Indian Institute of technology Madras

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COMPUSTION

Lecture 21
Schvab-Zeldovich Formulation 1

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

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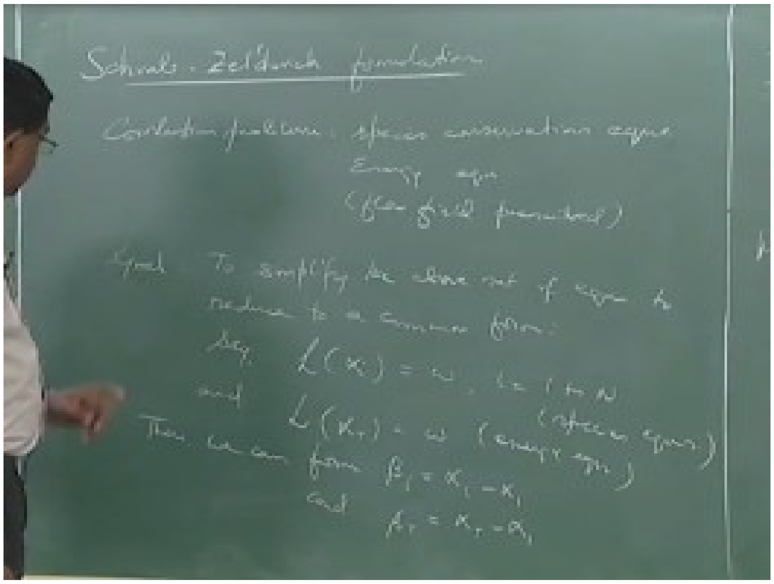

Schvab - Zeldovich formulation

Combustion problem: species conservation eqns
Energy eqn
(flow field prescribed)

Goal To simplify the above set of eqns to reduce to a common form:
Say, $L(\alpha_i) = \omega$, $i = 1 \to N$ (species eqns)
and $L(\alpha_T) = \omega$ (energy eqn)
Then we can form $\beta_i = \alpha_i - \alpha_1$
and $\beta_T = \alpha_T - \alpha_1$

Mainly the combustion problem now, so combustion problem of essentially having the species conservation equation equations rather and energy equation of course energy conservation equation. So this is what we want to now focus our attention on we simply say flow field is prescribed and let us not worry about the two-way interaction where we are assuming a density dependent temperature that influence is to flow back again the moment we will just say as far as the combustion problem is concerned the flow field is prescribed and the question is it possible for us to now simplify this set of equations right what do you mean by simplifying how do how do you want to simplify this?

Well if you think about it the species conservation equations is something which contains the capital V the diffusion velocity with the species diffusion velocities which are in turn given by the multi-component diffusion equation, so you now have these n equations relating to three n equations for the three components of this multi-component diffusion vector equation okay and that those are those are an excise where as this is NY ice you know have to have an additional a set of n equations to relate excise and why is so that is complicated enough alright and then you have this energy equation which has like lots of terms that are on the right hand side and each of those terms has lots of terms in turn and so on.

So it is actually a very low long equation our goal believe it or not okay at this stage is to try to simplify these two sets of equations to look almost the same not even similar, is that possible? Can we can be even dream up of making this set of equations and sop bowl of additional equations that it comes along with to look like an energy equation that is very long actually so it is possible if you now make lots of assumptions right but the goal here is goal to simplify the above set of equations to reduce to do a common form right reduced your common form in fact let me tell you what the form that we are looking for is say a operator L script L of something like an α I okay equal to ω and α.

So this is i = 1 ton right so obviously that is a species equations right species equations then let us suppose that we can now form a as per t which is also equal to ω okay and this is the energy equation right and that is one equation what we expect is αi should be related to why I in some way okay the primary are known corresponding to the species equations why I being the mass fraction of species I and α T should be related to temperature in some sense in a fairly direct way so long as we can actually establish those kinds of relationships and then say this stands for temperature that stands for species concentration then and then you now are able to write these two equations in this form okay then we can now form then we can form okay we can form βI = α I - α 1 you pick the first one okay first of the α okay.

And then subtract that from all other α well then you form a β I corresponding to that okay and β T = α t - α 1you pick the first of these α that is okay, alright and then subtract from α T to form a β T okay, now look for l the script l are to be a linear operator okay further now if you really think about it if you know if you know some basic fluid mechanics what you would expect is the nonlinear terms in fluid mechanics are primarily coming from the convective term in the momentum equation okay.

If you are prescribing the velocity field in the species conservation and the energy conservation equations then on the convective terms in those species equations and energy equation or not there they are not nonlinear because your velocity there are known the momentum equation you have a product of velocity times velocity derivatives and the velocity was an unknown any time you have a product of an unknown and it is with itself or its derivatives then that shows up as a nonlinear term.

