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

Lecture – 40 Turbulent Non-Premixed Flames II

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Dissipation and scalar transport for mixture fraction z. So, we remember that we did this for the reactive scalar and we found out that the gradient transport assumption was not very good, because that was a reactive scalar with source terms, but of course, mixture fraction is a passive scalar. So, we can use the gradient transport assumption and if we do that what we will get is that if we use this assumption u double prime the Z prime favre average is equal to a turbulent diffusivity.

Now, this is of course, not true it is not initiates system model from gradient transport assumption and this is turbulent diffusivity modeled in analogy with eddy viscosity whereas, Dt is equal to nu t by turbulent Schmidt number nu t is that is the turbulent eddy viscosity, and this is a turbulent Schmidt number then one can derive an equation of mean mixture fraction is essentially if you can derive an equation for the ys, you can essentially derive an mixture equation on mean mixture fraction. You can essentially derive an equation of mixture fraction then from that you can essentially derive an equation a mean mixture fraction of course; here actually it can be shown that it is a conserve scalar.

So, essentially all the source terms cancel out that is the whole purpose of defining in a mixture fraction that it is a conserve scalar. So, you get the temporal term with the convection by mean flow. So, this is just an equation of this mixture fraction is essentially another just another concept for a scalar or a coupling function similar to that coupling function formulations that we did, but it is just in terms of the scalars or in terms of if two etcetera and essentially everything cancels out and we are left with these equations ok.

So, this is the transport this is the essentially the have a equation for mean mixture fraction of course, here we have neglected the molecular mean molecular term, because we consider the turbulent diffusion term to be much stronger than the mean molecular diffusion, but we can as we said before that it can be absorbed within this Dt term also ok.

Now, we also need an equation of Z prime we will see why. So, for that first we need to derive an equation of Z we need to derive an equation of the variance of the Z that is Z prime square that is this thing. But first derive an equation for Z double prime and that is given by this, you should derive this you discuss these terms already its similar to this reactive scalar terms, because it emerges from the reactive scalars itself, but of course, with the so, without the source term ok.

Now, here of course, we have if we consider that this rho d etcetera and their mean gradients are neglected for simplicity. So, essentially the first two terms on the rihs can be combined to obtain a term which is proportional to this thing, and then by multiplying the whole thing by multiplying by twice rho Z prime, we can get an equation for Z double prime square. And then we use the continuity and average and then we get an equation for this the Favre average Z prime square this is once again as you have seen this is a once again similar to the kinetic energy thing because kinetic energy was essentially the u prime that is the fluctuating a velocity squared a averaged ok.

So, it is essentially this the scalar counterpart of the kinetic energy turbulent kinetic energy. So, now essentially then one what we can do is that we can go with essentially with these things, we can essentially go with and derive that equation and that is given by.

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That is the equation of this is the transport equation for Z prime square Favre averaged, and that is given by transient term convective term, I will describe this terms in a while please hold ok.

So, now, let us call this as T1 T2 and T3. So, the left hand side of course, this is the transient term and this is the convection of the variance of Z by the mean velocity that is u; u Favre averaged on the right hand side you get this 3 terms and this you know once again needs an explanation just like the way we explained the previous where previous reactive scalars.

So, T 1 is essentially a turbulent transport term T 2 you see once again this is similar to the Reynolds stress terms if it were in terms of velocity this is similar to the Reynolds stress terms and this is like the this is a tilde of course, like the mean velocity gradient. So, here you essentially have a flux of the velocity and joint covariance of velocity fluctuation and scalar fluctuation mixture fraction of fluctuations, and that is supported with this mean mixture fraction gradient.

So, this causes essentially it can be shown that essentially when the this essentially causes the production of the Z prime fluctuation. So, once you have this terms and the

non zero once we have this terminology to this essentially increases acts as a source for Z prime fluctuations. Z through the fluctuations and once again this will essentially a dissipation term, but let us write this down this is essentially the mean this is the production of scalar fluctuations ok.

And the once again you hear we have neglected the mean molecular transport term for simplicity, but of course, you will see that the mean in molecular diffusivity does not vanish and it arrives and it comes back in the Favre averaged scalar dissipation rate term that is which this term. So, this is essentially chi tilde is essentially 2D by the way here D essentially we have assumed that Lewis number equal to one. So, d is essentially di.

