thermal instability etcetera which is happens only because, when the when the Lewis number is below certain range and below certain value does when is less than unity etcetera.

So, it is important to understand the concept of non unity Lewis numbers and have coupling function formulations for non unity Lewis numbers and the other thing that will come out of it is that this will be give you the idea of the local coupling function formulations. So, that is what we shall we shall proceed into now and rest we will do the local coupling function formulations and that will do the derivations for that.

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So, the local coupling function; function formulations the need arises this is the local formulation now the local coupling function formulation need arises because as we have said that in the previous case the restrictive assumption for arriving at the coupling function formulation was that the diffusivities has to be always all equal the D i js is equal to D and also Lewis number is equal to 1 right. So, that was a restrictive assumption.

So, what we will do now is that- that we will do it only in terms of locally why do we essentially neglect convection neglect the convection in the sense that. So, the idea is that we will separate the flow into this where the combustion is happening in 2 parts right. So, here suppose this is a pipe this is combustor in which combustion is happening in this manner in this part. So, this is your flame right. So, we will say what we will say is that that all these regions all omega is that is your species production rate or species generation reaction rate etcetera species production rate species consumption rate of the species independent reaction rate these are all 0 here. So, only part these and is not equal to 0 in these regions.

So, we will have when this is equal to 0 we do not need to bother about the source term essentially. So, it is identically equal to 0, right. So, in these regions where do you need an coupling function when you know that the reaction rate is 0 we only need to bother about the source term when we know that there is a flame and then it is not equal to 0. So, we will only apply the coupling function in this sort of this thin regions, but in this sort of thin regions the most important thing is that you see this because of the large activation energy the regions are actually very thin and the flame essentially is very thin and when the flame is thin the temperature rises very sharply in a small amount of in a in a small region right.

So, it is a very compact region and. So, what we can do is that we can apply the local coupling function the coupling function formulation only in this part of the regions and not in this part because there may rise this reaction at a 0 itself and what we will assume is that because the temperature rises in a very sharp regions. So, if you plot the temperature here and the temperature, so, if you plot and this is your temperature axis and this is the x axis. So, you see that the temperature rises very sharply like this right

So, this is a very sharp gradient that you see here. So, when you have a very sharp gradient here higher derivatives will become important as a result the diffusion process become important is because it appears as a second derivative inside your governing equations where as your first derivatives which is like convection that is becomes less important. So, we will neglect convection in this region and we will consider only diffusion.

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So, that is the essence of the local coupling function n formulation. So, the local coupling function formulation essentially we can apply it because flame is compact because of the large activation energy and then we can do it. So, we will consider now this distinct diffusivity formulation where dou rho (Refer Time: 22:46) dou T density h s if you remember the distinct diffusivity formulation this was the generic formulation plus divergence of n rho v vector h s minus lambda by C p gradient of h s is equal to D p D T pressure term transient pressure term and summation i is equal to 1 to h i 0 W i this was the heat release rate term remember it. So, we consider steady satiate.

So, this is equal to 0, this is equal to 0 and also we neglect convection because we consider higher derivatives of course, you see that this term has 2 this is second derivative there is only first derivatives. So, we neglect here and this is only within the flame region. So, it is not value of an entire flame its only in the flame region we neglect this. So, the equation that we get is essentially this 1, so, setting all these transient terms to be equal to 0 transient to be equal to 0 sorry for that.

So, setting all these transient terms equal to 0 and setting convection to be equal to 0 because only we are interested now in the coupling function formulation inside the flame outside the flame there is no need for coupling function formulation, because reaction rate itself is 0 and we will not; this coupling. So, only within the flame we neglect essentially the convection and this is becomes a equation that is its balance between your gradient of second derivative of essentially the h s that is a conduction and the and reaction.

Similarly, for the species governing equation from the distinct diffusivity formulation this was the equation rho Y i plus divergence of. So, this is the species is a sample enthalpy this is a species equation once again transient term convection term diffusion term is equal to species production consumption rate for i is equal to 1 2 up to n of course, we neglect this when because it is we consider steady state we can neglect this because you consider convection to be not important.

So, arrive at this quantity. So, now, with the same non dimensionalisation that is h s is equal to h s tilde is equal to h s divided by q C this is equal to the h s divided by Y n B divided by times q C n that is this was a normalisation if you remember h s tilde is equal to h s by Y n this is important because this will be required in our next analysis of a flame also q C n non premixed flame as such. So, this is the normalisation and if you remember Y i tilde is equal to Y i divided by Y n times one by sigma this is Y n B this was one by sigma i n, whereas sigma i n was given by W i nu i double dash minus nu i dashed divided by W n nu n double dashed minus nu n dashed.

Now, if you apply this normalisation I will erase all these normalisations if we apply these normalisations in these equation these normalisation in this equations ok what you get essentially is i will just write it down that and if you assume that this is is specially non it does not vary in space similarly this is constant in space does not change in space. So, that it can take these out of the gradient we can take these out of the gradient you get Laplacian of sensible enthalpy non dimensionalised sensible enthalpy is equal to C p by lambda times W n.

Remember that form of W n which we discussed and del square Y i by Lewis number of i species is equal to minus C p by lambda W n so, and whereas, Lewis number of ith species is nothing but lambda by rho C p times D i. So, as you see that these and these are essentially same things just with a minus sign. So, we can just add these 2 things up and deform a new quantity beta i to be equal to beta i is essentially h s n tilde sorry h s is here it is a superscript not a subscript plus sorry this is tilde Y i tilde by Lewis number of i and this gives del square beta i to be equal to 0 right Laplace equation, right.

