Fundamentals of Combustion for Propulsion
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Lecture – 26
CFD Modeling aspects – Modeling approaches

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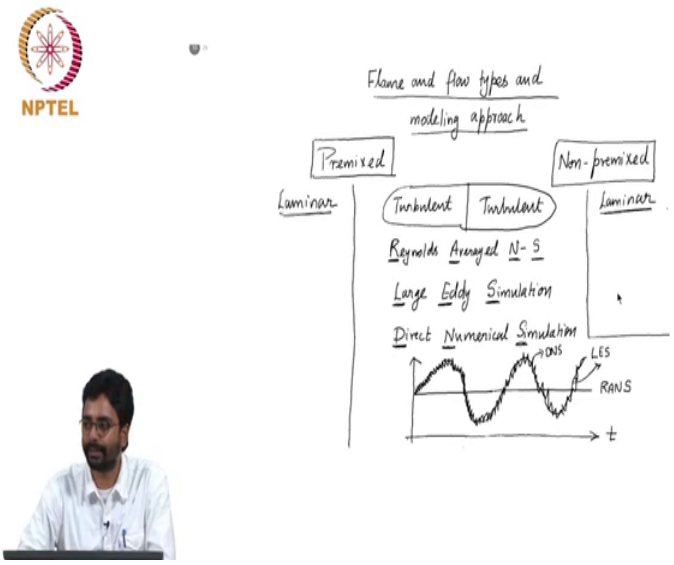

Now, let us move on to the effect of turbulence on premixed and non premixed flames. Let we will look at the general features first and then move on to specific aspects. So, we have different two different flame types and premixed and non premixed. And within this within each category the flame can either be laminar or turbulent ok. We know how to deal with laminar premixed flames these days, it is even easy to compute the structure of un strained and strained laminar premixed flames with detailed chemistry and all the full multi component diffusion.

And for laminar non premixed flames also the calculations can be done by starting with the mixture fraction approach. And creating what are called flame lit libraries with detailed chemistry and transport properties.

But when it comes to the effect of turbulence on the premixed and non premixed flames, we have one of these three approaches. See turbulence remember is flow in which the flow and other scalars fluctuate. And they fluctuate in a very specific way that the spectrum of the fluctuation should generally have continuous behavior with a certain power law ok.

Otherwise it is just white noise does not constitute a turbulent flow or flows with discrete modes are also not turbulent flows; they are just unsteady laminar flows turbulent flow has a very specific definition this was discussed earlier. And therefore, there are three approaches to modelling turbulent flames one has to look at only the mean field its called the Reynolds average Navier Stokes approach. Where what we solve for is only the mean value of a particular quantity; that is shown as a simple horizontal line here.

Imagine temperature or velocity or one of these variables. What is solved for is only the average value. But in reality it may have fluctuations of different frequencies and different length scales as shown in the same plot ok. And the next level of detail is detailed simulation is large eddy simulations, where what is captured is just easier to explain here.

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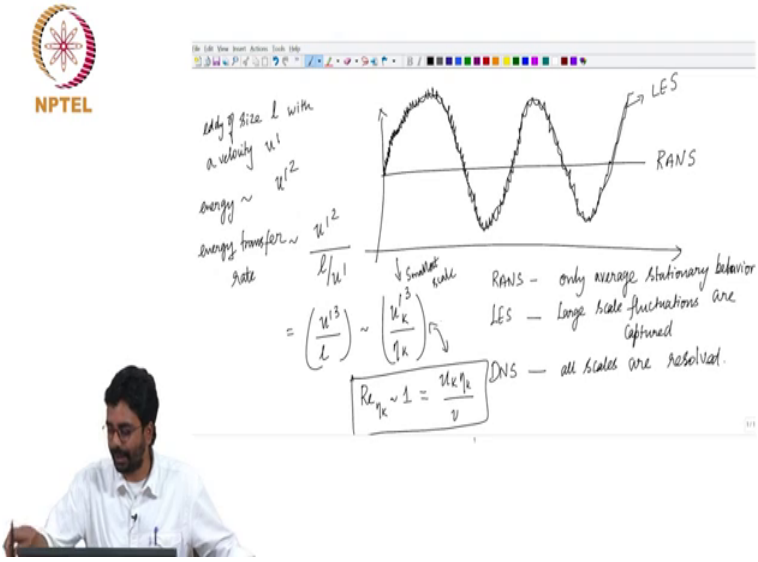

eddy of size l with a velocity u'

energy ~ u'^2

energy transfer rate ~ $\frac{u'^2}{l/u'}$

$= \left(\frac{u'^3}{l}\right) \sim \left(\frac{u'^3_k}{\eta_k}\right)$

$$\boxed{Re_{\eta_k} \sim 1 = \frac{u_k \eta_k}{\nu}}$$

RANS - only average stationary behavior

LES — Large scale fluctuations are captured

DNS — all scales are resolved.

