Turbulent Combustion : Theory and Modelling
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Lecture – 53
Turbulence-Chemistry Interaction (Contd...)

Welcome back. So, let us continue the discussion. And we have finished turbulent premixed flame and the modelling of that. And now we will move to the discussion on turbulent non premixed flame.

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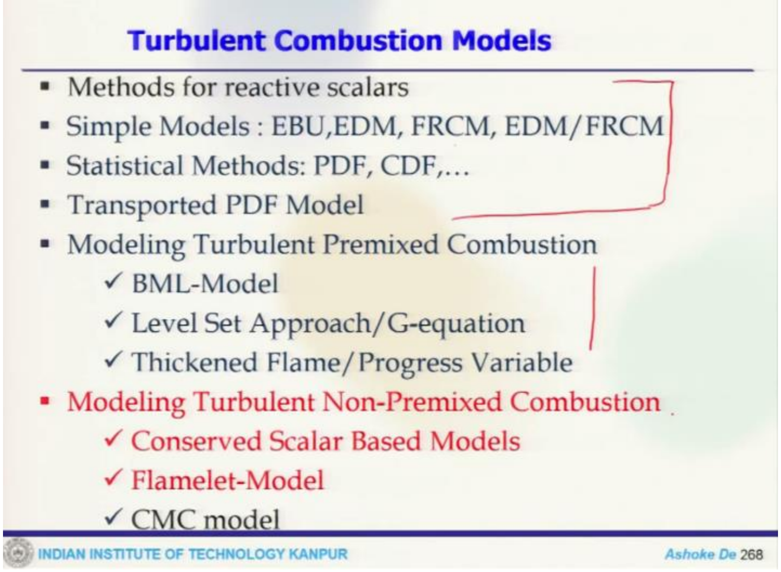

Turbulent Combustion Models

- Methods for reactive scalars
- Simple Models : EBU,EDM, FRCM, EDM/FRCM
- Statistical Methods: PDF, CDF,…
- Transported PDF Model
- Modeling Turbulent Premixed Combustion
  - ✓ BML-Model
  - ✓ Level Set Approach/G-equation
  - ✓ Thickened Flame/Progress Variable
- Modeling Turbulent Non-Premixed Combustion
  - ✓ Conserved Scalar Based Models
  - ✓ Flamelet-Model
  - ✓ CMC model

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So, as you can see or you recap from this particular diagram, we started off reactive scalars and we did the discussions on transported PDF approach, statistical methods, and simple models like EBU, EDM, finite rate chemistry and EDC. Now, these are the models which are applicable, again applicable does not mean they are going to be accurate, but they can be applied to any mode of the combustion with their associated pros and cons.

And then there are models which are very specific to the premixed combustion that we have discussed in details, how one develop those models and what are the issues behind that what is the theoretical background or these things. Now, we move to the turbulent non-premixed combustion. Now, these models are also very specific to the turbulent premixed flames.

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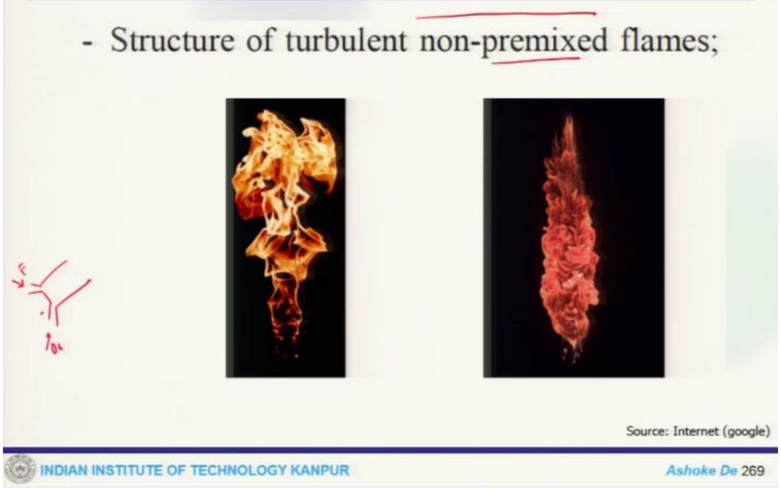

Turbulent non-premixed Flames

- Structure of turbulent non-premixed flames;

Source: Internet (google)

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Now, just to give you an idea, how this typical turbulent non-premixed flames looks like. So, this is quite different from the principle of operation of the premixed flame, because premixed flame your fuel and oxidiser they are premixed before they are sent to the or injected to the combustion chamber. But in this case, you have the combustion chamber where fuel is injected separately.

And so, this is your fuel this is your oxidizer so they come separately and then inside the chamber they come in contact through the diffusion process or the mixing takes place and then the reaction along this stoichiometric line. So, this is a basic difference between only premixed to non-premixed, and that is why the flame structures are quite different like our other system, this non-premixed flames are basically easy to control.

So, they are not also dangerous, but obviously, there are certain issues which will be associated like you can see this kind of early flames which is you are a lot of unburnt fuel sitting there. So, and also emission becomes an issue. And when you burn hydrocarbon fuel, you get carbon and all these things. This is another image where you can see using experimental diagnostic techniques that flames fronts are the images are captured.

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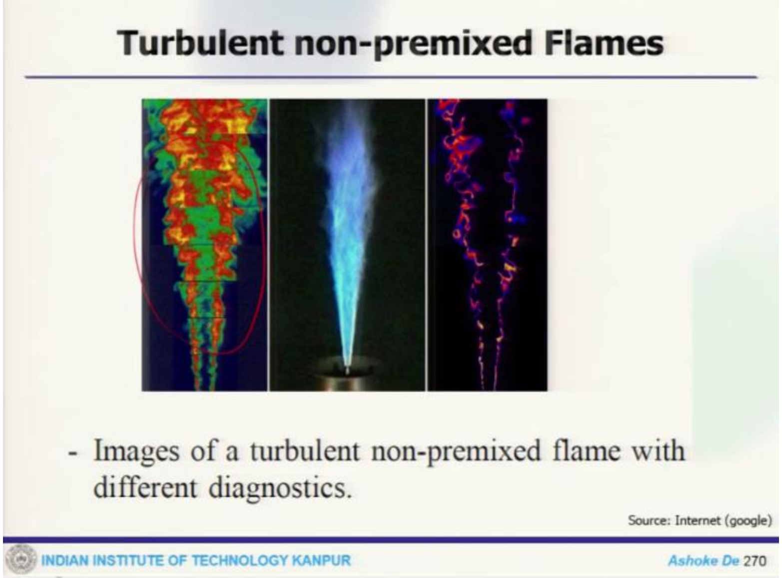

Turbulent non-premixed Flames

- Images of a turbulent non-premixed flame with different diagnostics.

Source: Internet (google)

So, this is a very image in the laboratory scale banner and this is the reaction zone, and this is the overall flame structure. But two thing which is common while talking about the premixed flame and non-premixed flame is the importance of the turbulent scales. Which are and that is why we did detail discussion and under turbulence their scales picture and all these things now, you can see how this turbulence actually impact is this flame front.

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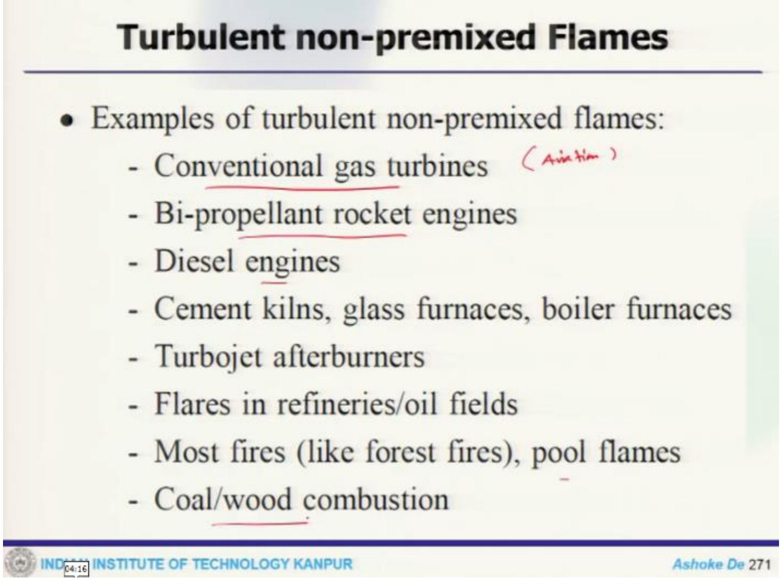

Turbulent non-premixed Flames

- Examples of turbulent non-premixed flames:
  - Conventional gas turbines (Aviation)
  - Bi-propellant rocket engines
  - Diesel engines
  - Cement kilns, glass furnaces, boiler furnaces
  - Turbojet afterburners
  - Flares in refineries/oil fields
  - Most fires (like forest fires), pool flames
  - Coal/wood combustion

Now, these are some of the examples we have kind of come across this example earlier also. And like your conventional gas turbine which uses in gas turbine in your aviation industry, then your rocket engines bi-propellant rocket engines your diesel engine that means, glass furnaces, boiler furnaces, turbojet burners, oil fuels, pool flames, combustions and all these things. Now, as I mentioned, there are some of the things which are actually can be challenging.