But in the species equation and the energy equation if your flow field is prescribed that constitutes a linear term with a variable coefficient or a non constant coefficient that is all okay, so as far as the convective term is concerned which typically poses the non-linearity in fluid mechanics in the momentum conservation as far as the combustion problem is concerned we can expect it to be linear that is fine all right it is the other nonlinearities that be a lot of worry about like for example if you had a radiation term with the T to the power 4 or if you had this e $^{-ea\ /}$rut right the exponential term of the reaction rate depending upon temperature and so on those are the villains that we should be looking out for but we expect that that should actually be on the right hand side okay the L itself could be linear.

So if you now look for this L to be a linear operator then we get l α 1 = ω but L of β I = 0 and L of β T = 0 here I going from 2 to n because you can now subtract one equation from the other right you can try basically subtract the first equation from all other equations and then now form your pairs of α as for I - α 1 or as the t - α 1 and then plug in the β the right-hand side is the same for all of them so if you now subtract one from the other you get a zero right what is the advantage with zeros I really like zeroes do not be right.

So the moment you now have zeros the first of all it means that this really means that we are now looking at homogeneous equations right which are lot easier to think about when mathematically speaking when compared to in homogeneous equations where you have source terms influencing the mathematical nature of the equations otherwise okay, so first of all you are dealing with homogeneous equations that is like a big boon but implicitly we are also thinking it does not have to be zeros but thank God the nonlinear term goes away it was a right-hand side that was nonlinear we have this e to the minus e exponential of minus e rt which is a huge nonlinear term.

I trying to get rid of this in most of the equations that was posing this tiff problem right that was the one that was actually trying to vary in a highly nonlinear fashion that means it becomes very sensitive within a very narrow range of temperatures and you have to take like very small steps in time or space or both in order to try to should a variation somewhere they are near the flame and so on all those things you do not worry about for these equations.

You still have that stuck in one equation representing this for the representing the severity for the rest of the set and if you were to follow this then here we would recall β I and β T as coupling functions because they couple α together okay, β is couple α I and α 1 and β T couples α T and α 1 right.

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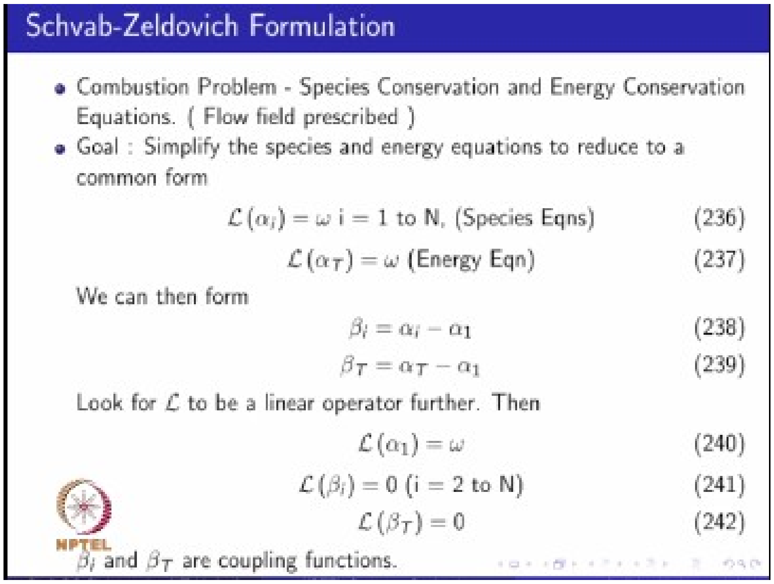

Schvab-Zeldovich Formulation

- Combustion Problem - Species Conservation and Energy Conservation Equations. (Flow field prescribed)
- Goal : Simplify the species and energy equations to reduce to a common form

$$\mathcal{L}\left(\alpha_i\right) = \omega \text{ i = 1 to N, (Species Eqns)} \qquad (236)$$

$$\mathcal{L}\left(\alpha_T\right) = \omega \text{ (Energy Eqn)} \qquad (237)$$

We can then form

$$\beta_i = \alpha_i - \alpha_1 \qquad (238)$$

$$\beta_T = \alpha_T - \alpha_1 \qquad (239)$$

Look for $\mathcal{L}$ to be a linear operator further. Then

$$\mathcal{L}\left(\alpha_1\right) = \omega \qquad (240)$$

$$\mathcal{L}\left(\beta_i\right) = 0 \text{ (i = 2 to N)} \qquad (241)$$

$$\mathcal{L}\left(\beta_T\right) = 0 \qquad (242)$$

β_i and β_T are coupling functions.

So these are called coupling functions, so our goal is essentially to simplify the above set of equations to reduced you a common form that is LF α = 0 ω for both the species and the energy together and then form the coupling functions so that we could actually get a homogeneous set of equations for a whole number of large number of equations except just one okay sounds very incredible at this stage if you now think back on what the equations are but the question is how do we simplify so this is the starting point right.