So, the RANS you get only these ok. In LES you get recover some of the large scales large scale behavior is only you will get in LES ok. And the so, you have RANS is only average stationary behavior is captured. LES is large eddy simulations large scale fluctuations captured. The DNS direct numerical simulation all scales are resolved the DNS simulation for a variable like this would look like this there will be several other frequencies. I think you get the broad idea, it will capture the large scale motion as well as the intermediate scale and all the way down to the smallest possible scale which is the Kolmogorov scale ok.

So, this is these are the three approaches that are used, what is commonly used in practice is or what can be done with the computational resources that are normally available is a RANS simulation. Slowly industries are moving towards LES simulations DNS remains as an academic activity ok.

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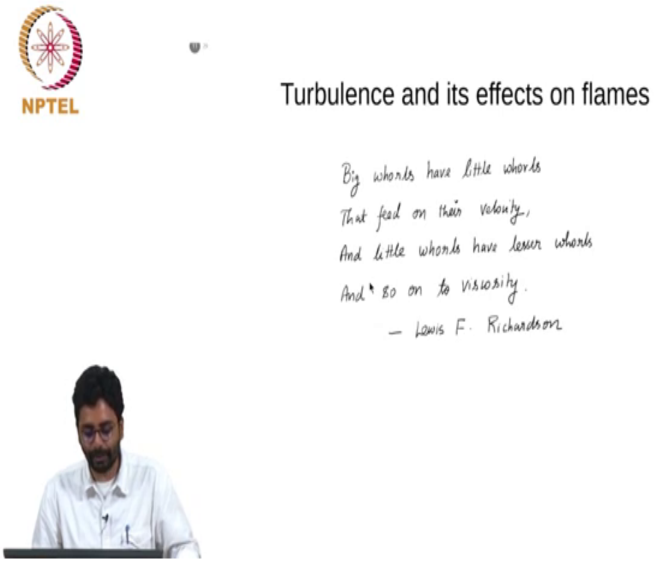

Turbulence and its effects on flames

Big whorls have little whorls
That feed on their velocity,
And little whorls have lesser whorls
And so on to viscosity.
— Lewis F. Richardson

I thought this poem by Lewis Richardson who has a meteorologist captures the essence of turbulence. This he wrote to bring out the message that a turbulent flow has a spectrum of length and timescales with energy exchange between different scales ok. So, big whorls have little whorls that feed on their velocity. And little whorls have lesser whorls and so on to viscosity ok.

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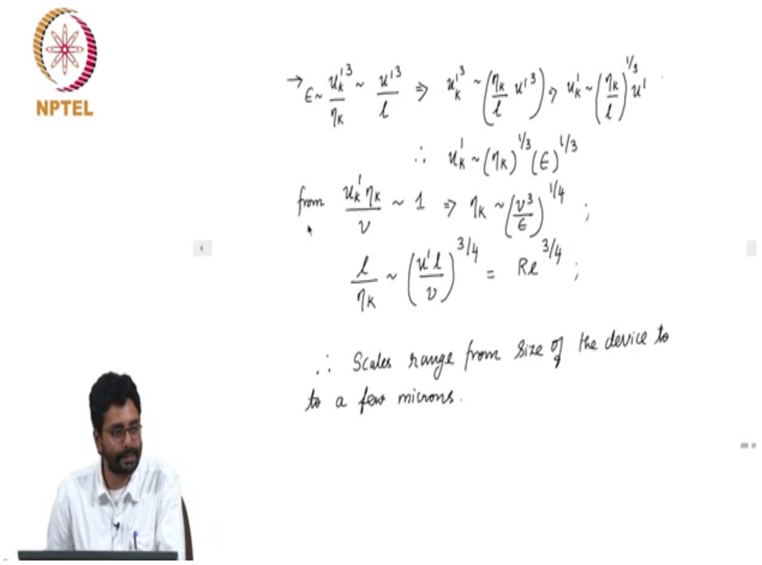