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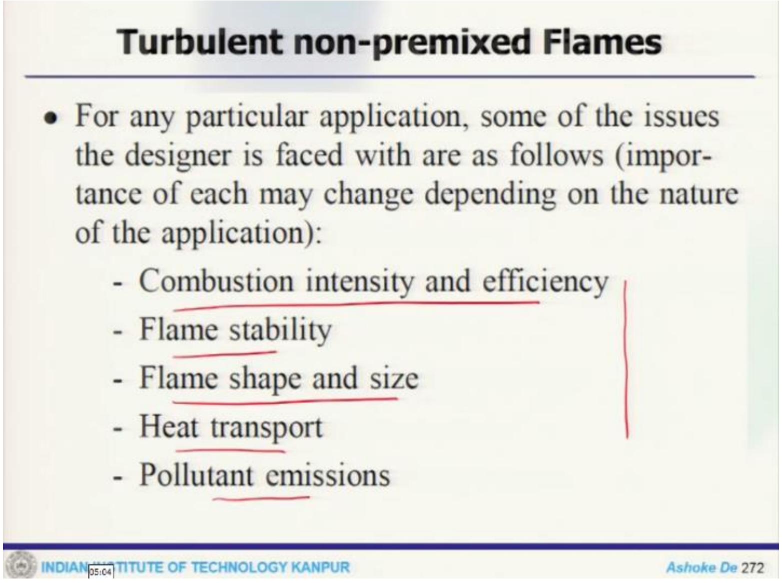

Turbulent non-premixed Flames

- For any particular application, some of the issues the designer is faced with are as follows (importance of each may change depending on the nature of the application):
  - Combustion intensity and efficiency
  - Flame stability
  - Flame shape and size
  - Heat transport
  - Pollutant emissions

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One is that and this is also important to change of depending on the nature of the applications. One is the flame stability, combustion intensity and efficiency, flame shape and size, heat transfer pollutant emissions. So, these are obviously, not only problem dependent, these are also dependent on the kind of fuel it is used. So, in a nutshell one can think about they are depending on the operating conditions, which include not only the geometric conditions also the flow conditions and other parameters.

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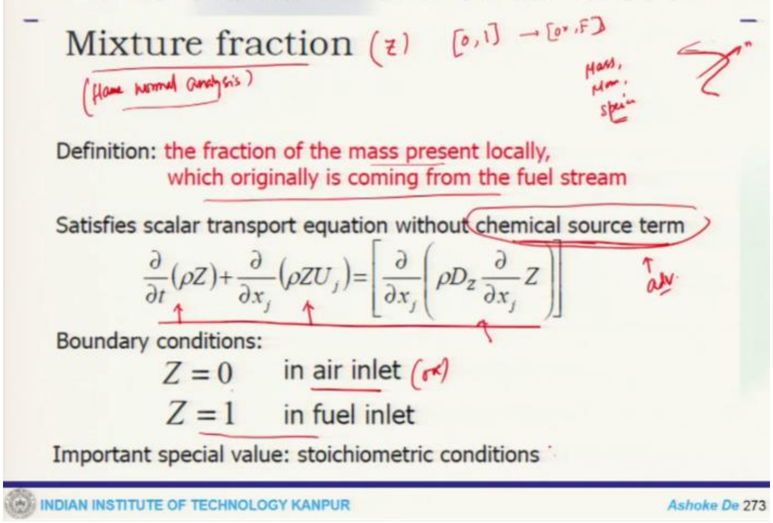

Turbulent Non-Premixed combustion

Mixture fraction (z) [0,1] → [or, F]

(flame normal analysis)

Mass, Mom, species

Z''

Definition: the fraction of the mass present locally, which originally is coming from the fuel stream

Satisfies scalar transport equation without chemical source term

$$\frac{\partial}{\partial t}(\rho Z)+\frac{\partial}{\partial x_j}(\rho Z U_j)=\left[\frac{\partial}{\partial x_j}\left(\rho D_Z \frac{\partial}{\partial x_j} Z\right)\right]$$

adv

Boundary conditions:

$Z=0$ in air inlet (ox)

$Z=1$ in fuel inlet

Important special value: stoichiometric conditions

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Now, in turbulent non-premixed flame the one of the popular approach is the mixture fraction kind of approach, which is an conserved scalar typically denoted by z and 1 has a like premixed variable, this is also a non-premixed variable or conserved scalar is a scalar variable and which also goes between 0 to 1 from oxidizer to fuel. So, this is how it is varies. So, what it allows you the fraction of the mass present locally which originally is coming from the fuel stream and for this mixture fraction, you have a scalar transport equation without the source term.

So, theoretically we solve mass, momentum and species conservation and these species conservation equation when convert to a mixture fraction phase, this is again to mind it this is in flame normal analysis. This is not one point statistical analysis this is a flame normal analysis that means, if you have a flame front like this, so, this is your flame normal, where you transform the things in that phase and from physical phase to that and you come across the transport equation of this.

And this transport equation of the scalar filter mixture fraction, these involves in the physical phase. This is like your conserved term. This is convection due to mean velocity. This is diffusion. So, there is no source term which is one of the biggest advantage because this is the chemical source term which appear in your species mass transfer equation that creates lot of trouble I mean how to close that particular equation and to close that particular term.

And that is why we have seen there are so many variance of different kinds of models in different reason to close down the source term. Now, the advantage of this particular conserved scalar approach is that you come across a transport equation, this is without the source term and you can actually get without this chemical source term. So, this is a real advantage, so, that the stiffness of the system is reduced. And the boundary conditions for that at the air inlet, it would be zero or oxidizer inlet and z equals to 1 in the fuel inlet.

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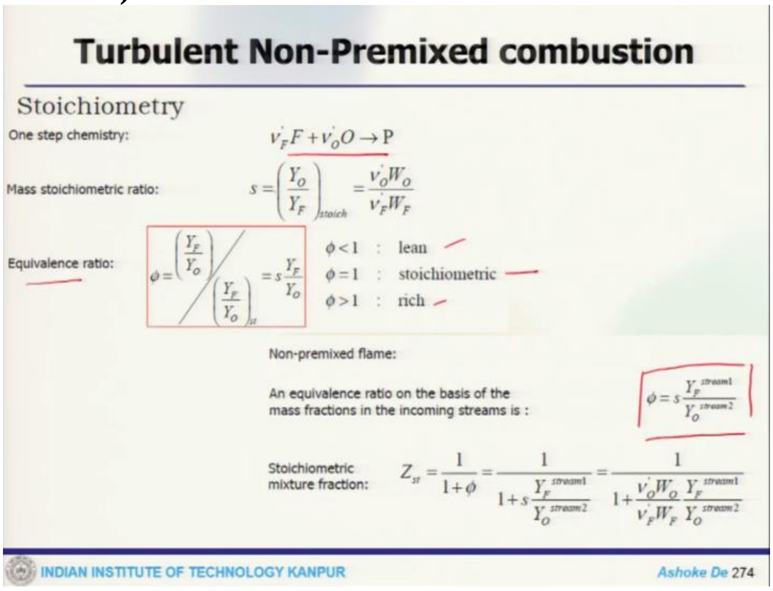

Turbulent Non-Premixed combustion

Stoichiometry

One step chemistry: $\nu_F' F + \nu_O' O \rightarrow P$

Mass stoichiometric ratio: $s = \left(\frac{Y_O}{Y_F}\right)_{stoich} = \frac{\nu_O' W_O}{\nu_F' W_F}$

Equivalence ratio: $\boxed{\phi = \left(\frac{Y_F}{Y_O}\right) \Big/ \left(\frac{Y_F}{Y_O}\right)_{st} = s\frac{Y_F}{Y_O}}$

$\phi < 1$: lean

$\phi = 1$: stoichiometric

$\phi > 1$: rich

Non-premixed flame:

An equivalence ratio on the basis of the mass fractions in the incoming streams is : $\boxed{\phi = s\frac{Y_F^{stream1}}{Y_O^{stream2}}}$

Stoichiometric mixture fraction: $Z_{st} = \frac{1}{1+\phi} = \frac{1}{1+s\frac{Y_F^{stream1}}{Y_O^{stream2}}} = \frac{1}{1+\frac{\nu_O' W_O}{\nu_F' W_F}\frac{Y_F^{stream1}}{Y_O^{stream2}}}$

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An important special value is the stoichiometric conditions. Now, in the stoichiometry, if you consider this one step reaction where fuel oxidizer, go to product, your mass stoichiometric ratio defended oxidizer by fuel at stoichiometry which is:

$$\frac{\nu_O W_O}{\nu_F W_F}$$

And then you can define the equivalence ratio which is: $S\frac{Y_F}{Y_O}$. So, φ is 1 which is a stoichiometry condition, φ less than 1 it is a lean condition and φ greater than 1 is could be a rich condition.