So we will now have to make a lot of assumptions 11 assumptions to be precise okay which are mostly simplifying assumptions, so we now make these assumptions and I want you to listen to this very carefully there are lower assumptions that we are going to make all right. So it could be as if you can you can expect an exam question or a PhD qualifiers question what are the 11 assumptions of the Schvab Zeldovich formulation because they are the 11 assumptions okay so we will make those 11 assumptions number one, number two whenever we make assumptions keep in mind we get into the habit of questioning those assumption how they good assumptions or are they bad assumptions are we making them mainly because we want to simplify the matter right or they just simplifying assumptions or are they physically tenable that means over can we justify them from physical grounds are they reasonable right.

We will have to go through that when we make those Levin assumptions the third is there a way we can relax these assumptions some of them many of them all of them right, so those will be your homework problems right, so I will try to point out to you which are the assumptions you can you can relax and has been relaxed in the literature okay and I will also point out to those literature and then you can you can say well work out the Schvab Zeldovich formulation with this assumption relaxed that is like one particular question in an exam okay.

So if you thought that you really mucked it up then the next question in the next exam will be workout the fobs Olivet formulation with relaxing the other resumption so you can keep doing this okay, and it will be it to be a pretty good piece of work actually okay. So do not do not take it lightly it is very important so I am not going to relax all the assumptions I am not that crazy okay.

So I will point out to some assumptions that can be relaxed, so the first assumption that you're looking for is a negligible body forces we also should be looking for why we are making these assumptions right so and then I will also point out to some things that we are not assuming as you go along so in that sense to draw to that extent the formulation is general enough because we are not making assumptions for example to tell you right away we are do not have to make assumptions about constant species we could have temperature dependent species that are different for different species all right that is what is great that means you can actually get the adiabatic flame temperatures predicted fairly well and then you’re your formulation should be able to show the temperature in your flow field.

So that is pretty good here the reason why we take one is actually neglect body forces is it shows up in your it shows up in this new set of equations it shows up in the multi-component diffusion equation right, so our goal is to try to simplify the multi-component diffusion equation to look like Flick’s law all right.

So that we can directly substitute the Flick’s law form of the multi-component diffusion equation into the species conservation equation right away just like how we did it the first time for a binary mixture. Then we do not have to deal with the multi-component diffusion equation separately anymore. So the question is what will allow us to simplify the multi-component diffusion equation to look like Flick’s law.

You remember the multi-component diffusion equation had four terms the first of those or what was the one that was going to give rise to Flick’s law then there was a pressure gradient term, then there was a temperature gradient term which was the solid effect, and then there was a body force term. So if you want to get rid of pressure gradient term and then you have to get rid of the body forces term, then you have to get rid of this solid effect okay.

So the first thing that we are trying to do here is to neglect body forces. Now if you get when back and actually looked at that particular term you had a FI vector - FJ vector. So you do not necessarily have to neglect body forces all together it is sufficient if the body forces were the same on all this same species right. So if not okay equal on all species that is assumption that we try to make okay.

Again negligible, so rate and do for effects terms involving DT, I right, this is this is the solid effect is actually neglected so that you can simplify our multi-component diffusion equation into your Flick's law, the ∂ for effect actually shows up in the energy equation which also we try to neglect primarily the justification being DTI over ρ DIJ is typically fairly small it has one order magnitude less than unity all right.

Therefore, it is insignificant or negligible most of the time, pressure gradient diffusion, pressure gradient should say negligible pressure gradient diffusion right, negligible pressure gradient diffusion. This term was looking more like YI - XI times grad P/P there are many ways by which you can neglect this one you simply say this term does not contribute a lot to the multi-component diffusion equation right, no matter how much it is you say it is very you now evaluate it and find that it is very.

The other way of trying to get rid of this term is to say that there you have equal molecular weights that means YI = XI, but there is a worse assumption than just saying that this is negligible right. The third way of actually trying to justify this is just the previous class we found that for low mach numbers the pressure is almost a constant, it affects only your flow field, but it is not really get into you your combustion field a lot right.

So as far as the combustion problem is concerned we could simply say the grad P is very small right that is the reason why we want to say the diffusion associated with it is even smaller right, okay. So that is reasonable, now neglect negligible bulk viscosity and viscous dissipation, these are related, but slightly different bulk viscosity effect can be neglected for incompressible flows when you are now looking at low mach numbers.

We are now talking about low incompressible flows so you can say that the divergence is equal to zero, so you do not really have dilatation effects coming in so bulk viscosity, the effective bulk viscosity is negligible, and this also shows up in the viscous dissipation if term and we are now saying the viscous dissipation itself is pretty small.

If you now do an order of magnitude analysis unless you are looking at situations of tribology like, when you now have a two surfaces that are actually in very close clearances and you had a fluid in between like in lubrication and so on, or if you have like re-entry effects where your mach numbers are so large and the boundary layer is so thin with a steep gradient effectively you looking for very large gradients of velocity that is when viscous dissipation is significant, otherwise you do not have to worry about it not typically in order in our application.