So, you see that with this coupling function formulation and this normalisation that is a part of this normalisations you have converted this very complicated state of coupled equations of course, there has been assumptions that it is transient time 0 convection is 0, but even then n you have converted this whole thing into this very simple Laplace equation, whereas del square beta i is equal to 0 and beta i essentially 0 conserved scale. So, I strongly encourage that you do this derivation yourself you can take a look into the book also it is basically I have followed from professor laws book C K law in combustion physics from Cambridge university place.

So, but this will give you a very strong sense of the different balance of this species and the enthalpy that is happening it might look little bit complicated in at first glance, but this is very important because it gives you a full sense of how this things how basically the you can form a conserved scale of even from non conserved quantities which an individual will not conserve. So, you can add them up and then the. So, you add them up carefully and with a proper weighting. So, you can create conserve quantities the reason is the reason is very simple fundamental the reason is that when you consider as reaction consumption of one means production of another right. So, it is damped property that you have utilised and these things are all related it is not that those species are essentially independent rather than enthalpy is in essentially independent right.

So, because of utilising that we have arrived at this from a very complicated set of equations. So, these were the 2 equations first we essentially got from the full set of equations we should remember from the full set we are we simplified it into this form which is the diffusivity form and from that we arrived at this simplified form we also considered the; so this was the this was the full complicated form of this sensible enthalpy equation from that by applying the fact that your transient term is 0 when transient term is 0 we apply that, we came at and we considered convection to be 0 because inside a flame only this steep gradients matter.

So, the diffusion terms matter. So, essentially the flame is a balance between your diffusion and reaction thermal it is thermal diffusion and the heat release rate whereas, and then you consider the species equation where we basically consider the transient term to be 0 and then the convection term to be 0. And once again it become a balance between species diffusion and the species consumption or production and then we normalised this enthalpy and normalised the species mass fraction. And then we arrived at this coupling function which is beta i is equal to h s tilde plus Y i tilde by Lewis number of the i-th species and then we arrived at this Laplace equation which is a beautiful simplification from this complicated forms.

So, ultimately we arrive at this del square beta i equal to 0 and this is very important from that we have done and then in the next class what we will do is that we will utilise this to arrive at to solve for basically the non premixed flames. So, this much for the governing equations that is. So, if you remember we used what we have done in this class in these 2 couple of this 3 4 classes of governing equations is that we have consider the Reynolds transport theorem to convert the conservation loss from a system to a system that is packet of fluid moving in space to a controlled volume through which the packet is moving.

And then we arrived at loss for essentially we arrived at loos for mass conservation continuity equation momentum conservation species conservation and energy conservation and then we have arrived at a different terms we have arrived at constitutive relations which can close these equations and then we have applied different kind of simplifications from. So, that we can arrive at useful forms of this equations and these useful forms we have again further simplify it for distinct specificate formulation distinct diffusivity formulation and then we landed up in a problem because we found that the species equation and the momentum and the energy equation was coupled.

The momentum equation did not come we did not explicitly consider because we found that in combustion here pressure is mostly constant. So, we do not need to bother about the momentum equations as such species conserved in space of course, the density changes. And the velocity changes, but main equations that we need to consider is essentially the species and the sensible enthalpy equation we also arrived at the sensible enthalpy equation by considering the internal energy equation, and then converting the internal energy equation to specific enthalpy equation the total specific enthalpy equation.

And then from this specific enthalpy is subtracted the enthalpy of formation to arrive at the sensible enthalpy equation and then from the sensible enthalpy equation we arrived at further simplifications using the distinct diffusivity or the distinctly specificate and then we removed the transient terms and then we considered the this then we also arrived at a generic coupling functions when we consider the diffusivities are equal.

So, when then we can apply that generic coupling functions for generalised equations when the diffusivities were constant where essentially are same and then if we then we also argued that the in some cases diffusivities may not be same. So, then we arrived at the local coupling function formulation and for that we argued that the for most part of the fluid when there where there is no flame we do not need to bother about the species we do not need to bother about the fact that the reaction rate couples the species or the products or omega i that is a species production rate or the consumption rate couples the species mass fraction equation with the energy equation that is a sensible enthalpy equation we do not need to bother about this because there is no flame.

So, that becomes active only inside a flame right. So, at thus that part we can simply set omega i or the W i to be omega W i is to be essentially equal to 0, but inside the flame what we do is that where we cannot said this to be equal to 0 because that is where the species is being produced is species is being consumed, but we erase that we argue for the fact that, because activation energy is large the flame is a actually a very thin occupies a very thin region in space and if it is if it is contained in a very thin if it is the flame is very thin that is its thickness is very it goes a very small volume and it is a very thin structure.

So; that means, which is not a fact of the large activation energy or the combustion reactions so, but if it is a thin structure it means that the temperature or the species gradients temperature or species gradients are very high there. So, temperature species change very rapidly inside the flame as a result of which it is not only the diffusion process that matter and convection process does not matter as much.

So, we neglected convection we considered steady state and we arrived at the simplified equations and this simplified equations for the sensible enthalpy sensible gradient equations for species. And from that again we applied this non dimensionalisation of sensible enthalpy non dimensionalisation of species and arrived at this simplified laplace equation for the coupling function beta i.

So, that is in a summary what we have done and then we will please remember this coupling function please note it down derive these things which will which will give you immense confidence in how the combustion governing equations where can how different parameters themselves. I strongly suggest you to do the derivations on yourself and then once you are ready will come and discuss about non premixed flames using these coupling functions.

Thank you very much.