$$\rightarrow \epsilon \sim \frac{u_k'^3}{\eta_k} \sim \frac{u'^3}{l} \Rightarrow u_k'^3 \sim \left(\frac{\eta_k}{l} u'^3\right) \Rightarrow u_k' \sim \left(\frac{\eta_k}{l}\right)^{1/3} u'$$

$$\therefore \quad u_k' \sim (\eta_k)^{1/3} (\epsilon)^{1/3}$$

$$\text{from } \frac{u_k' \eta_k}{\nu} \sim 1 \Rightarrow \eta_k \sim \left(\frac{\nu^3}{\epsilon}\right)^{1/4} ;$$

$$\frac{l}{\eta_k} \sim \left(\frac{u' l}{\nu}\right)^{3/4} = Re^{3/4} ;$$

$\therefore$ Scales range from size of the device to to a few microns.

So, now let us look at a simple way to actually understand what does the range of scales that are present in turbulent flows. So, the largest scale will have a dimension, that is approximately the length scale that is of relevance to the problem in the case of a liquid rocket motor it could be the injector diameter.

And in a gas turbine it could be the length scale associated with the injectors or the liners or one of these macroscopic features of the geometry. And the smallest scale is where the viscous dissipation becomes significant ok. So, the energy contained in an eddy of size l is u dash squared k it is the kinetic energy that is contained in the eddy. And it has a turnover time of l over u dash ok.

So, an eddy of size l with the velocity u dash will have approximately energy contained. In this eddy is the kinetic energy which is u dash squared by 2 we are going to do a scaling analysis. I am going to leave out the 2 divided by the time this is the energy is u dash squared. And the energy transfer rate is u dash squared by the turnover time for the eddy; which is l by u dash which is equal to u dash cube by l.

This is the rate of transfer of energy from the largest eddy to the next size eddy ok. And this energy transfer will happen remember Richardson's poem that smaller eddy is feed on the energy of the larger eddy. And then these larger eddy is the role of viscosity is negligible viscosity becomes important only if you go to smaller scales ok.

So, this is the energy transfer rate from the large eddy towards the smaller sizes. And this energy transfer will happen up to a point up to a point beyond which viscosity takes over ok. And when viscosity takes over the inertial effects and the viscous effects are comparable. And therefore, the Reynolds number at the smallest scale will be of the order of 1; because that is when viscous dissipation can become significant.

And till that point inertial forces will dominate. And therefore, this smallest scale is defined by the condition that the Reynolds number at that scale should be about 1 ok. And by combining these two equations you can get an idea of what is the spectrum of scales and that is what I have summarized here.

The rate of transfer of energy from the largest eddy towards the smaller sizes is u dash cube by l. Will go all the way up to a certain scale and then at that scale it will get dissipated by viscosity ok. And you can rearrange this equation to show that the size of the largest eddy the ratio of the size of the largest eddy to the smallest eddy will be proportional to the Reynolds number raised to 3 by 4 power. Therefore, larger the Reynolds number larger is the separation of scales.

So, similarly you can show for timescales also, that the timescales will depend on the number of flows. So, larger the Reynolds number larger is the separation of the scales. So, scales range from size of the device to a few microns, depending on the Reynolds number yeah.

Student: We have exchanged the (Refer Time: 09:45).

Reynolds number of the order of 1 is where viscous dissipation will dominate and can significantly convert the kinetic energy contained in eddys into heat. Then the Reynolds numbers are large viscous effects the Reynolds number is a ratio of inertial forces to viscous forces. So, when the Reynolds numbers are large, the inertial forces dominate the amount of energy that is dissipated by the viscous forces is negligible. Only when Reynolds number becomes of order of 1 viscous forces will dominate.

Student: (Refer Time: 10:17) is like viscosity from critical parameter that is essentially popping out because of nonequilibrium flow. The moment you have a different nonequilibrium (Refer Time: 10:29) two layers of flow then only say viscosity pops out if you want you say Reynolds number comes into picture of 1.

Yeah.

Student: Then viscosity has no (Refer Time: 10:37).

Not ok, not really actually it is when Reynolds number becomes 1 that the viscous forces dominate yes. A state of active non equilibrium is maintained this is the I would like to you know construct an analogy with the flame example that we discussed earlier. So, you have a conical flame and the temperature at the flame is different from the temperature away from the flame.