Five negligible radiant heat flux right QR vector right, now of course this is going to be a nonlinear term if it represent. So you are going to have a T^4 and T is an unknown so you are now looking at a nonlinear effect there. So try to get rid of it, okay, but of course when can say this is okay. So long as you are dealing with a gaseous medium this is reasonable okay.

But the moment you have things like surfaces you have to think a little bit harder okay. So if you have surfaces you have to look for whether those surfaces are transparent or opaque or if they are closer to black, if their emissivity is closer to black emissivity right. So if that is the case, then you cannot neglect this. So not valid when in problems with phase interfaces right not valid in problems with phase interfaces.

Well of course you will find in the literature there are lots of problems with phase interfaces that are being solved after neglecting radiant heat flux and you still get good results, it is not terribly bad okay. But in general the radiant heat flux is significantly small think about this you now look at a flame the fact that you are able to see the flame is because you have radiation coming and hitting your eye all right.

And you are like wait a minute, I could I could see the flame only because of radiation it is there how could I say how could I not take that into account the answer is that is quite small in magnitude. So we do not have to worry too much about this. Six we assume a steady flow we did that when we were trying to do on the low mach number assumption okay, so whatever we did in the previous class where we came to the conclusion the pressure remains almost a constant for low mach numbers is typically called the low mach number assumption right.

So the low mach number assumption was actually derived for steady flows which is something that we also adopt over here. The point I mentioned the other day was you do not have to do that okay. And similarly we do not have to do that here as well, you can relax this assumption can be relaxed, you should be able to relax this assumption and derive a unsteady equivalent or an unsteady Schvab-Zeldovich formulation okay, that is a homework problem for you.

And keep in mind what are we looking for, we are looking for a L, the script L operator right that should be linear and typically the time derivative δ/δt is a linear term it is not showing up any non linearity. So you should not have a problem with unsteady flows at all. So it should be able to relax this assumption. Then we say binary diffusion coefficients of all pairs of pgs right, or equal, that is there is DIJ = DIJ = D.

Not even saying that we have DIJ = DI that is to say we are not saying that the binary diffusion coefficients are the same as the multi-component diffusion coefficients. We call the multi-component diffusion coefficients are derived quantities, whereas the binary diffusion coefficients are more fundamental okay which come from kinetic theory. But we are saying here that all of them are going to be equal for all pairs of species, and this is very important for you to be able to plug in your multi-component diffusion equation into your Fick's law and then plug that into this species conservation equation.

Otherwise what happens is you now have this XI is equal to, sorry grad XI is equal to some coefficient times VI - V J, and you could draw a Fick's law only for a binary speed binary mixture where again DAB=DBA. And since only two of them are there and they are equal it is just as good as this assumption, and then you could have obtained Fick's law that is what we did before.

But here we have to get past that for a truly multi-component mixture more than two species, therefore, this assumption is necessitated okay. The question is it okay, the answer is not terribly bad typically you have to start worrying about this assumption if you are dealing with things like hydrogen as part of your mixture right. Let us say you have a mixture of hydrogen and hydrocarbon going through combustion, then the pairs of species involving hydrogen may typically have a higher diffusivity when compared to others.

And then that is machedly different whereas if you are dealing with most species of the order of the same molecular weights not necessarily equal you can expect that this assumption is a very reasonable assumption not bad at all okay. Eight low speed or low mach number low mach number this implies that momentum equation reduces to $P=\text{constant}$ to first order which means we could now say let me get a flow field that is prescribed I do not have to worry about solving for the flow field in addition to the combustion problem.

So I am looking only at the combustion problem, so that that is something that came from the previous class. Nine unity lowest number right, so question is what is lowest number right. So Lewis number Le is $k/\rho CpD$. Now keep in mind that D should really be like DIF in reality alright, so correspondingly you should have a Lewis number that is like LeIJ okay. But many times as we have seen earlier the DIJ can be replaced by like KDI that is like the multi-component diffusion coefficient rather than the binary diffusion coefficient.

In this case again we will now have to recognize that Le should be written as LeI that means it is different for different species. So you are looking at a Lewis number that should be really species dependent, and many times people talk about a fuel Lewis number or an oxidizer Lewis number that are distinct from each other right.

So what does this Lewis number really telling us $k/\rho CP$ is the thermal diffusivity and DIJ or D here is the mass diffusivity okay. So in SI units $k/\rho CP$ is going to be like meter square per second, and the mass diffusivity also has the same units meter square per second, and therefore, Le is a non-dimensional number which actually indicates the capability of a species to conduct heat just as well as it can diffuse right.

So we are now looking at comparing the capability of the species to actually transport enthalpy as it can transport mass right. So that they do not have to be necessarily the same right, depends on how well it can conduct versus what at CP is in comparison to what would how much it can diffuse itself as a mass right. Why would you want to now compare these two, and what you are now basically saying is this should be equal to 1.