Now, for a non-premixed flame and equivalence ratio in the basis of the mass fraction in the incoming stream is defined like:

$$\varphi = S\frac{Y_F^{stream1}}{Y_O^{stream2}}$$

So, the stoichiometric mixture fraction if one tries to calculate it, it would be 1/(1 + φ). So, which is nothing but:

$$Z_{st} = \frac{1}{1+\frac{\nu_O W_O}{\nu_F W_F}\frac{Y_F^{stream1}}{Y_O^{stream2}}}$$

So, you can simplify with this expression that we have got earlier.

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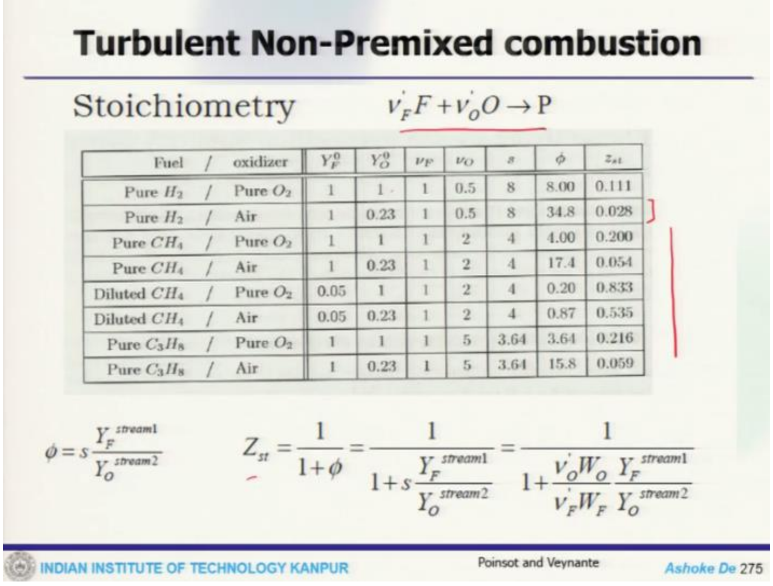

Turbulent Non-Premixed combustion

Stoichiometry $\nu'_F F + \nu'_O O \rightarrow \mathrm{P}$

Fuel / oxidizer	Y_F^0	Y_O^0	ν_F	ν_O	s	ϕ	z_{st}
Pure H_2 / Pure O_2	1	1	1	0.5	8	8.00	0.111
Pure H_2 / Air	1	0.23	1	0.5	8	34.8	0.028
Pure CH_4 / Pure O_2	1	1	1	2	4	4.00	0.200
Pure CH_4 / Air	1	0.23	1	2	4	17.4	0.054
Diluted CH_4 / Pure O_2	0.05	1	1	2	4	0.20	0.833
Diluted CH_4 / Air	0.05	0.23	1	2	4	0.87	0.535
Pure C_3H_8 / Pure O_2	1	1	1	5	3.64	3.64	0.216
Pure C_3H_8 / Air	1	0.23	1	5	3.64	15.8	0.059

$$\phi = s\frac{Y_F^{stream1}}{Y_O^{stream2}} \qquad Z_{st} = \frac{1}{1+\phi} = \frac{1}{1+s\frac{Y_F^{stream1}}{Y_O^{stream2}}} = \frac{1}{1+\frac{\nu'_O W_O}{\nu'_F W_F}\frac{Y_F^{stream1}}{Y_O^{stream2}}}$$

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Now, for the single step reaction, now you can take different combination of this like an equivalence ratio is this and then Z stoichiometry you can find out. And this is heavily dependent on kind of oxidizer you use and that is what is tabulated here. If you let us say look at pure hydrogen to pure oxygen, this is 1, this is 1, this is 0.5, s should be 8, φ would be 8, Z stoichiometry is 0.111. At the same time, if you look at pure hydrogen when it is burning with the air, gets stoichiometry is quite low.

And the reason is, you have oxygen now by mass fraction is 0.23 because your oxidizer now contains 77% Nitrogen by mass. And this is true for any particular fuel. And that already we have seen, while looking at the fundamental flame properties like adiabatic room temperature and such things that if you have a fuel which is burning with the air and we have a fuel which is burning with oxygen, they would give you a different flame temperature. So, this table shows you that when different fuel you burn and now given a fuel you can now calculate these things very easily.

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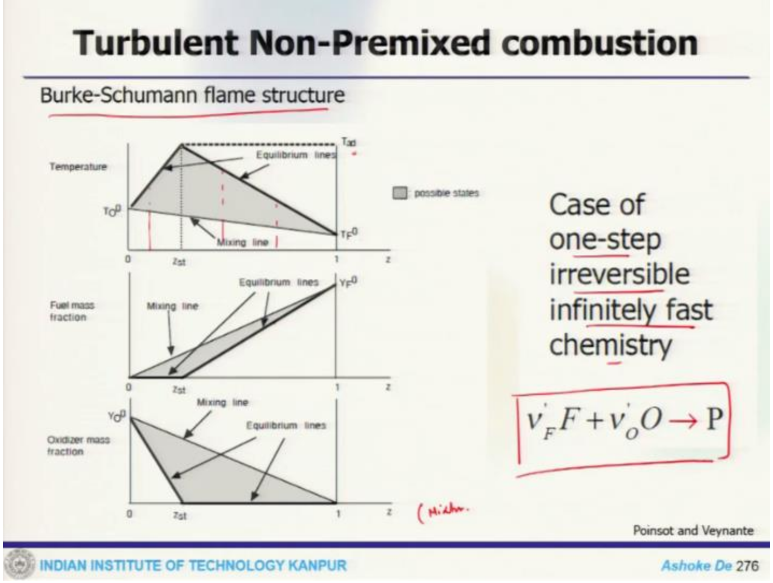

Turbulent Non-Premixed combustion

Burke-Schumann flame structure

Case of one-step irreversible infinitely fast chemistry

$$\boxed{\nu_F^{'}F+\nu_O^{'}O\rightarrow \mathrm{P}}$$

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So, now, we have not this single step reaction, we consider the single step reaction and this is a famous flame structure which is known as Burke-Schumann flame structure. Now, these case is one step, this is a one-step reaction, irreversibly infinitely fast chemistry. So each of these terms receives one step, irreversible, infinitely fast chemistry. That means fuel oxidizer come in contact they actually burn and prepare of the product. So, if you look at the situation what happens?

So, first let us look at the oxidizer mass fraction and when it comes to burning state that gets stoichiometric to be immediately 0 and this is in the mixture fraction phase. So, why oxidizer mass fraction in Z. Similarly, fuel mass fraction if you look at it, this is 1 at the beginning when the reaction takes place it is 0 and these lines corresponds to equilibrium line and this is the mixing line that means, if there is nothing happens the mixing line like that and this is the same mixing line for the oxidizer.

Now, if you look at the temperature, this is oxidizer temperature and fuel temperature along Z stoichiometric there will be a peak this is your adiabatic flame temperature and these are the equilibrium lines. So, one can looking at a particular Z value one can find the temperature at different location. So, this is true simple analysis for one step reactions, where you get this irreversible one step infinitely fast reaction and that time the temperature profile we like that and name or by knowing in particular mixture fraction value one can always estimate the temperature, fuel concentration, oxygen concentration and everything.

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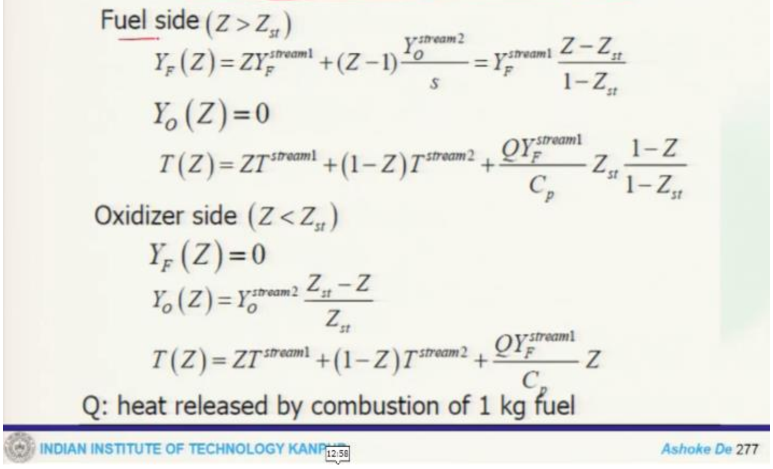

Turbulent Non-Premixed combustion

Burke Schuman model equations

Fuel side $(Z > Z_{st})$

$$Y_F(Z) = ZY_F^{stream1} + (Z-1)\frac{Y_O^{stream2}}{s} = Y_F^{stream1}\frac{Z-Z_{st}}{1-Z_{st}}$$

$$Y_O(Z) = 0$$

$$T(Z) = ZT^{stream1} + (1-Z)T^{stream2} + \frac{QY_F^{stream1}}{C_p}Z_{st}\frac{1-Z}{1-Z_{st}}$$

Oxidizer side $(Z < Z_{st})$

$$Y_F(Z) = 0$$

$$Y_O(Z) = Y_O^{stream2}\frac{Z_{st}-Z}{Z_{st}}$$

$$T(Z) = ZT^{stream1} + (1-Z)T^{stream2} + \frac{QY_F^{stream1}}{C_p}Z$$

Q: heat released by combustion of 1 kg fuel

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Now, if we do little bit detailed analysis of this Burke Schuman flame equations. So, our fuel side which is Z stoichiometric if you go back here, this is the Z stoichiometric and this is our fuel side.