For example, in the reactant side the temperature is lower on the flame the temperature is higher. So, there is a gradient in temperature. This gradient in temperature is maintained by continuous supply of reactance to the flame. If you stop that the gradient disappears. In fact, everywhere the temperature becomes the same. Similarly in a turbulent flow, you are adding energy by the kinetic energy that is provided to the largest scales.

For example imagine fuel injector like the one that we that you use in liquid propellant rockets. Let say 10 millimeters in diameter and liquid hydrogen or gaseous hydrogen is coming in with 100 meters per second. That contains a certain kinetic energy associated with the length scale of the diameter of the injector.

And now this energy cascades through smaller and smaller scales as to how these smaller scales are produced itself is an interesting topic it is produced by vortex stretching. So, the energy gets transferred from the larger scale to till a point where viscosity will convert this kinetic energy into heat. In fact, viscosity has no role in the side of the larger scales. Because Reynolds number is at very large the inertial forces are much higher than the viscous forces. Once you reach length scale that is much smaller for.

Student: (Refer Time: 12:31).

For gradients to actually dissipate away the heat the Reynolds number must be 1; its viscosity dominates when Reynolds number is 1, when Reynolds number is large viscosity has marginal role.

Student: I have a included like rho vd is equal to delta v that is why (Refer Time: 12:47) now its not.

Its not delta v.

Student: Sir its not delta v.

It is the length scale of the eddy.

Student: (Refer Time: 12:53).

Student: So, then this is absolutely the picture.

Correct, any other questions? No, the reason why I wanted to there is a relationship between the large scale and the small scale is, to look at mixing rates or estimate a timescale for mixing.

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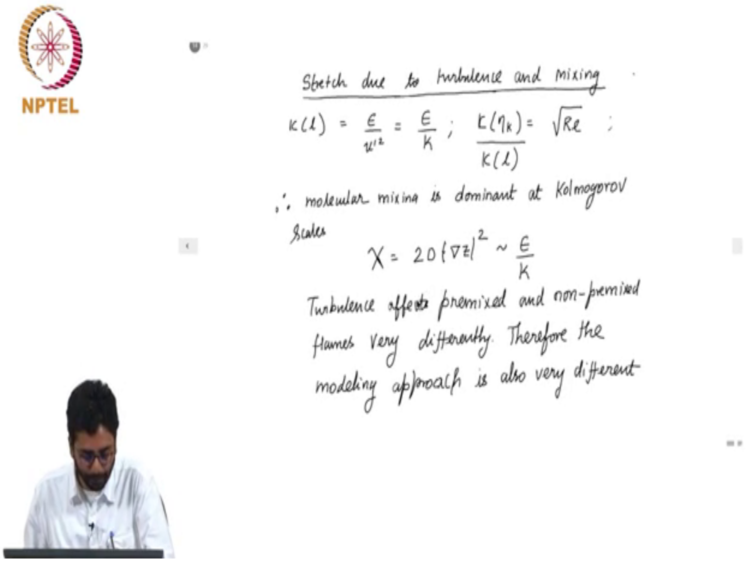

Stetch due to turbulence and mixing

$$\kappa(l) = \frac{\epsilon}{u'^2} = \frac{\epsilon}{k} ; \quad \frac{\kappa(\eta_k)}{\kappa(l)} = \sqrt{Re} ;$$

∴ molecular mixing is dominant at Kolmogorov scales

$$\chi = 2D|\nabla Z|^2 \sim \frac{\epsilon}{k}$$

Turbulence affects premixed and non-premixed flames very differently. Therefore the modeling approach is also very different

So, a typical timescale for mixing is length divided by velocity. So, we can calculate mixing timescale for the largest scale and for the Kolmogorov scale ok; which is what I have done here you can.

So, kappa of l will be l over u dash and you can express that in terms of the dissipation rate and the kinetic energy of turbulence epsilon by k. I am using this because this is what you typically use when you are doing calculations with RANS models k epsilon model ok. The epsilon is the dissipation rate remember that it is u dash cube by l and k is the intensity of turbulence which is u dash squared.

So, the stretching rate or the inverse of the stretching rate at the integral scale or the largest scale is epsilon by k. And you can similarly calculate the stretching rate at the Kolmogorov scale which will be eta k divided by uk we have derived expressions for both of this in the previous slide. And if you take the ratio of these two, it will be proportional to the square root of the Reynolds number.