This is a very, very important assumption I can be relaxed that is a good news okay, but it is a very important assumption why, because our goal is to actually look at the species conservation equation and the energy conservation equation and try to express them in a single form. How do you hope to do that if you know you do not expect the species to actually transport enthalpy just as well as it can transport the mass.

Because in your, these equations are essentially remember the convection, diffusion, reaction these are the three things. And if you had some sort of an intuition you would say that ω stands for reaction not just because it is a symbol, but I have been saying that this is the one that is containing the non-linearity in the rainiest term that is essentially from the reaction.

So if you now say convection, diffusion, and reaction and this is going to contain the reaction, then this is going to contain the convection and the diffusion. And sure enough prescribing a velocity you now simply have a non constant coefficient for the convective term coming from the flow field, and the diffusion term should be linear just as well as a convection term.

So we expect this to turn out to be linear that means we are looking for two terms here both of them linear, one of them coming from convection, the other one coming from diffusion right. If now these two terms should look similar for the species conservation equation, and the energy conservation equation, then we should be looking for the transport terms to be comparable.

So if you now have a species which is actually diffusing so fast, but it does not really conduct heat a lot that means it is having a non unity Lewis number less than 1 okay. Then the transport term, so the country or the diffusion terms in the species conservation equation and the energy conservation equation they are not going to match up all right, you are going to have a problem.

So the only way we can actually try to get these two together to look similar is if you now have a Lewis number. In fact in most of the earlier literature I will show you early like as late as even the 70s or 80s or even now some work, so many theoretical works that are getting published they would make a unity Lewis number assumption.

And sometimes when they relax this assumption and publish they would even put it in the title, like they would say blah, blah, blah, blah, blah for non unity Lewis numbers as if it is a big achievement that they have done, that they relax this assumption right. So that indicates the importance of this assumption okay, that is indicating the importance of this process of what is called as preferential diffusion when you now say the Lewis numbers are first of all not equal to one and not equal to each other.

So if you now say preferential diffusion you now allow for a oxidizer Lewis number to be different from a few Lewis number for example right, and sometimes you have this analysis that is done where you now assume that the oxidizer Lewis number is unity, but the fuel Lewis number is not unity or vice versa maybe okay. So many times you need this assumption in different ways, but it is still possible for us to think of writing not exactly in this form of course, but you will still be able to write something like a convection, diffusion and reaction okay except that the diffusion terms alone may be different by a factor of the Lewis number, if the Lewis number were non unity.

And that would be like the counterpart of the Schvab-Zeldovich formulation. We may not be able to form coupling terms all right. So it is possible to actually work with non unity Lewis numbers and proceed in the manner, if you know make all the other assumptions relax this assumption and see what happens it is worth pursuing that okay. Then we assume a chemical changes occur in a single reaction step, Σ=1 to n, UI’ script MI gives rise to ΣI=1 to n, μI’’ script MI, this is one step.

We do not entertain multi step chemical kinetics okay, that helps us in dealing with trying to split the enthalpy into the formation enthalpy, and the sensible enthalpy and deal with the formation in therapy term. So you now get a single heat release rate term because of the single step kinetics it is essentially what is happening is you now assume like there is only one reaction that is happening in the flame although there are lots of reactions that are happening.

But if you were to entertain many reactions each of those reactions is going to give rise to your heat release right, and some of them could actually absorb heat. So they are like a net heat release that you should be looking for, whereas we want to deal with only one heat release rate term not multiple heat release rate terms okay. So that is what this assumption let u you do try relaxing does either okay.

So we will talk a little bit about that as we as we go along, the eleventh assumption is a fairly straight forward assumption, no external heat flux that is a Q.=0, this was showing up as a solitary term only in the energy equation it was not there in the species equation. So if you now keep this then it is not possible for you to make them look alike right. So we have to get rid of this, this is reasonable again okay.

We get into this kind of situation only in some odd ball cases where you have to keep some externally heat generating mechanism or machinery within your domain all right, that is like some electrical heating or nuclear heating or let us say our heating or something of that sort which is not due to the combustion all right. Therefore, we do not have to worry about this and the most circumstances good.