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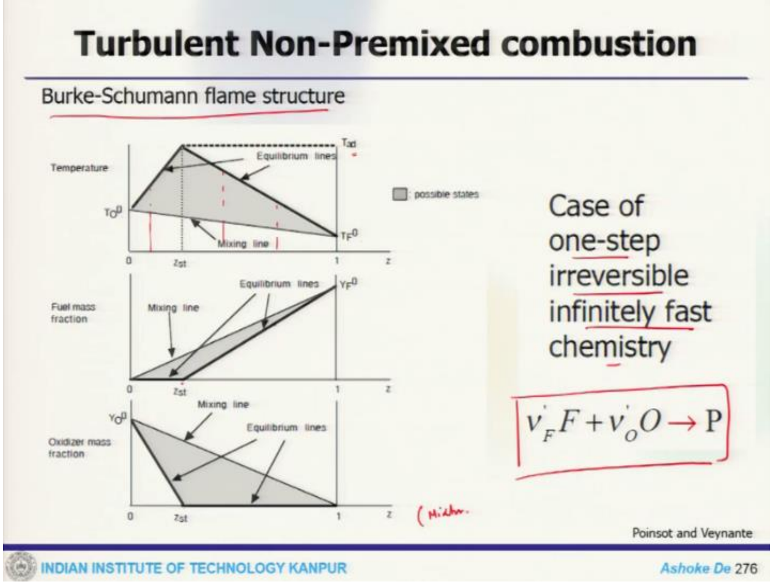

Turbulent Non-Premixed combustion

Burke-Schumann flame structure

Case of one-step irreversible infinitely fast chemistry

$$\boxed{v_F'F + v_O'O \rightarrow \mathrm{P}}$$

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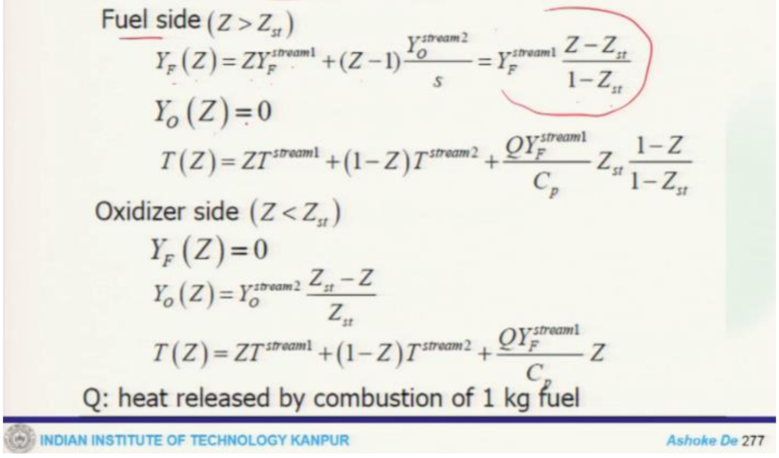

Turbulent Non-Premixed combustion

Burke Schuman model equations

Fuel side ($Z > Z_{st}$)

$$Y_F(Z) = ZY_F^{stream1} + (Z-1)\frac{Y_O^{stream2}}{s} = Y_F^{stream1}\frac{Z-Z_{st}}{1-Z_{st}}$$

$$Y_O(Z) = 0$$

$$T(Z) = ZT^{stream1} + (1-Z)T^{stream2} + \frac{QY_F^{stream1}}{C_p} Z_{st}\frac{1-Z}{1-Z_{st}}$$

Oxidizer side ($Z < Z_{st}$)

$$Y_F(Z) = 0$$

$$Y_O(Z) = Y_O^{stream2}\frac{Z_{st}-Z}{Z_{st}}$$

$$T(Z) = ZT^{stream1} + (1-Z)T^{stream2} + \frac{QY_F^{stream1}}{C_p} Z$$

Q: heat released by combustion of 1 kg fuel

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So, for the fuel side:

$$Y_F(Z) = ZY_F^{stream1} + (Z-1)\frac{Y_O^{stream2}}{s}$$

So, which can be simplified as:

$$Y_F(Z) = Y_F^{stream1}\frac{Z-Z_{st}}{1-Z_{st}}$$

So, this is how you simplify that. Oxidizer at that Z is 0. That because beyond Z stoichiometric, oxygen is always 0.

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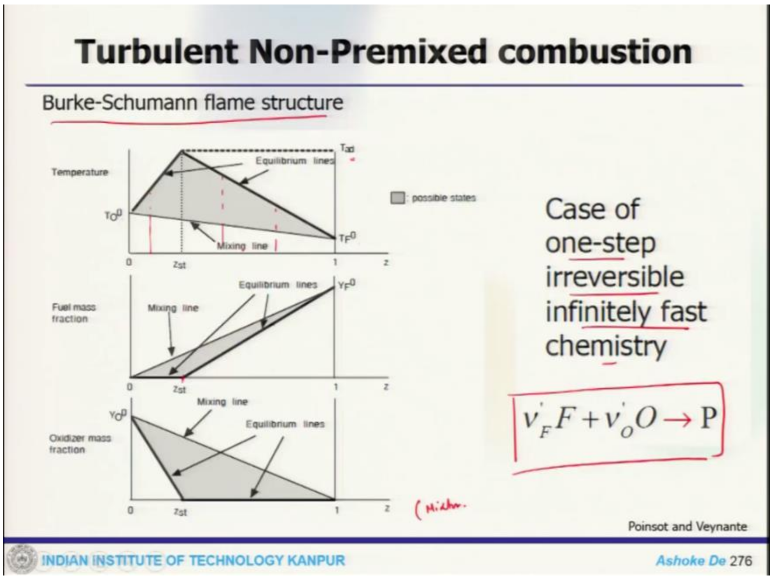

Turbulent Non-Premixed combustion

Burke-Schumann flame structure

Case of one-step irreversible infinitely fast chemistry

$$\boxed{\nu'_F F + \nu'_O O \rightarrow P}$$

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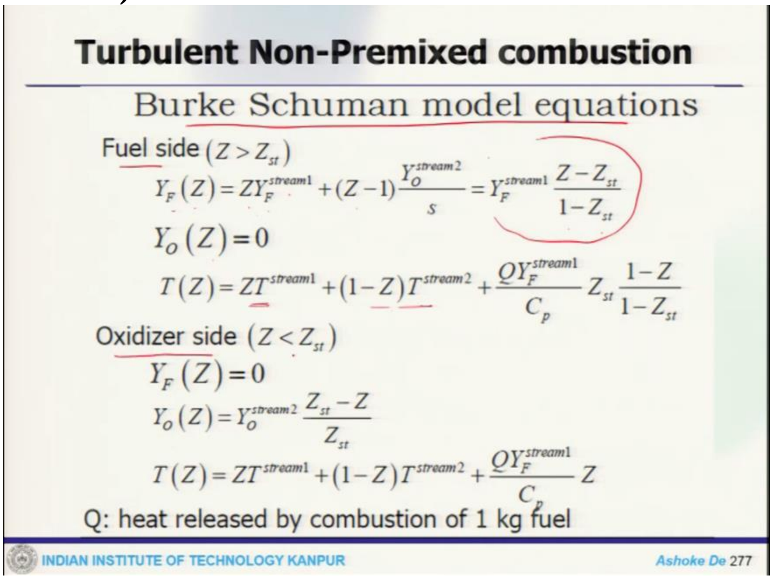

Turbulent Non-Premixed combustion

Burke Schuman model equations

Fuel side $(Z > Z_{st})$

$$Y_F(Z) = ZY_F^{stream1} + (Z-1)\frac{Y_O^{stream2}}{s} = Y_F^{stream1}\frac{Z - Z_{st}}{1 - Z_{st}}$$

$$Y_O(Z) = 0$$

$$T(Z) = ZT^{stream1} + (1-Z)T^{stream2} + \frac{QY_F^{stream1}}{C_p}Z_{st}\frac{1-Z}{1-Z_{st}}$$

Oxidizer side $(Z < Z_{st})$

$$Y_F(Z) = 0$$

$$Y_O(Z) = Y_O^{stream2}\frac{Z_{st} - Z}{Z_{st}}$$

$$T(Z) = ZT^{stream1} + (1-Z)T^{stream2} + \frac{QY_F^{stream1}}{C_p}Z$$

Q: heat released by combustion of 1 kg fuel

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And temperature would be:

$$T(Z) = ZT^{stream1} + (1-Z)T^{stream2} + \frac{QY_F^{stream1}}{C_P}Z_{st}\frac{1-Z}{1-Z_{st}}$$

So, this will come the contribution from the stream 1, this is the stream 2, that is oxidizer stream, fuel stream and this is because of the reaction the amount of heat which is released. Now, similarly, on the oxidizer side which is Z less than Z stoichiometric that means this zone.