Therefore the there are two conclusions one is that mixing rates are much much higher at the smaller scales ok. And larger the Reynolds numbers this disparity will this separation of scales will be wider and wider. So, molecular mixing is dominant at Kolmogorov scales and remember that molecular mixing is required for chemical reactions to happen.

It is not just sufficient to bring a bulk of fuel in contact with bulk of the oxidizer, it is important to mix them thoroughly for all the fuel and oxidizer to react. So, this is quantified by what is called the scalar dissipation rate. So, chi equals to 2 D grad z squared and this is proportional to epsilon by k. So, turbulence therefore, remember that in a premixed situation mixing has already happened.

So, that the mixing rates are very different at integral scales compared to the mixing rates at Kolmogorov scales. Will have marginal effects on the dynamics of premixed flame. But on the other hand if you look at non premixed flames, that molecular mixing is significant at Kolmogorov scales and that there is marginal mixing at integral scale; means that there will not be any reactions at integral scales the reactions happen because of mixing at. The flame structure is dependent on mixing at the Kolmogorov scales ok.

Student: This sign after 2 D (Refer Time: 15:51).

That.

Student: (Refer Time: 15:53) of spacious component (Refer Time: 15:53) if it.

I did not I missed that part. I just want to go back to. This comes from the conserved scalar equation where we showed that I am sorry I missed that.

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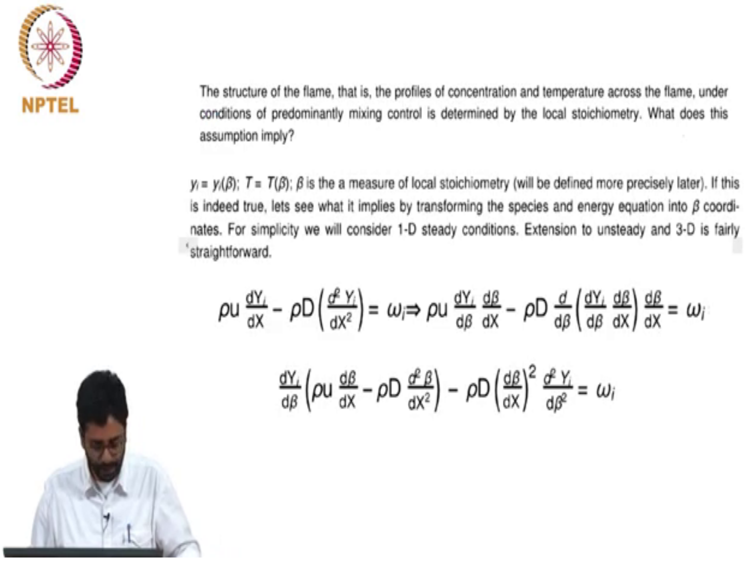

The structure of the flame, that is, the profiles of concentration and temperature across the flame, under conditions of predominantly mixing control is determined by the local stoichiometry. What does this assumption imply?

$y_i \equiv y_i(\beta)$; $T \equiv T(\beta)$; β is the a measure of local stoichiometry (will be defined more precisely later). If this is indeed true, lets see what it implies by transforming the species and energy equation into β coordinates. For simplicity we will consider 1-D steady conditions. Extension to unsteady and 3-D is fairly straightforward.

$$\rho u \frac{dY_i}{dX} - \rho D\left(\frac{d^2 Y_i}{dX^2}\right) = \omega_i \Rightarrow \rho u \frac{dY_i}{d\beta}\frac{d\beta}{dX} - \rho D \frac{d}{d\beta}\left(\frac{dY_i}{d\beta}\frac{d\beta}{dX}\right)\frac{d\beta}{dX} = \omega_i$$

$$\frac{dY_i}{d\beta}\left(\rho u \frac{d\beta}{dX} - \rho D \frac{d^2\beta}{dX^2}\right) - \rho D\left(\frac{d\beta}{dX}\right)^2 \frac{d^2 Y_i}{d\beta^2} = \omega_i$$

You remember this equation. So, we showed that a conserved scalar will satisfy a convection diffusion equation. Therefore, rho u d beta d X minus rho D d square beta d X square is equal to 0; that is what we showed for a conserved scalar. So, the first term on the left hand side will be 0.

So, the reaction rate under purely mixing control situation is equal to negative rho D d beta d X squared d square Y by d beta square i.