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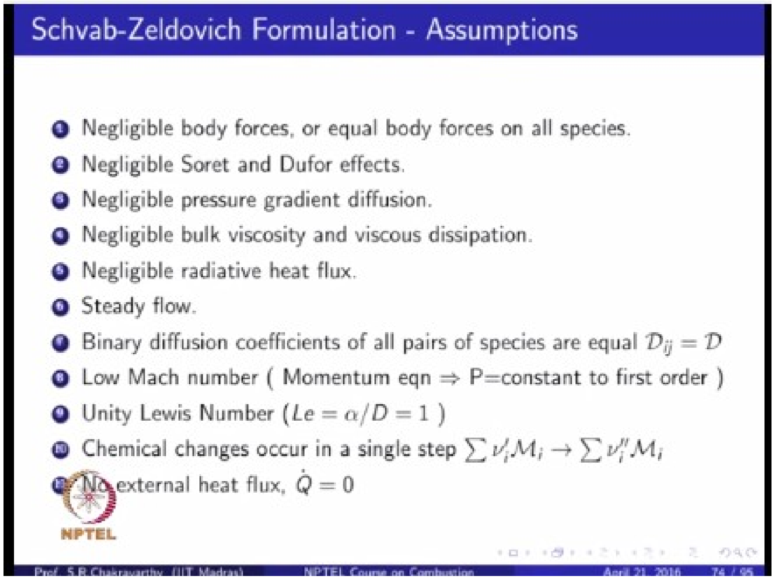

Schvab-Zeldovich Formulation - Assumptions

1. Negligible body forces, or equal body forces on all species.
2. Negligible Soret and Dufor effects.
3. Negligible pressure gradient diffusion.
4. Negligible bulk viscosity and viscous dissipation.
5. Negligible radiative heat flux.
6. Steady flow.
7. Binary diffusion coefficients of all pairs of species are equal $\mathcal{D}_{ij} = \mathcal{D}$
8. Low Mach number (Momentum eqn $\Rightarrow$ P=constant to first order)
9. Unity Lewis Number ($Le = \alpha/D = 1$)
10. Chemical changes occur in a single step $\sum \nu_i' \mathcal{M}_i \rightarrow \sum \nu_i'' \mathcal{M}_i$
11. No external heat flux, $\dot{Q} = 0$

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So we now have done through the 11 assumptions, now we go through the algebra, how do you crack the machinery to make this look like, we make these two equations look alike. So it is going to look, it is going to involve some magic all right, so you have to kind of watch out for how these manipulations happen and we will go through this, now when maybe in the next hour as well, and maybe by the end of them they should be we should be getting there to see whatever we are looking for.

Yeah, correct. The equations can still be considered linear, if you now have like two species equations you assumed a nonentity Lewis number all right, but the Lewis numbers were equal right. You now have two species equations which are still in which can be severe, where you can still form the coupling functions all right. And then you have the Lewis number, the equal Lewis number for each of those still sticking together.

It is only that you cannot make it look similar to the energy equation. So as far as the species equations are concerned they can begin to look similar right. And I am still saying I am not having a unity Lewis number, I am having non unity Lewis number. But non unity but equal you see, so there are such conditions. There are also other situations where it is possible for you to deal with like saying one of the lowest numbers is equal to one other Lewis number is not equal to 1, there you try to couple that equation with energy equation where the Lewis number of that particular species is equal to 1, but you keep the other one okay.

So typically, in fact what we will find is in the problems that we deal with, let us say we want to do like a pre-mixed flame or a diffusion flame and so on in the course, our starting point will be the shrubs elder which formulation okay. At that time we should look forward to seeing if we can relax the lowest number unity assumption for some of the species or say equal Lewis numbers but not necessarily equal to one and so on.

The point I wanted to make was what you will find us we will pick and choose some equations to form coupling functions and not worry about others all right. So this will depend on the way you assume your Lewis numbers all right. So it is pretty interesting the way we can deal with it okay.

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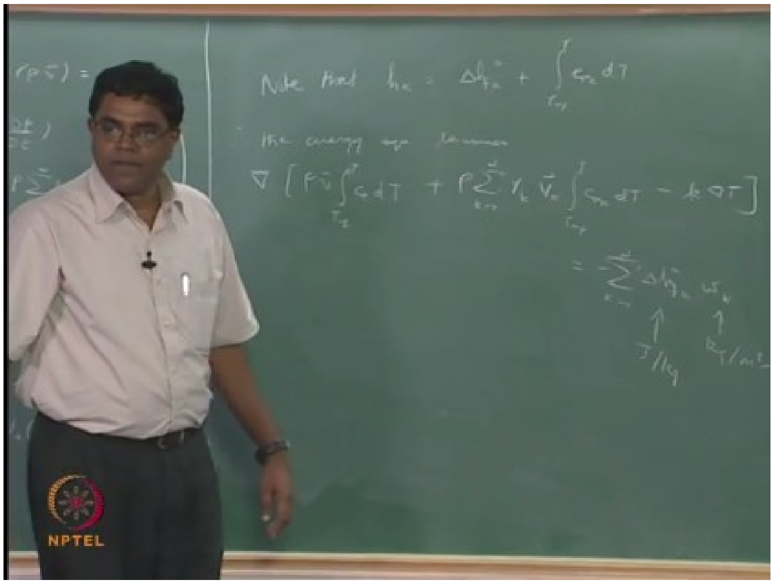

So now given the situation we now start with the overall continuity equation it simply leads to divergence of ρV vector = 0 right, we still deal with 3D, we will have a vector form of equations so that means it is a three-dimensional formulation nothing no assumptions on that right. Now let us look at energy equation with all the assumptions if you have made so no Q. viscous dissipation ϕ and DP/DT you get this DP/DT only for compressible flows, because we are now looking at a low mach number situation you should not have to worry about this.