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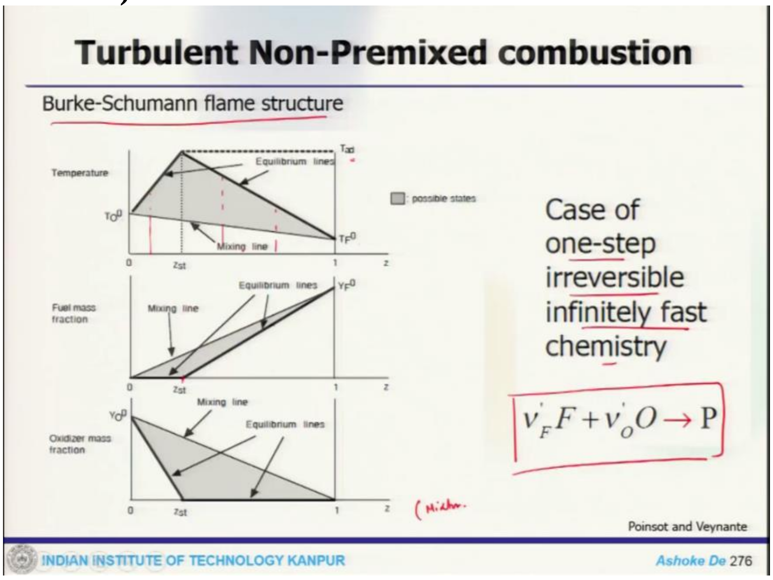

Turbulent Non-Premixed combustion

Burke-Schumann flame structure

Case of one-step irreversible infinitely fast chemistry

$$\nu_F' F + \nu_O' O \rightarrow P$$

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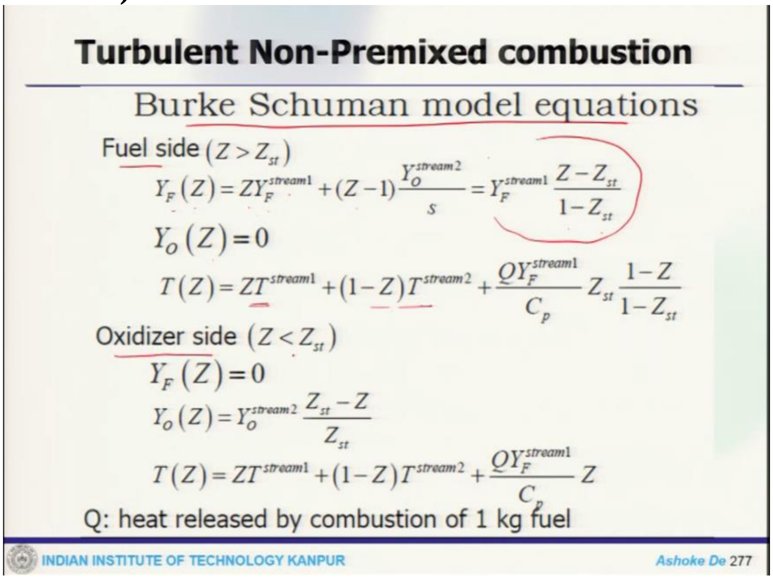

Turbulent Non-Premixed combustion

Burke Schuman model equations

Fuel side $(Z > Z_{st})$

$$Y_F(Z) = ZY_F^{stream1} + (Z-1)\frac{Y_O^{stream2}}{s} = Y_F^{stream1}\frac{Z-Z_{st}}{1-Z_{st}}$$

$$Y_O(Z) = 0$$

$$T(Z) = ZT^{stream1} + (1-Z)T^{stream2} + \frac{QY_F^{stream1}}{C_p} Z_{st}\frac{1-Z}{1-Z_{st}}$$

Oxidizer side $(Z < Z_{st})$

$$Y_F(Z) = 0$$

$$Y_O(Z) = Y_O^{stream2}\frac{Z_{st}-Z}{Z_{st}}$$

$$T(Z) = ZT^{stream1} + (1-Z)T^{stream2} + \frac{QY_F^{stream1}}{C_p} Z$$

Q: heat released by combustion of 1 kg fuel

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Here, fuel is completely 0, oxidizer can be estimated as always:

$$Y_O(Z) = Y_O^{stream2}\frac{Z_{st} - Z}{Z_{st}}$$

And T(Z) is this. So, Q is the heat released by combustion of 1 kg of fuel.

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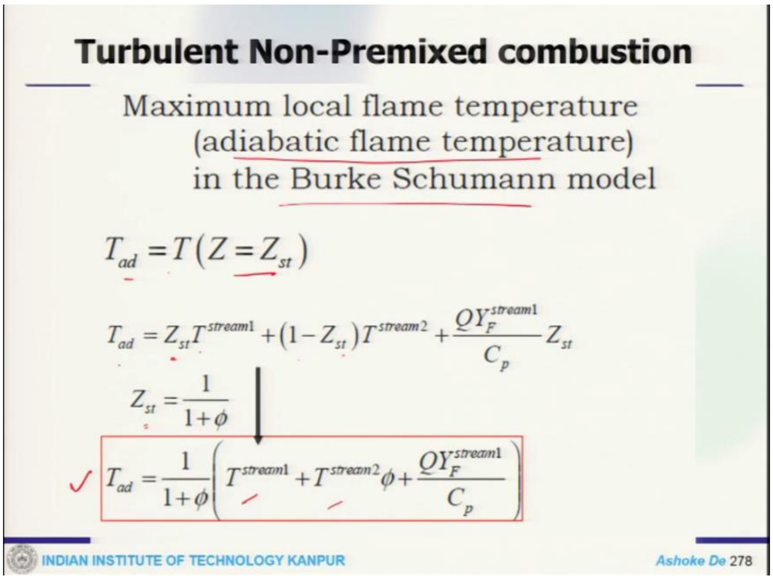

Turbulent Non-Premixed combustion

Maximum local flame temperature (adiabatic flame temperature) in the Burke Schumann model

$$T_{ad} = T(Z = Z_{st})$$

$$T_{ad} = Z_{st}T^{stream1} + (1-Z_{st})T^{stream2} + \frac{QY_F^{stream1}}{C_p}Z_{st}$$

$$Z_{st} = \frac{1}{1+\phi}$$

$$✓\ \boxed{T_{ad} = \frac{1}{1+\phi}\left(T^{stream1} + T^{stream2}\phi + \frac{QY_F^{stream1}}{C_p}\right)}$$

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Now, one can also get the local flame temperature or the maximum local flame temperature or adiabatic flame temperature in the Burke Schumann kind of model. So, that T adiabatic would be:

$$T_{ad} = Z_{st}T^{stream1} + (1 - Z_{st})T^{stream2} + \frac{QY_F^{stream1}}{C_P}Z_{st}$$

And Z stoichiometric is 1/(1+φ). So, if you use that, so, this one actually reduces to this equation for T adiabatic can be estimated as 1/(1+φ) multiply by this.

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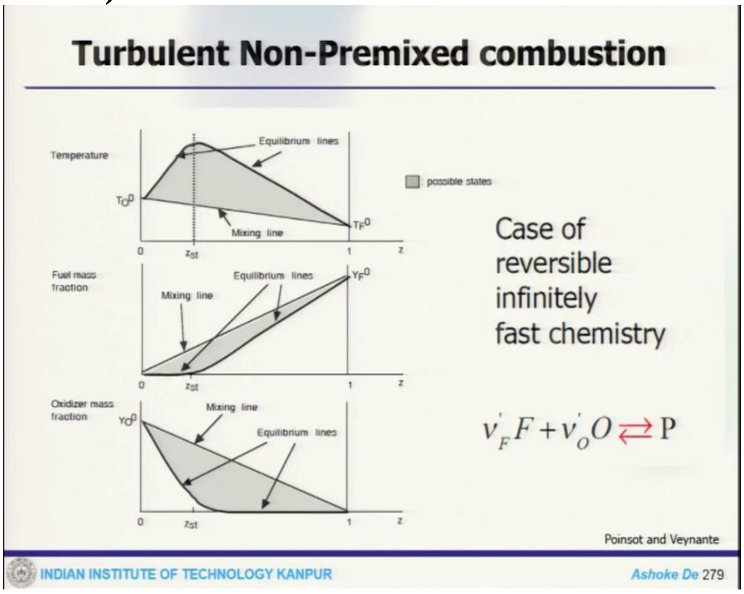

Turbulent Non-Premixed combustion

Case of reversible infinitely fast chemistry

$$\nu'_F F + \nu'_O O \rightleftarrows P$$

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So, that means this theoretical calculations allow you to estimate the adiabatic flame temperature for any fuel for the global reaction, which assumed to be. So, now we can have a situation where your equation system is against single step, but it is now reversible but is still infinitely fast. So, previously the case was your one step reaction where it is irreversible, but infinitely fast. Now, this case we take as one step reaction but reversible that means, the product can be disassociated from fuel and oxidizer.