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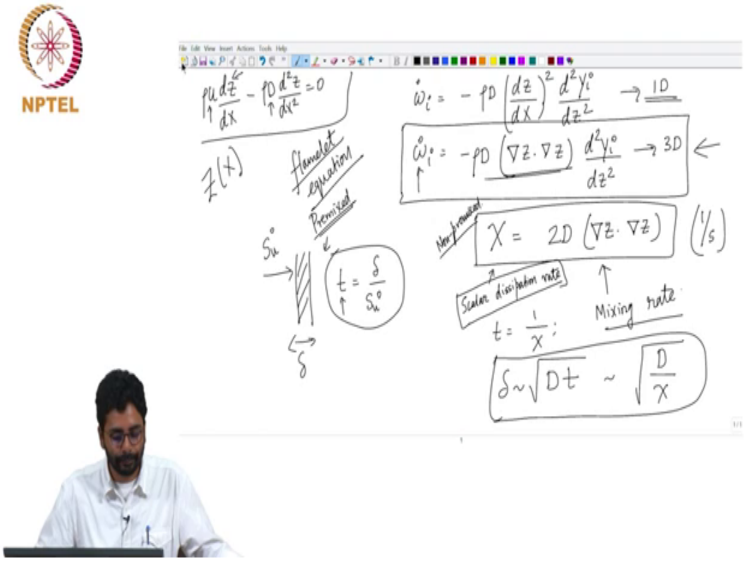

So, omega dot I is negative rho D d square beta, let me not use beta I will use the normalized scaler which is Z; keep making to me sorry I think this is correct ok. So, this is for a 1 D case right. And if I generally set to 3 dimensions this is D Z by D X dot D Z by D X. It is actually the gradient of z dot the gradient of Z in 1 dimensions; it is simply dz by dx squared this is for 3 D this by the way is called the flamelet equation ok.

From here you can identify a quantity called chi which is 2 D grad Z; this is a very important quantity. Remember that unlike the premixed flame, if we have a premixed flame I had no difficulty we had no difficulty in assigning a thickness to it and it had a characteristic speed is S u 0. Once I have [vocalized- noise] length scale and the velocity scale, I can define a time scale as delta over S u 0 ok; which we also showed depends on the reaction rate ok.

So, we could in a straightforward way we could connect the time scale of the flame to the reaction rate, but diffusion flames are tricky. Because the reaction rate is limited by the mixing rate and mixing itself is dependent on the flow. And when the flow conditions change the structure of the diffusion flame will change the reaction rate will change. And therefore, the timescale for mixing is different for different flows.

So, its not easy to find an intrinsic length and velocity scale for a diffusion flame, the convenient scale is this as you can see this is dimensions of one over seconds ok. And this is the mixing rate and a convenient time scale is for a diffusion flame is 1 over chi and the length scale is D over chi.

Let me write clearly always remember this length scale is, length scale in a diffusive situation is square root D t, which in this case will be D over chi. But there is no universal value scalar dissipation rate for diffusion it depends on the flow conditions. Therefore, its different under different conditions this is the scalar dissipation rate.

Student: Its essentially talks about the diffusion of the spacious or non spacious to another spatial equation.

Yes.

Student: Where.

The rate of mixing the rate of diffusion.

Student: (Refer Time: 20:29).

Yeah.

Student: But where we have not talked about the low interaction with the mutual (Refer Time: 20:37).

The Z is Z is governed by this equation which is passing here, Z as a function of X. You remember this controlled by or is governed by convection diffusion balance without a source term and the flow effect comes through this equation. So, from here we will get a Z as a function of X; which will give as a grad Z grad Z squared therefore.

Student: (Refer Time: 21:19).

The mixing rate is. In fact, intimately connected to the flow.

Student: Intrinsically (Refer Time: 21:23) yes.

Connected to the flow and the mixing of the flow any other questions? This distinction between pre mixed and diffusion flames is important this is the premixed situation this is the non premixed.

Student: Sir.

Yeah.

Student: How we can define from (Refer Time: 21:45) by (Refer Time: 21:47).

Yeah.

Student: (Refer Time: 21:48) actual situation how do you attain that.

Its too bad actually this e we well what I mean by that is that the mathematics is not as nice as this. But the simplest way to deal with that is you define one more scalar ok.

So, when the number of variables for which the diffusivities or the transport coefficient you know. If you are forced to choose different values for you may be interested in the specific phenomena, which can be captured only if you account for that effect you have to define additional scalars to keep track of that particular variable.