Then you have a ρV vector. ∇H = ∇.grad T) - ∇. ρΣ k=1 to n, 1k VK okay, this is coming from your divergence Q vector, and Q vector had k grad T – K grad T and you had this term and you have the dufor effect and the QR you have the dufor effect and the QR outside of the grad Q. you had the body force work you had the viscous dissipation and you had the pressure work, so all those all those have gone.

So we are left with only these two, keep in mind what are you looking for, we are looking for giving this equation to look like convection, diffusion, reaction okay. Now the reaction rate term is actually embedded in here, this is going to be now written as H = ΣYK HK, where HK is the specific enthalpy of species k which can in turn be written as ∇HF K0 plus the sensible enthalpy for that right, and then the ∇H(K0) term is the one that is going to contribute to the heat release so that is where the reaction term is coming from in the energy equation okay.

The job of the reactions in the energy equation is to give rise to the chemical heat release that is embedded in here right. So this contains both the convection term and the reaction term that we are looking for, this is the diffusion term that we are looking for from an energy point of view. This is the essentially the energy transport term okay that is something that we have to deal with it is not something that we were looking for.

It is not there in the species conservation equation okay, but you do have a capital VK showing up in the species conservation which will now have to be replaced by a Fick’s law having a gradient YK. So this is going to be a little bit more involved then it seems okay. So now note that h=Σ YK HK all right. Now therefore, Σ YK HK divergence ρV vector equal to zero starting from here.

I just multiply these two right and right hand side of this is equal to 0, therefore this should be equal to 0. Now add the above to the energy equation right, and then you have, so what do you get if I can now add this to this which is essentially zero okay, I can now try to take the divergence out you see you have a ρV. grad H here we have a this is H times divergence ρV.

So if you now add these two together we can get a divergence of ρV times the H you see, so I can get this divergence of ρΣ HK YK, and then what happens, why did I do want to do that, because however, divergence of ρ times this right. I should now be able to combine these two v+VK right. And I also note that this is like a divergence term. And so if I now have a divergence that is outside I should not be able to write this also inside k gradient T=0.

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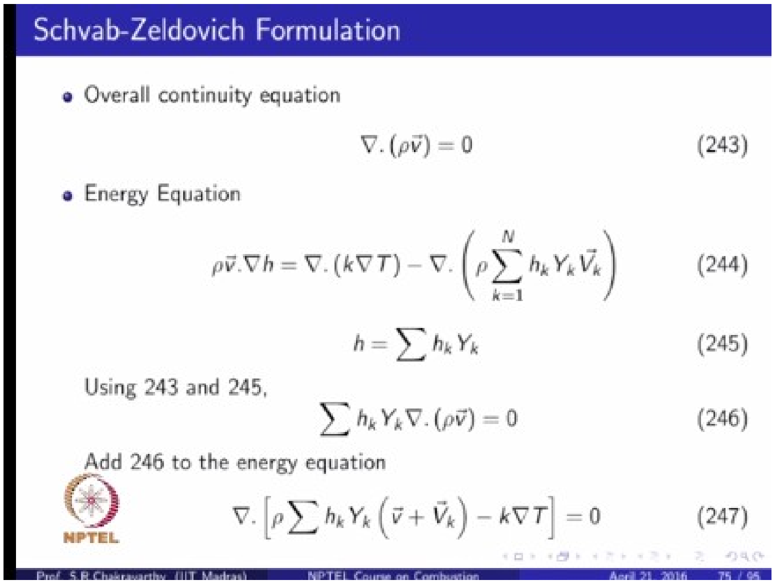

Schvab-Zeldovich Formulation

- Overall continuity equation

$$\nabla.(\rho\vec{v}) = 0 \tag{243}$$

- Energy Equation

$$\rho\vec{v}.\nabla h = \nabla.(k\nabla T) - \nabla.\left(\rho\sum_{k=1}^{N} h_k Y_k \vec{V}_k\right) \tag{244}$$

$$h = \sum h_k Y_k \tag{245}$$

Using 243 and 245,

$$\sum h_k Y_k \nabla.(\rho\vec{v}) = 0 \tag{246}$$

Add 246 to the energy equation

$$\nabla.\left[\rho\sum h_k Y_k\left(\vec{v}+\vec{V}_k\right) - k\nabla T\right] = 0 \tag{247}$$

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Now let us call this A, keep this why would I want to do this, because I am now going to begin to realize that HK can be written as ∇H(K0) plus the sensible enthalpy all right ∇H(K0) times YK, times V, if you now have this term I can now try to look for supplying the species conservation equation to get its right-hand side to come and plug in here okay.