So, thermal diffusivity equal to molecular diffusivity and of the diffusivity walls species also equal. So, that assumption is there. So, this is the term grabbed Z prime average times grabbed Z prime averaged now the integral scalar times kl you can use this. So, essentially in this term this is the convective this is a transient term, this is a convective term, this is a turbulent transport term, this is the production term this is the production term and this is the dissipation term. So, what thia scalar fluctuations are produced by this presence of mean mixture fraction gradients, and it is destroyed or dissipated in the fine scales by this scalar dissipation rate chi.

So, that is the mechanics of how scalar fluctuations are produced and dissipated and one can be what can be shown also that is essentially it takes essentially this this essentially takes the a large scale a large scale mixture fraction gradients and then it basically essentially creates this scalar a fluctuations at large scales and essentially this will be dissipated at the small scales ok.

So, once again here also you will see that there is a cascade of essentially scalar fluctuations. So, now, then we can define an integral time scale using this as a tau Z is equal to Z prime square Favre average by the scalar dissipation rate, and tau the time scale is essentially tau k Favre average divided by mean dissipation rate turbulent kinetic energy dissipation rate and those can be as we have seen before those can be connected through these things whereas, this is of an 2.0, but sometimes 3.0 proportionality constant and using this one can write the scalar dissipation rate is essentially Cx tilde times epsilon by k times Z prime square ok.

This is often called the scalar dissipation rate anomaly because you see that scalar dissipation rate is a small scale quantity, but here you do not have any diffusivity essentially. So, it is essentially dependent only on the mean dissipation rate and the of the turbulent kinetic energy dissipation rate on the turbulent kinetic energy average, and thus a scalar fluctuation and the variance of scalar fluctuations. So, this is the thing.

And then we will use this we have essentially derived what we have done here is that we have derived an equation for Z, we have derived the governing equation I am not derive we have just written down rather the governing equation, but we have shown you although what are the steps to derive you should derive the we have we have shown the steps to for the governing equations for Z tilde and Z prime a Z prime square tilde ok.

There is a mean mixture fraction, Favre averaged mixture fraction and the Favre variance of mixture fraction of fluctuations this we have obtained this this is a very important step we will see why.

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Using this we can show that we can essentially use the Flamelet model. Now what is the Flamelet model now the Flamelet models are basically we consider a full flame, that is if you say consider a jet flame like this fuel which is a air coming out air coming out.

So, this is a gas turbine combustor and you will have this is a flame. So, we will see you will consider that each of these are essentially a flamelets. So, this whole flame. So, these

are essentially is a temperature like this. So, a whole of this flame. So, temperature goes down when you go away from the flame temperature goes down when you go away from the flame on this side also .

So, you have the flame here. So, this whole big flame is essentially an ensemble of infinitely large number of flamelets. So, that is the idea of this Flamelet model that the whole flame is essentially composed of many flamelets, and flamelets are essentially thin reactive diffusive layers these are essentially thin reactive diffusive layers which are embedded in an otherwise non reacting turbulent flow field. So, the otherwise the flow field is non-reacting. So, where you have got this flamelets and these are embedded in the non-reacting flow field. And the Flamelet structure is justified if the thickness of the inner layer of the fuel consumption layer where the reaction layer happens which is essentially infinite small in the fast reaction rate, limit is much much smaller than the Kolmogorov line scale.

So, it is a Kolmogorov line scale does not disturb your inherent Flamelet structure. So, inherent flame structure our Flamelet structure is justified only in that case. So, what we will do is that this Flamelet model is essentially a.

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A combination of the of you will see that is equation of Z and Z prime square that we have obtained, and plus this one d chambered flame solutions that we obtained in the mixture fraction space. So, this coupled with this 1D laminar flame, these are essentially our Flamelets solutions and this gives rise to Flamelet model ok.

So, that is the whole idea behind this Flamelet model.

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So, we will see essentially that the Flamelet concept focus on the location of the flame surface and not reactive scales. In this Flamelet concept will not in the there are essentially two versions of the Flamelet model that we will discuss in the first one we will not even go to solve for the reactive scalars, what we will do is essentially solve for the mixture fraction the average we will solve for the Z and the Z prime square. We will not even solve for the mixture fractions later we will do that we will not even solve for the a reactive scalars we will solve for the mixture fractions.