Or if the number of variables if number of additional scalars becomes equal to the number of variables that you already have you solve the original equations that is it. But the point to keep in mind is even for such a problem, you might want to actually get solution by this approach and use that as the initial solution.

And then add one more layer of detail to actually you know see the difference between the behaviour. When Lewis number is 1 and when it is not 1 if you just start with a case, where Lewis number is not one you may be assigning effects to Lewis number, which may be explained only by a simple calculation.

So, hierarchical approach where you start with the simplest model and this is the simplest model to start with. In fact, one effect of Lewis number not being one will be that the behaviour of the flames under stretch will become different from what it is when Lewis number is 1; because rate of transport of mass and rate of transport of heat will be different the same. If you choose a small control volume and look at the energy balance when Lewis number is 1; Lewis number is is not 1. Its possible that for under certain conditions the there will be loss of energy from the control volume or there will be addition of gain of energy where it would be other questions?.

Student: When a how we can (Refer Time: 23:53).

I will discuss that when I discuss the flamelet model itself.

Well we do not have to actually wait it is calculated by solving this equation, with a reaction mechanism for different values of the scalar dissipation rate ok. So, one configuration which is used to generate these flamelet libraries is what is called the upholstered configuration which is a slightly different version of the porous cylinder flame. That we saw the idea is to create an opposing jet of fuel and oxidizer that is what was done in that is what was shown in the porous cylinder case.

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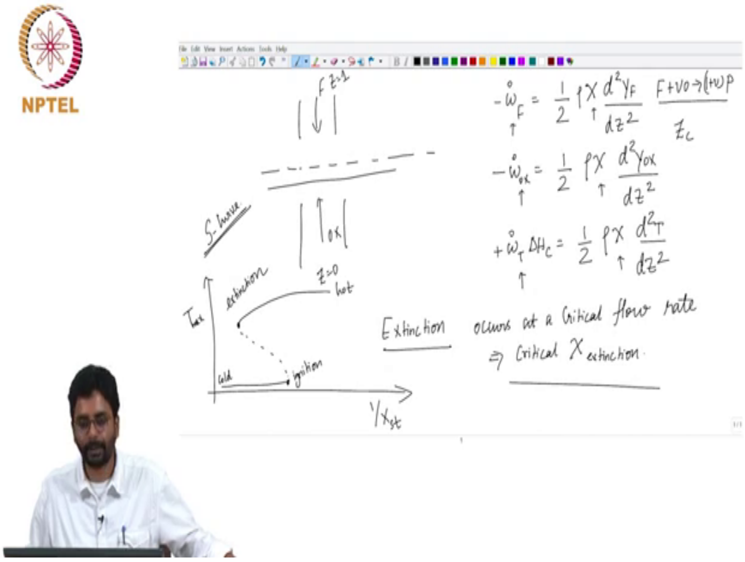

$$-\underset{\uparrow}{\dot{\omega}_F} = \frac{1}{2}\rho \underset{\uparrow}{\chi} \frac{d^2 Y_F}{dZ^2} \qquad \underline{F + \nu O \rightarrow (1+\nu) P}$$

Z_c

$$-\underset{\uparrow}{\dot{\omega}_{ox}} = \frac{1}{2}\rho \underset{\uparrow}{\chi} \frac{d^2 Y_{ox}}{dZ^2}$$

$$+\underset{\uparrow}{\dot{\omega}_T} \Delta H_c = \frac{1}{2}\rho \underset{\uparrow}{\chi} \frac{d^2 T}{dZ^2}$$

Extinction occurs at a critical flow rate

$\Rightarrow$ Critical $\chi_{extinction}$

Another way to create it is by having two jets going in opposite directions; one is issuing fuel other is issuing oxidizer this configuration was discussed in the in one of the earlier lectures. You ensure that the momentums are balanced. So, you have a stagnation plane and the flame is usually on the oxidizer side, because of this stoichiometry being much greater than 1 ok.

So, the structure of the flame in this configuration see remember that here the mixed fraction is 0 here the mixed fraction is 1 flow is actually 2 dimensional. But when you see it in the Z coordinates its 1 dimensional. Where the profiles are simply governed by this equation which we just saw see and so on. You can write an equation for this maybe plus ok. You can solve these equations for a certain reaction scheme for different values of chi ok.