So I will now be able to write something like, for the term that has the ∇H(K0) alone I should now be able to write this is like a Σ WK ∇H(K0), so WK is coming from the right hand side of the species conservation which will now look which left hand side is this I plug the right hand side of that here right, for only that term which has the ∇H(K0) that will simply mean the chemical heat release rate term is nothing, but the reaction rate term times the heat release from that reaction.

That is correct, because a heat, a reaction is going to give rise to a certain heat release per unit mass of the fuel or any of the reactants, if you now multiply that by the rate of change of that species mass per unit time right, then you should get the heat release rate. So we will try to look for that manipulation soon, so you now say species conservation can be written as divergence ρYI times v+VI = WI, I=1 to n right.

Now let us just start this thing this is B okay, so what I am basically saying and I will stop, so basically note that, so note that HK=∇H(K)= ∇H(K0)+ integral T up to T cpk dT right. So this is the sensible enthalpy term, this is the standard heat deformation. Therefore, if we now plot this in here right, in the energy equation and notice that you now have a ρYI v+VI combination with the ∇H(K) wherever you have that, you know put your WI.

Well I guess, I am sorry I missed symbol, so let us just have k instead of I K right. So what you are looking for is whenever you have this combination you now try to put WK, whenever you have ∇H(K0) over there. And if you are not split this then what is going to remain is only this term on the left-hand side, the right hand side is simply going to be ∇H(K0) times WKΣ of that.

So the energy equation becomes divergence of ρ integral ρ, we now say Σ, well actually I think I can get rid of the Σ for the first term. If I now try to pull this V out and open up this brackets ΣHK YK will simply again be H and that will correspond to simply – so we are now looking at only the sensible enthalpy term kept on the left-hand side. So we now some over the cpk becomes CP, but anyhow to keep the cpk as it is with the VK.

So we will just do that ΣK=1 to n, YK VK and then keep your sensible enthalpy term as it is for the cpk. And then of course you can also have this - KD grad T that you have to keep – K grad T, and what we did was to keep get the standard heat deformation part to the right hand side and notice that that part alone actually stands for WK, so you can now easily write this as –Σ K=1 to n ∇H(K0) WK.

So this obviously is the chemical heat release term rate term, because this actually tells you how much is the heat that is released right. So this is actually like J/kg, and this is like kgs/m^3 sec right. So if you now get rid of these two K kilograms this is the amount of heat released per unit mass of that species K, and this is the mass of species K that is getting converted per unit time, per unit volume. So together this will actually mean J/sec/m^3 or watts/m^3 you see.

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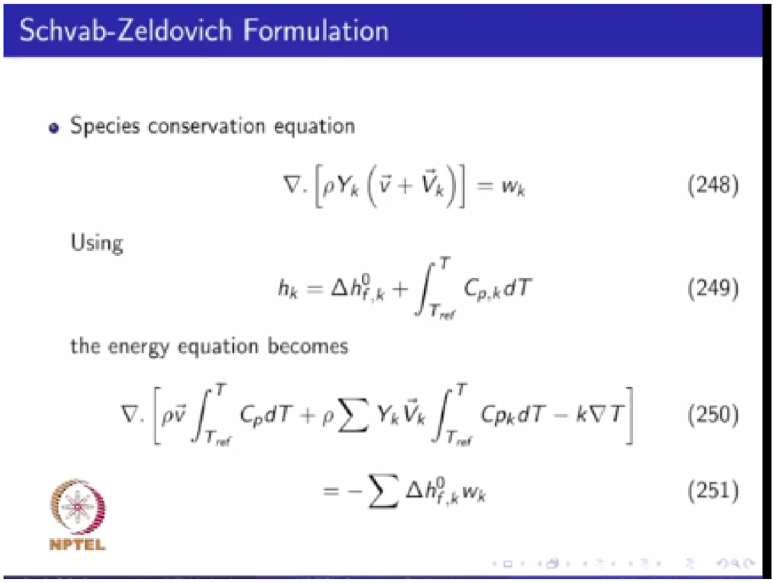

Schvab-Zeldovich Formulation

- Species conservation equation

$$\nabla . \left[\rho Y_k \left(\vec{v} + \vec{V}_k\right)\right] = w_k \qquad (248)$$

Using

$$h_k = \Delta h^0_{f,k} + \int_{T_{ref}}^{T} C_{p,k} dT \qquad (249)$$

the energy equation becomes

$$\nabla . \left[\rho \vec{v} \int_{T_{ref}}^{T} C_p dT + \rho \sum Y_k \vec{V}_k \int_{T_{ref}}^{T} Cp_k dT - k \nabla T\right] \qquad (250)$$

$$= - \sum \Delta h^0_{f,k} w_k \qquad (251)$$

So this is the volumetric heat release rate right. So that is how and then you summit over for all the species that are getting produced or consumed okay. So this effectively is now for the first time we are now beginning to see the chemical heat release rate isolated in the energy equation here okay, this is a good point to stop.

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