So, the essentially first important thing is that essentially to find out the location of the flame surface, and what is the location of the flame surface? The ZST the iso contour or the isosurface Z st stoichiometric will be my location of the flame surface. Now this location is defined as the isosurface as we have said is the nonreacting scalar quantity Z and this nonreacting scalar quantity Z is a is a conserved scalar because it does not have any source term in the transport equation and the statistical moments of the reactive scalars will be obtained using the statistical distribution of the scalar Z how we will obtain the statistical distribution of the Z by the Z prime and the Z double prime square equations.

And then we have to obtain we have to find out somehow by which we can relate psi i the reactive scalar as a function of Z this can be either done through some kind of a like a model that is we assume that the solution of the one d flame that we have done is valid everywhere and or the other way is to basically solve for psi i is a function of Z we will do both ok.

Now, what the other thing is that there is one more step in between, that is just by knowing Z prime and Z double prime square we this psi i is a function of Z 1 psi i from 1 z. So, to map that essentially we need to know a distribution of Z and we will have to find out how we can describe a distribution of Z. So, essentially. So, what the advantage is that is that you see you the problem was with reactive scalars handling reactive scalar, shows that the reactive scalars we could not apply the classical non reacting turbulence modeling strategy. Because a they did not obey sometimes the gradient transfer assumption they have is a huge closure problem for the mean reaction rate.

So, as soon as you define go to a you basically then you have a take a d 2 and instead of directly attacking to solve for the mean reactive scalar space that is instead of trying to solve for psi i which creates problems we do not go for that approach, rather we go for solving for the non reactive scalar or essentially this conserved scalar which is this Z prime Z tilde, that is the Favre average Z and this one. And then we map this reactive scalar write to Z using either the 1D flame solution or an equilibrium solution that we obtained or by solving for this will show both.

So, this is the Flamelet approach is it clear to you it is a very beautiful concept see that because psi i process problems you have problems with closings psi i it does not it does not obey your classical gradient transporter assumption it does not obey your closer, but the reaction that cannot be closed properly, and we have to result to some like ad hoc modeling things like eddy breakup model eddy dissipation concept is return.

So, a more elegant approach is that you go for a scalar you go for a concern scalar which obeys gradient transport assumption and which does not even our source term what is that scalar that scalar is Z mixture fraction. So, then you basically solve for Z tilde and then you solve for Z prime, and then you map your reactive scalar onto this is Z now of course, we have to do one to one mapping and for that you need only Z and Z prime is not enough you need to basically find the pdf of Z, and you will see that that pdf of Z can be formed just by using the knowledge of Z averaged there is the Favre average Z and Z prime in the variance of z.

So, using this you can find essentially the pdf of Z, and then you can essentially map the reactive scalar into Z space one to one and then you can find out the reactive scalar at each point in space. So, that is the beauty of this Flamelet model of course, it has its own inherent assumptions and you are assuming that it each point is essentially the Flamelet behaves as if it is a one d flame.

So, but that those assumptions can be defined as more and more as you will see later. So, that is the thing. So, the basic most important thing is that you can if you can use a conserved scalar then a lot of problem get solved problem is essentially elevated because of this site because sidestepping this closure problems.

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So, we will see that or we will see use the models essentially based on the presumed shape pdf approach, and that will require the knowledge of Favre means Z average and Z prime squared which we have already obtained.

And using the gradient transport assumption hypothesis in the Favre average mixture fraction we have obtained this equation here rho barre is essentially if you see rho barre is essentially rho average. So, that on make a discrimination between these two sometimes you use rho barre it is typically we use rho typically we use bar for time average then rho bar for ensemble average.

So, here your rho bar is equal to rho angular brackets and of course, you have used that d is essentially less than Dt. So, the equation of for Z prime square is this which you we just obtained and now if you remember if we go back here you see this temperature.

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For the 1D chambered flame or for a burke Schumann flame that is a which we can might have read in books or for the equilibrium solution, here temperature is essentially a linear function of Z ok.

So, or the enthalpy actually will be a linear function of Z. So, why do not we use this assumption? So, we can use this assumption essentially to refine out and we can write this as a do establish a relation between enthalpy and Z this is very important. So, we say that h at any point is essentially h 2 that is your fuel stream, h 2 plus sensible this is sensible enthalpy by the way time Z plus h 1 minus h 2. So, h at any point is essentially a linear function of Z you know h and you know your boundary conditions h 1 and h 2 you find out the h at that point.