Now, what happens if you look at the plot of the oxidizer in the mixture fraction phase. This is how it varies instead of the Z stoichiometric the reaction live. There is a nice curvature you can see instead of that steepness and these are the mixing lines which correspond to that. Similarly, flame aspects you look at it will come down around Z stoichiometric not that steep and goes to 0 slowly to oxidizer side and the temperature would also do not show that peak hot we used to or we have seen which is happening at irreversible case.

So, compared to that there is a temperature will be also less and this is along that Z stoichiometric and these are the mixing lines. So, you see immediately there is a change and that change is coming primarily because of these, it‘s reversibility, which allows that means not only this way, that reason is when the product dissociates that also consume some of the energy this side this part of the reaction can produce let's say amount of heat and the side of the this is conjunct Q_2 so overall Q would be Q_1 - Q_2.

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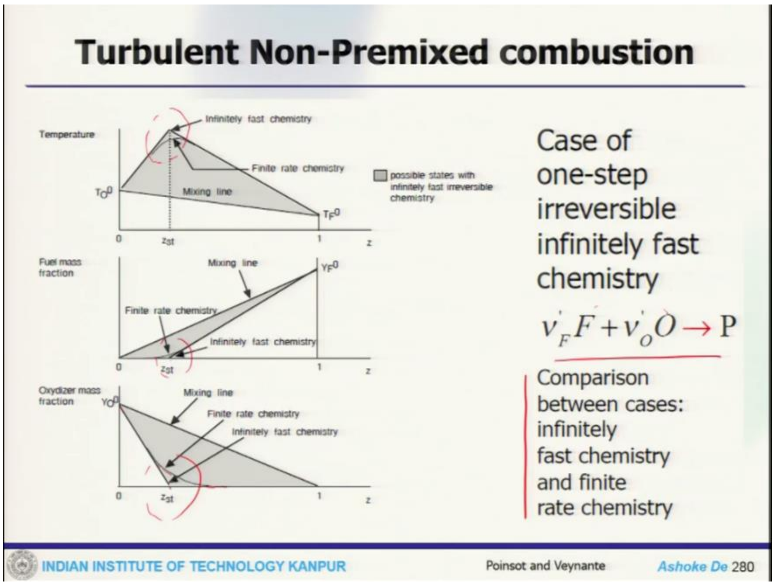

Turbulent Non-Premixed combustion

Case of one-step irreversible infinitely fast chemistry

$$\nu_F' F + \nu_O' O \rightarrow \mathrm{P}$$

Comparison between cases: infinitely fast chemistry and finite rate chemistry

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Poinsot and Veynante

So, this is why also that effect is immediately shown in the temperature plot. Now we can look at a case whether it is a one-step reaction and this is irreversible and infinitely fast chemistry, where we can compare between the cases of infinitely fast chemistry and finite rate chemistry. So, but the reaction is still single step and irreversible. Now, if you recall, it is infinitely fast that means fuel and oxidizer come in contact and it will produce the product.

So, this is all in mixture fraction rate this is how oxygen will come at this stoichiometric to become immediately 0. Similarly, fuel or Z stoichiometric to become 0 that means, these two guys are come in contact and burn and the temperature will be peak there. But when you look at the situation, when it said, final rate chemistry oxidizer does not come to zero immediately at Z stoichiometric rather this goes nicely and then becomes zero.

Whereas, if you look at the fuel also similarly does not go immediately at zero at the moment it was like that and the temperature formation also like that. So there is a huge impact of the chemistry what you can see even for a diffusion, whether it is an so that means the assumption that we are going to make that has a lot of impact in your fuel mass fraction and temperature production. So whether it is a fast chemistry or finite rate chemistry, or it is a reversible or irreversible that will have.

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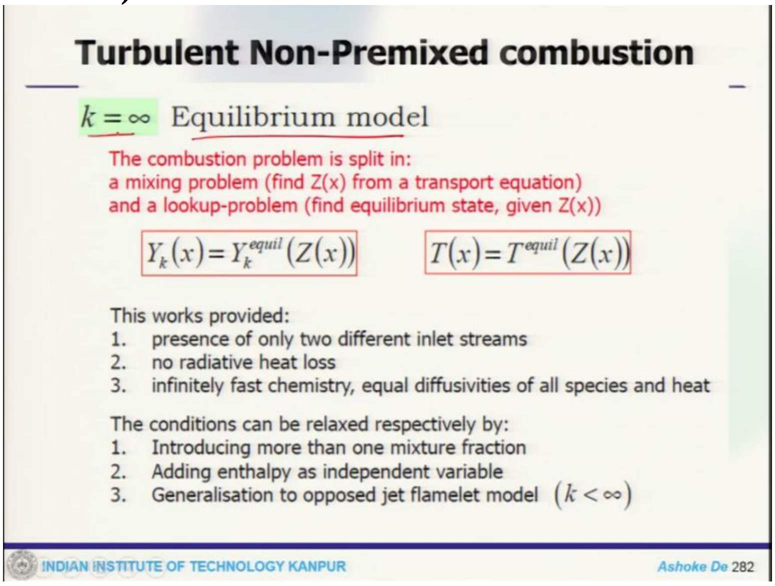

Turbulent Non-Premixed combustion

$k = \infty$ Equilibrium model

The combustion problem is split in:
a mixing problem (find Z(x) from a transport equation)
and a lookup-problem (find equilibrium state, given Z(x))

$$\boxed{Y_k(x) = Y_k^{equil}(Z(x))} \qquad \boxed{T(x) = T^{equil}(Z(x))}$$

This works provided:

1. presence of only two different inlet streams
2. no radiative heat loss
3. infinitely fast chemistry, equal diffusivities of all species and heat

The conditions can be relaxed respectively by:

1. Introducing more than one mixture fraction
2. Adding enthalpy as independent variable
3. Generalisation to opposed jet flamelet model $(k < \infty)$

Now we can see this temperature what is Z plot and we combine this case for a single step reaction, which is reversible and within situation where laminar flame with chemical mechanism, single step we say fast chemistry which is sort of an equilibrium kind of situation and there will be finite rate chemistry which is non-equilibrium. If it is fast chemistry, then K goes to infinity. If it is non-equilibrium finite chemistry, K equals to infinity, then one scenario it could be irreversible situation.

Other situation is the reversible one and irreversible situation which is equilibrium temperature goes up z stoichiometry and come to fuel. Now, here when you take the finite rate chemistry, this is the limit of my infinitely fast rate chemistry limit this is finite rate chemistry limit, but these two are four different states when you have a low strain, you get high temperature when you are high strain and you get low temperature that means now strain has huge impact on flame front. So, this is another important aspect when you look at it.

Now, the reversible case, obviously, the temperature limit would be less, because of this reversible reaction some of the energy which is again consumed back. Now, if you see this is infinitely fast chemistry limit that is still quite high compared to finite rate chemistry limit and finite rate, low strain still produces high temperature, high strain produces low temperature. So, that means when you have a high strain that flame is exposed to that strain. So the effect of your mixing indirectly impacting the flame front. Now, I will elaborate these things slightly more.

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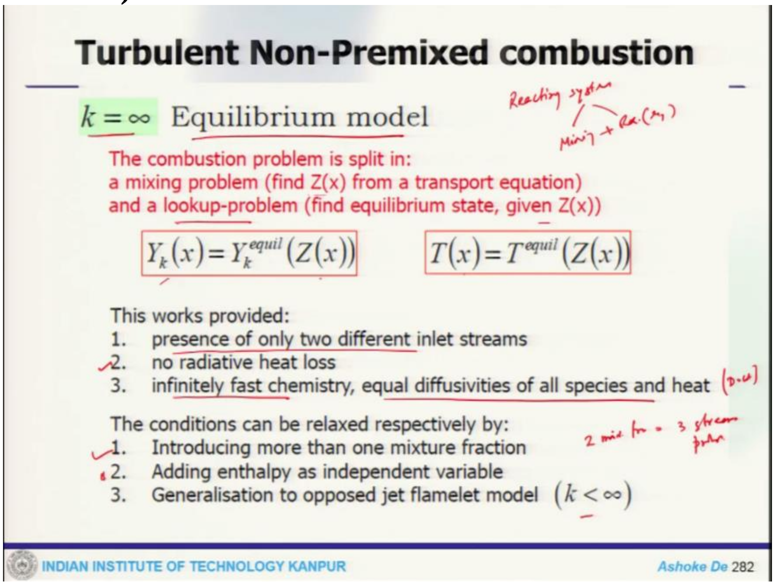

Turbulent Non-Premixed combustion

$k = \infty$ Equilibrium model

Reacting system
Mixing + Rea.(eq)

The combustion problem is split in:
a mixing problem (find Z(x) from a transport equation)
and a lookup-problem (find equilibrium state, given Z(x))

$$\boxed{Y_k(x) = Y_k^{equil}(Z(x))} \qquad \boxed{T(x) = T^{equil}(Z(x))}$$

This works provided:

1. presence of only two different inlet streams
2. no radiative heat loss
3. infinitely fast chemistry, equal diffusivities of all species and heat (D=c)

The conditions can be relaxed respectively by:

1. Introducing more than one mixture fraction
2. Adding enthalpy as independent variable
3. Generalisation to opposed jet flamelet model $(k < \infty)$

2 mix fr = 3 stream probm

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Ashoke De 282

So, this is our equilibrium model k would be where be infinity. Now, if that is an equilibrium model that when infinitely first situation, we can split the whole business into 2 problem. One is the mixing problem that means only look at the transport equation of these conserved scalar Z(x) and then we can find the equilibrium state from for a given Z(x) from the lookup table that means the whole reacting system is now broken into 2 pieces.

