Turbulent Combustion : Theory and Modelling
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Lecture - 51
Turbulence-Chemistry Interaction (Contd...)

Welcome back. So, let us continue the discussion on turbulent premixed flame. And we have look at the fundamentals like turbulent speed, displacement speed and all these. Now we are discussing the BML model and we have seen turbulent scalar flux closure and now we are looking at the source term.

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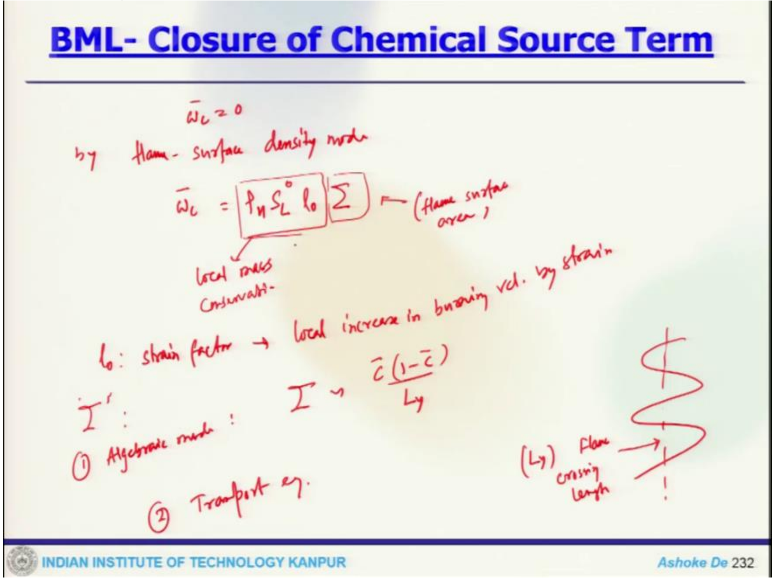

BML- Closure of Chemical Source Term

$\bar{\omega}_c = 0$

by flame- surface density model

$\bar{\omega}_c = \boxed{\rho_u S_L^0 I_0}\boxed{\Sigma}$ ← (flame surface area)

local mass conservation

I_0: strain factor → local increase in burning vel. by strain

Σ:

① Algebraic model : $\Sigma \sim \frac{\bar{c}(1-\bar{c})}{L_y}$

② Transport eq.

(L_y) Flame crossing length

So, this is how the source term one can close it. So, I mean the source term can be represented like in local mass conservation and the in terms of flame surface density. And once you write in terms of flame surface density, either one can use algebraic model like this, which is quite simple or transport equation like this. Where the transport equation of the flame surface density contents look convective term, local change, turbulent transport.

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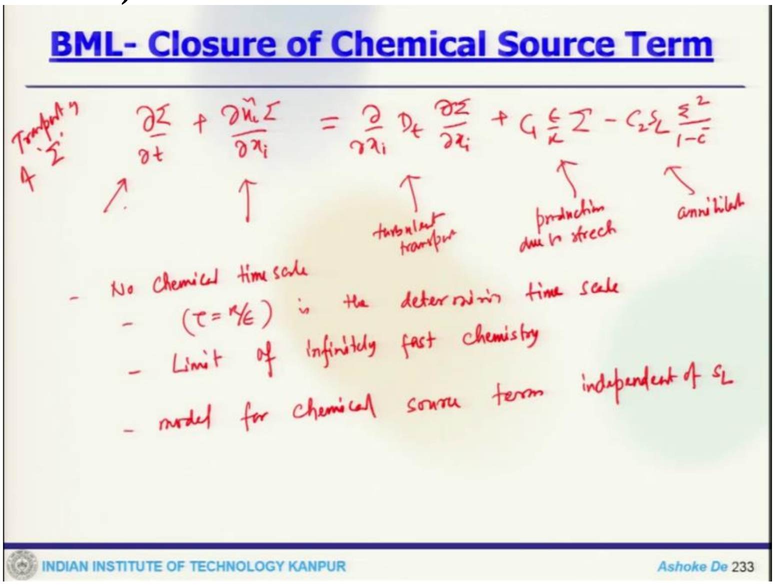