And we saw that that when you continue to increase the flow rate of the oxidizer and the fuel there is a critical flow rate, at which the flame will become extinct. So, the extinct the point of extinction occurs at a critical flow rate ok. And that corresponds to a certain critical value of the scalar dissipation rate the critical value of chi this is called the chi extinction ok.

In fact, if you compute the solutions, which I am not discussing in detail and plot as a function of peak temperature and 1 by chi stoichiometric will get a curve like this ok. This is a cold branch this is the hot branch this is a point of extinction if you this is a point of ignition called the s curve ok. And I did not go into the details because we will not be using it I just wanted to give you an overview of what it means, but we have gone into some detail now.

Student: (Refer Time: 27:37) extinction is that is single phase the mixture of fuel.

Here of course, I have assumed that I am looking at this reaction ok, but you can have multiple reactions. When you have multiple reactions you have to your conserved scalar will not be if it will instead be the mass fraction or the normalized mass fraction of the carbon element or oxygen element or hydrogen element. Because even when multiple reactions happen, all reactions put together the number of elements are conserved species need not be conserved.

So, the way to derive the equation is instead of starting from well instead of combining the species equation. Convert the species equation into element mass fraction equation, which you can do by converting the mass fraction to mole fraction and multiplying by.

Student: (Refer Time: 28:31).

Any other questions? So, we have gone from the definition of scalar dissipation rate and we have looked at the basic scales of turbulence. And therefore, the scalar dissipation rate is nothing, but the inverse of the timescale for mixing or simply the rate of mixing. And in most turbulent situation because of the relationship between the stretch rate or the mixing rate at the Kolmogorov scale to its ratio at the integral scale being proportional to the square root of the Reynolds number. And the stretch rate at the integral scale itself being proportional to epsilon by k.

The mixing rate can simply be related to the turbulent timescale ok, which will be k by epsilon and this connection or this connection between mixing rate. And the turbulence parameters is what is used in many turbulent diffusion flame models ok. Remember that when you are in imagine that you are solving you are simulating flow through practical combustion device using RANS models ok.

So, you need the average reaction rates. And since the reaction rates are in exponential function of temperature, if you simply calculated the reaction rate at the average temperature; it will not be representative of what is actually happening in the system. Because you are plugging in the average value into an exponential function ok

So, if the temperature fluctuates around the average value there can be a large change in the reaction rate. And this is the fundamental limit fundamental problem with turbulent combustion modelling ok. So, what is done is that when you identify the limiting phenomena and identify the timescales and the length scales associated with the phenomena.

It simplifies the procedure for calculating average reaction rates ok. So, remember that omega dot is equal to minus if omega naught is actually proportional to the scalar dissipation rate, when the phenomena is largely mixing controlled. And therefore, if we can get an estimate for the timescale of mixing from simple turbulence parameters, you can get an estimate or we can get an accurate estimate for the reaction rates.

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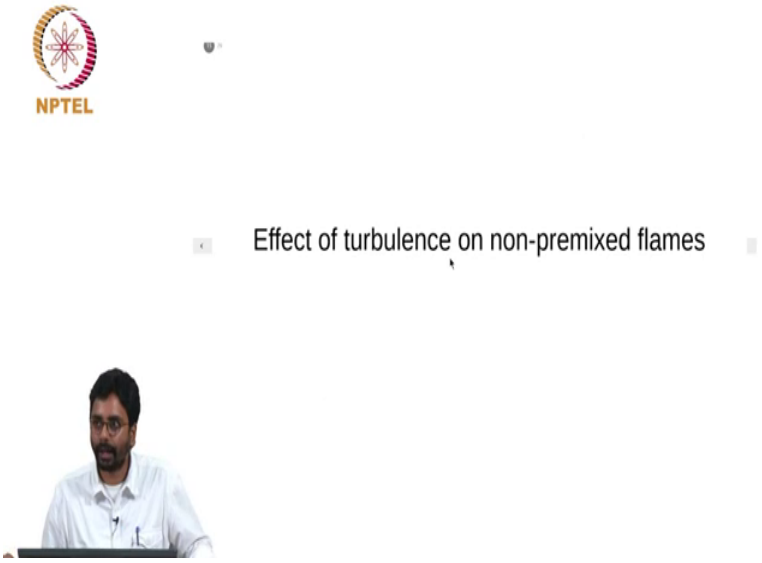

Effect of turbulence on non-premixed flames

I think we will take a break now and come back in 15 minutes and continue with this.

Thank you.