One is the mixing and another is the reaction to the equilibrium reaction. So, these 2 combinely look at the whole flow fuel. So, this is what happens and when you find out that state here your species mass function will be equilibrium and the function of Z temperature also going to be function of Z this particular concept or the way of handling the system this works nicely provided you have only presence of 2 different streams.

Second, there is no radiative loss. Third is infinitely fast chemistry equal diffusivity all species that means, this will lead to an assumption of di is same. It is a sort of a constant di business. So, these are the sort of an assumption and, but these conditions can be relaxed by introducing and then more than one mixture fraction that means, we can define another mixture fraction and then can somehow relax this particular inlet issue.

And that is what is very common even today, we can defined two mixture fractions and solve this things problem. So, like if we have 2 mixture faction we can solve three stream problem. Then we can add by enthalpy as an independent variable. So, where the radiative heat losses can be taken care of and also we can generalize into the upward jet flame let model to k is less than infinity. So, these are the modifications one can easily do and now, the question comes, how we evaluate the temperature from the mixture fraction.

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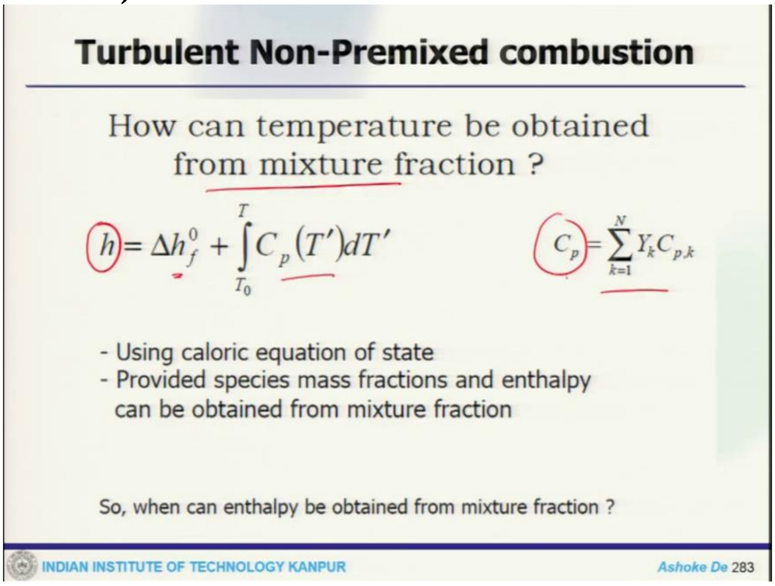

Turbulent Non-Premixed combustion

How can temperature be obtained from mixture fraction ?

$$h = \Delta h_f^0 + \int_{T_0}^{T} C_p(T')dT' \qquad C_p = \sum_{k=1}^{N} Y_k C_{p,k}$$

- Using caloric equation of state
- Provided species mass fractions and enthalpy can be obtained from mixture fraction

So, when can enthalpy be obtained from mixture fraction ?

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So, that is an important question to answer. So, we have enthalpy which is a calorific question of state which gives you enthalpy of formation plus the other part. Where mixture C_P is the total submission of over all the species Y_k and $C_{p,k}$. Now, using the mixture fraction, we can find out the C_P and enthalpy. So, this Chi we can find out. Now, when enthalpy can be obtained from the mixture fraction.

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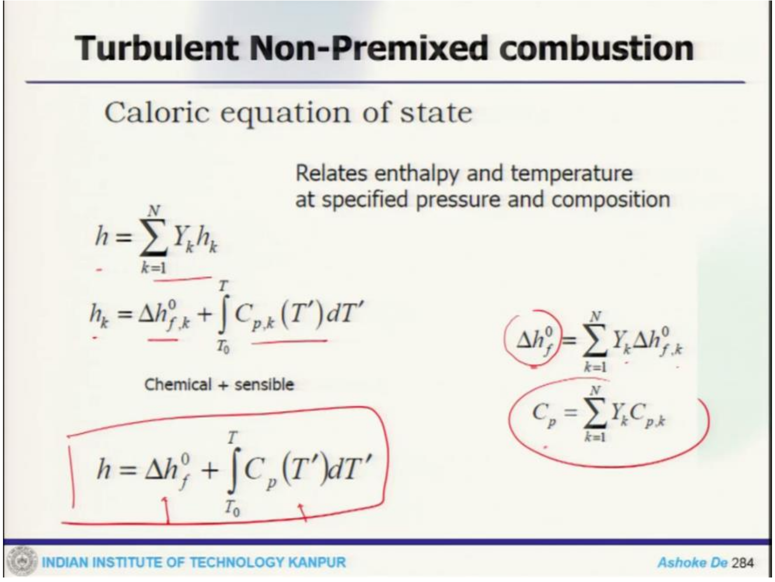

Turbulent Non-Premixed combustion

Caloric equation of state

Relates enthalpy and temperature at specified pressure and composition

$$h = \sum_{k=1}^{N} Y_k h_k$$

$$h_k = \Delta h_{f,k}^0 + \int_{T_0}^{T} C_{p,k}(T')dT'$$

Chemical + sensible

$$\Delta h_f^0 = \sum_{k=1}^{N} Y_k \Delta h_{f,k}^0$$

$$C_p = \sum_{k=1}^{N} Y_k C_{p,k}$$

$$\boxed{h = \Delta h_f^0 + \int_{T_0}^{T} C_p(T')dT'}$$

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So, we use our calorie equation of state and then relate the enthalpy. So, enthalpy is, some over all the species this is Y_k h_k and for individual enthalpy. It is the enthalpy of formation plus the sensible part. And now enthalpy of formation is also individual mass fraction to formation. So, that is the total Δh_f^0 and C_P would be total of these, so, that all we get h of chemical part and the sensible part for the mixture.

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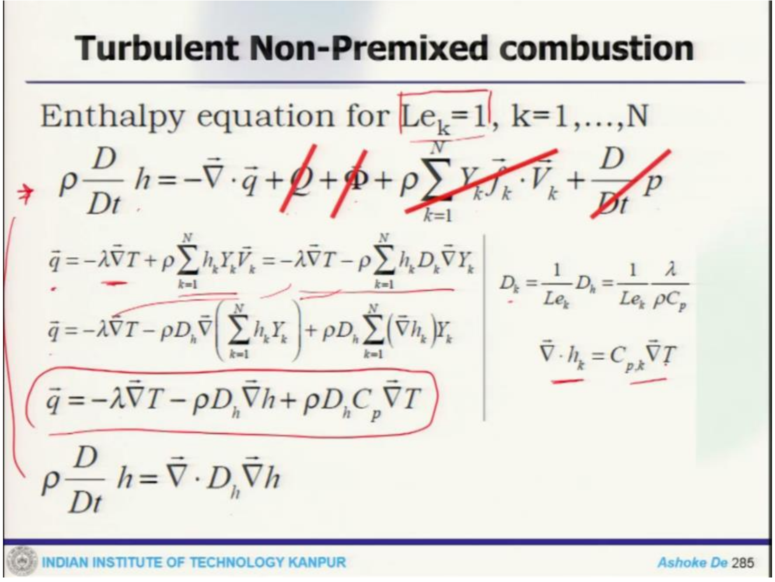

Turbulent Non-Premixed combustion

Enthalpy equation for $\boxed{Le_k=1}$, k=1,…,N

$$\rho\frac{D}{Dt}h = -\vec{\nabla}\cdot\vec{q} + \cancel{Q} + \cancel{\Phi} + \cancel{\rho\sum_{k=1}^{N}Y_k\vec{f}_k\cdot\vec{V}_k} + \cancel{\frac{D}{Dt}p}$$

$$\vec{q} = -\lambda\vec{\nabla}T + \rho\sum_{k=1}^{N}h_kY_k\vec{V}_k = -\lambda\vec{\nabla}T - \rho\sum_{k=1}^{N}h_kD_k\vec{\nabla}Y_k$$

$$\vec{q} = -\lambda\vec{\nabla}T - \rho D_h\vec{\nabla}\left(\sum_{k=1}^{N}h_kY_k\right) + \rho D_h\sum_{k=1}^{N}\left(\vec{\nabla}h_k\right)Y_k$$

$$\boxed{\vec{q} = -\lambda\vec{\nabla}T - \rho D_h\vec{\nabla}h + \rho D_hC_p\vec{\nabla}T}$$

$$\rho\frac{D}{Dt}h = \vec{\nabla}\cdot D_h\vec{\nabla}h$$

$$D_k = \frac{1}{Le_k}D_h = \frac{1}{Le_k}\frac{\lambda}{\rho C_p}$$

$$\vec{\nabla}\cdot h_k = C_{p,k}\vec{\nabla}T$$

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Now for Lewis number 1 case where the thermal diffusivity and the mass diffusivity they are same. So, once you assume that Lewis number 1 and this is our enthalpy equation this is what if you recall that we discussed about the governing equation all these are Dh/Dt for this is the flux q and viscous distribution and then there is effect due to mass diffusion and the pressure term. So, we neglect this term, this term and this term.