So, all you need to know is essentially what is the value of Z. So, similarly we write that the mean value is essentially h 2 plus mean Z I am sees this is of course; true this is the that is true this is also right. So, we can use this of course,; however, that if you have a more complicated case that if you have different boundary conditions for Z tilde and h tilde the Favre average Z in Farve average h you know you can may not have to use a different more generalized formulation for h and there can be heat loss due to radiation and unsteady pressure changes then you cannot use this.

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Presumed Shape Pdf Viewpoint - Also known as conserved scalar equilibrium model \widetilde{z}_i Presume the two parameter pdf in advance which in turn fix the functional form for pdf of two parameters in terms of known \tilde{Z} and \tilde{Z}'' Beta function pdf is widely used as Z varies between 0 and 1 $h = h_2 + 2(a,$ 12 $\odot \odot \oslash \circledast \odot \odot$

So, in that case what you uses that you use a Favre average education of enthalpy like which we have already known like this and here of course, the spatial variation of pressure is neglected in the small or not zero this is small mach number limit and dp dt the pressure averaged time is important for modeling. So, that has been retained for ic engine or diesel engines all for even thermo acoustic instability in gas turbine engines and the temperature changes due to radiation within the Flamelet structure also was strong influence on the prediction of no x formation and transporter term containing the molecular diffusivity has been neglected and non-unity Lewis number effects and neglected.

And no equation we have for we have we do not use an a equation for enthalpy fluctuation because in the non premixed turbulent combustion it is assumed that the fluctuations of enthalpy are due to mixture fraction fluctuations. So, that is a inherent assumption. So, this is just a sidestep that if you have a complicater situation, in which you cannot use this what to do , but in most cases if you use this then you can use the presumed shape pdf view point ok.

So, what we will do is that as I have said that that h is essentially h 2 plus Z times h 1 minus h 2. So, you need to know to know h at any point, all you need to know is that if these boundary conditions are available you need to know essentially what is this Z at this point. But when you have in a in rans in a in an average simulation of course, when you have done this equation of Z all you have essentially solved the equation of Z ok.

And that prime square of course, you must remember that only this solving this equation is not enough you have to solve for the averaged equation of u, that is the momentum equation the continuity equation also and along with the k equation and the epsilon equation also. So, only then can basically solve have this equation of Z prime and Z prime squared because you see that those equations you have already obtained this to get this to get this first you need to have mean U prime and mean k prime. So, you can obtain those whether renounce average Navier stokes equation ok.

So, that is of course, implied that only solving for Z and Z prime is not enough you have to solve for u prime u, u T u averaged equation and k averaged equation and epsilon averaged equation also so, but once you do that you have an you have a essentially a distribution of Z and Z prime square at each point in the flow, but that is not enough why because a enthalpy at each point is essentially i will function of Z at each point. So, what you need to do is that using this you need to basically generate all possible values of Z, what is that essentially that is a pdf of Z ok.

So, what we do is that we essentially assume a shape of pdf exist for a different for a given flow of flow turbulent flow. So, that is done by this presumed pdf model which is also known as the conserve scale equilibrium model, we will presume a two parameter pdf in advance which in turn fix the functional form for the pdf of two parameters known in terms of Z and Z prime. So, we will obtain a pdf something like this Z is a pdf of Z and this is only a function of Z average and Z prime square ok.

So, at each point as soon as you know this by solving all the rans equation that is by solving; that is by solving all these equations you obtain this pdf and then you can find out the h. Now I will just for simplicity i will just (Refer Time: 29:19) the steps. So, first you solve for the continuity equation averaged continuity equation this angular burke Schumann averaged solve for the averaged. Momentum equation it might be need to be solve in by in sync not alone in solver the average k equation in solve for the average epsilon equation ok.

And then you solve for the average or the favre averaged this this string should favre averaged or you can essentially solved the you essentially get this terms essentially here now this is the just of favre averaged also. So, uv w v equation you get and density you get you get and then you solve for essentially the turbulent kinetic energy using the methods which you have described before all this you solve and then you solve for this equation Z and Z prime ok.

But of course, you see in at in a real condition you can have numerous of this reactive scalars which you are not solving for. So, the computational load is also reduced. So, you solve for all these things. So, now, after this you have not solved for any of the reactive scalars. So, this not solved these governing equations to be solved ok the governing equation.