So, this will remain now q will be a contribution due to conduction and this component which you can write in this equation, $\lambda\nabla T$ and $\rho h_k Y_k$. So, one can expand this side. So, this will remain as it is, this can be taken into 2 components. So, finally, we get the flux part as:

$$\bar{q} = -\lambda\overline{\nabla}T - \rho D_h\overline{\nabla}h + \rho D_h C_P\overline{\nabla}T$$

So, then our enthalpy equation becomes:

$$\rho\frac{Dh}{Dt} = \overline{\nabla}.D_h\overline{\nabla}h$$

And we have used D_k as:

$$D_k = \frac{1}{Le_k}D_k = \frac{1}{Le_k}\frac{\lambda}{\rho C_P}$$

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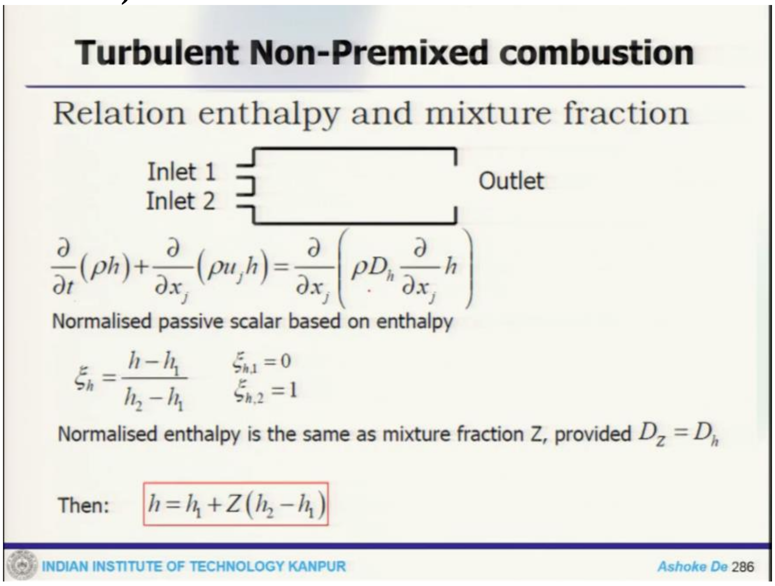

Turbulent Non-Premixed combustion

Relation enthalpy and mixture fraction

$$\frac{\partial}{\partial t}(\rho h)+\frac{\partial}{\partial x_j}(\rho u_j h)=\frac{\partial}{\partial x_j}\left(\rho D_h \frac{\partial}{\partial x_j} h\right)$$

Normalised passive scalar based on enthalpy

$$\xi_h=\frac{h-h_1}{h_2-h_1} \qquad \xi_{h,1}=0 \quad \xi_{h,2}=1$$

Normalised enthalpy is the same as mixture fraction Z, provided $D_Z = D_h$

Then: $\boxed{h=h_1+Z(h_2-h_1)}$

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So this is what we used for unity Lewis number system. Now you can find out the relation and the mixture fraction, so you have inlet 1 and you got inlet 2 and that outlet and this is our enthalpy equation, mixture enthalpy, steady convection and this is the diffusion term. This is what exactly we get mind it, this is for k equals to 1 for that situation and our normalized scalar on enthalpy would be:

$$\xi_k = \frac{h-h_1}{h_2-h_1}$$

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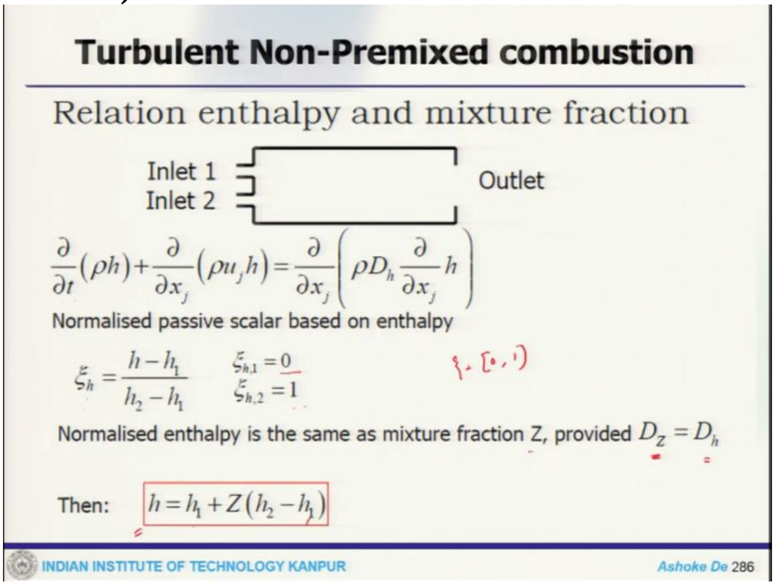

Turbulent Non-Premixed combustion

Relation enthalpy and mixture fraction

$$\frac{\partial}{\partial t}(\rho h)+\frac{\partial}{\partial x_j}(\rho u_j h)=\frac{\partial}{\partial x_j}\left(\rho D_h \frac{\partial}{\partial x_j} h\right)$$

Normalised passive scalar based on enthalpy

$$\xi_h=\frac{h-h_1}{h_2-h_1} \qquad \xi_{h,1}=0 \quad \xi_{h,2}=1$$

$\xi \in [0,1]$

Normalised enthalpy is the same as mixture fraction Z, provided $D_Z = D_h$

Then: $\boxed{h=h_1+Z(h_2-h_1)}$

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So $\xi_{h,1}$ would be 0 and $\xi_{h,1}$ this is how we normalize. So that the ξ actually goes between 0 to 1, like yours conserved scalar mean. Now this normal enthalpy is the same as the mixture fraction provided D_Z and D_h is same so we can write:

$$h = h_1 + Z(h_2 - h_1)$$

If it is purely at the inlet 1, then it will cancel out h_1 otherwise h_2 and in between it will varies like that, so, that is what you get in your these things and you can correlate the enthalpy on the mixture fraction.

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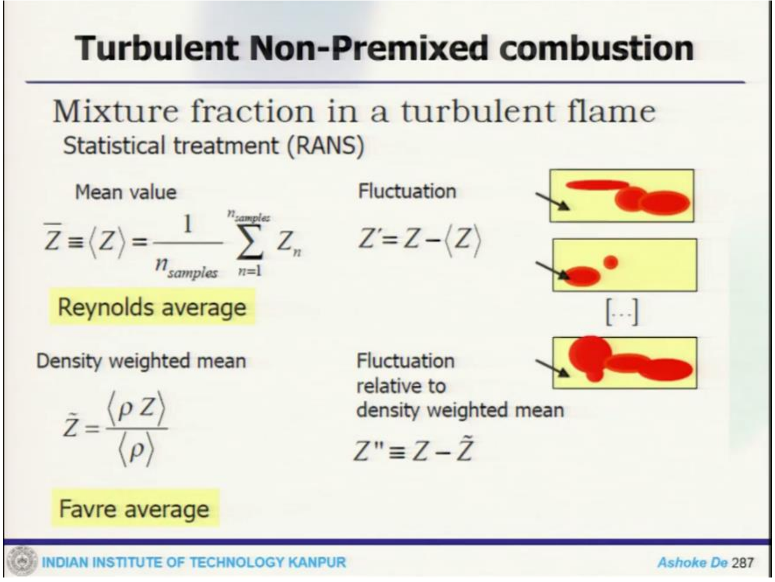

Turbulent Non-Premixed combustion

Mixture fraction in a turbulent flame

Statistical treatment (RANS)

Mean value

$$\bar{Z} \equiv \langle Z \rangle = \frac{1}{n_{samples}} \sum_{n=1}^{n_{samples}} Z_n$$

Reynolds average

Fluctuation

$$Z' = Z - \langle Z \rangle$$

[...]

Density weighted mean

$$\tilde{Z} = \frac{\langle \rho Z \rangle}{\langle \rho \rangle}$$

Favre average

Fluctuation relative to density weighted mean

$$Z'' \equiv Z - \tilde{Z}$$

Now we go to the turbulent situation where we can look at the mean value variance and all these things and we will continue the discussion from there in the next lecture. We will stop here today.