So, solving along with plus constitutive relations will solve this psi i not solved then how to get from this to this that is the point of the presumed shape pdf. So, as soon as you solve this. So, as soon as you solve this what you get you say that at each point in the flow you know you presume or assume a shape of a pdf of Z which is some something can be something like this and the pdf and this is Z and this pdf shape say which is f is given by two parameters Z prime and Z prime square average ok.

So, at each point now for each at each point we essentially at each point in the flow essentially our pdf of Z, and then you since you know that your h is equal to h 2 plus Z times h 1 minus h 2 at each point you can find out the value of h given the pdf of this and then using this we will show that how we can find out the mean of h, how we can find out the mean of psi i which we assume to be a function of which is will be our essentially a function of Z ok.

So, that is the idea of this presumed shape psf approach.

So, after you have solved for this Z prime and Z double prime you can essentially go to the instantaneous value of Z and from the instantaneous value of Z you go to h that is the idea. So, what we typically do is that we will to choose a beta function pdf is widely used as Z varies as Z varies between 0 and 1.

So, this is the pdf form that we will choose for an non premise combustion. So, this p tilde is the Favre pdf of Z at each point which is given by this form this gamma or essentially the gamma function whereas, alpha this is see that this is Z to the mixture Z is a mixture fraction two the (Refer Time: 33:11) alpha minus 1 times 1 minus Z to the power of beta minus one and gamma function of alpha plus beta divided by gamma of alpha times gamma of beta ok.

And whereas, this alpha you see mean Z and mean Z prime Z prime does not explicitly come, but it comes we here essentially where alpha is equal to Z Favre average Z times gamma whereas, beta is equal to 1 minus Z Favre average Z times gamma whereas, gamma here Z prime comes. So, Z is essentially Z non Z prime Z tilde essentially. So, Z tilde times 1 minus Z tilde divided by variance of Z ok.

Minus 1 which should be greater than 0. So, essentially is a function of Z tilde and Z prime square, and this is how the different pdf of Z looks like for different values of Z and gamma. So, for each point in the flow essentially assume that there is a pdf or for the entire flow you assume that this there is a pdf which is given by this this thing, and then once you do that ok.

And these are some of the properties that for large gamma it goes to Gaussian and alpha less than one it has a singular it is Z equal to 1 which is cannot be taken and for gamma beta greater than 1 it has singularity is Z equal to 1, but then the thing is that once.

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This pdf is obtained you can get assuming that this psi i by this 1D chambered flame model are we what we obtain that we can write that psi i is essentially only a function of Z, that because we have essentially we have shown that essentially Z behaves like an independent variable.

So, using this presumes shape pdf approach the mean of any reactive scalar is essentially a function of Z, as we have shown in the one the chambered flame calculations and can be calculated as this psi i tilde or the Favre average psi i at any point x in t is essentially integral 0 to 1, which is the d mean definition of from how to obtain a pdf is essentially psi i Z times this p tilde Z xt times dz is an exact equation actually ok. So, that is as long as this is only a function of Z.

So, mean density also be calculated something in a similar manner. So, you see that the conserve scalar model for non premixed combustion is a formulated to using 1 2 5 and the burke Schumann or the one the chamber flame chamber flame solution. So, that is the whole idea. So, now, you see that why the 1D chamber flame analysis is. So, important one we have a chamber of flame analysis you can go, using is just transformed that in the mixture fraction space and then you just solve for all this u tilde, u averaged, v average density average, p average, Z averaged and Z variance of Z and if you solve for k the turbulent kinetic energy epsilon and then as soon as you have that you construct this presumed pdf of Z, then by the assumption that you know as you know as these will all the local flames essentially behaves typically like a one d chamber flame and be covered the psi i is a function of psi i psi Z and immediately using that you can find out the model of the averaged value of psi i at each point in flow.

So without actually solving for psi i just by solving for Z, and because psi i as a function of Z which is can obtain this pdf of psi i. So, that is the whole point of this thing.

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So, laminar, this will consider take up in the in the next class that there can be alternative methods by which. So, here we had to that you see the limitation of this method, that here we have to assume that at each point in the flow the one d chamber flame on this burke Schumann solution in this simplified laminar solution is valid at each point in the flow. So, that is a little bit restricted assumption, but that can be relaxed when you essentially solve for psi i as a function of Z explicitly, without using result in to this solution we can also directly solve for psi i and that will be taken up in the next class. So, till then goodbye and see you in the next class again.