BML- Closure of Chemical Source Term

Transport eq of Σ

$$\frac{\partial \Sigma}{\partial t} + \frac{\partial \tilde{u}_i \Sigma}{\partial x_i} = \frac{\partial}{\partial x_i} D_t \frac{\partial \Sigma}{\partial x_i} + C_1 \frac{\epsilon}{\kappa} \Sigma - C_2 S_L \frac{\Sigma^2}{1-\bar{c}}$$

turbulent transport

production due to strech

annihilat

- No Chemical time scale
- ($\tau = \kappa/\epsilon$) is the determining time scale
- Limit of infinitely fast chemistry
- model for chemical source term independent of S_L

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Then, production due to stretch or flames stretch or annihilation. So, now, there is one thing there is no chemical time scale involved. So, the turbulent time which is τ, κ/ϵ is the determining time scale. So, as we can see κ/ϵ comes into the production of that, so there is a limit of infinitely fast chemistry. Now, using the transport equation, we can model for chemical source term which is independent of S_L. So that is what we can find it out.

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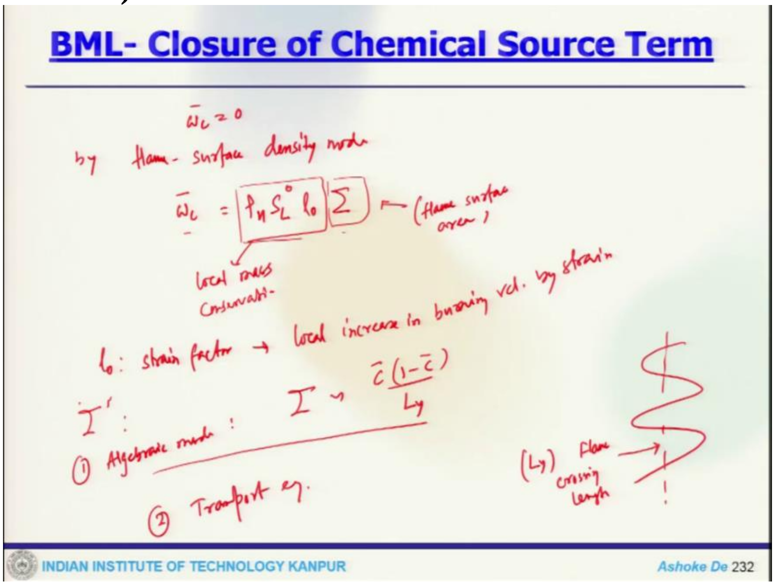

BML- Closure of Chemical Source Term

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(L_y) flame crossing length

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So that means when you use these source term closure, either use the simple algebraic expression or you can use the transport equation to close it. So, that is how we talk about the BML model.

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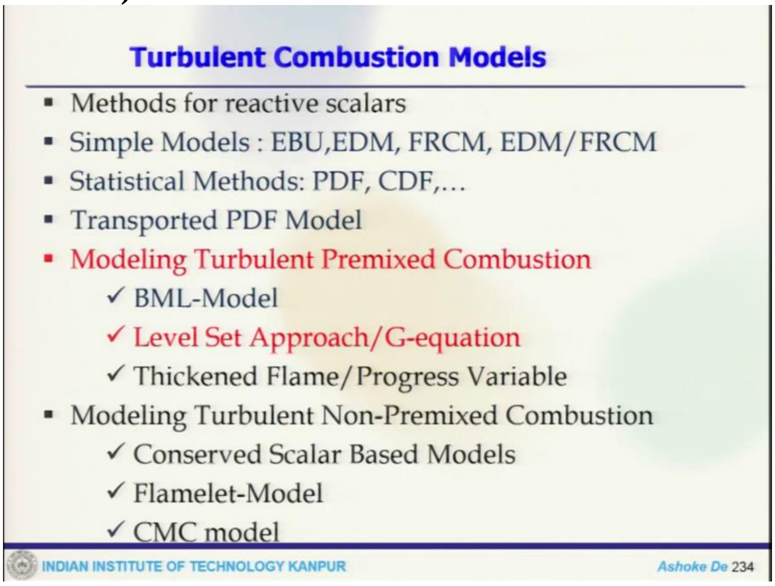

Turbulent Combustion Models

- 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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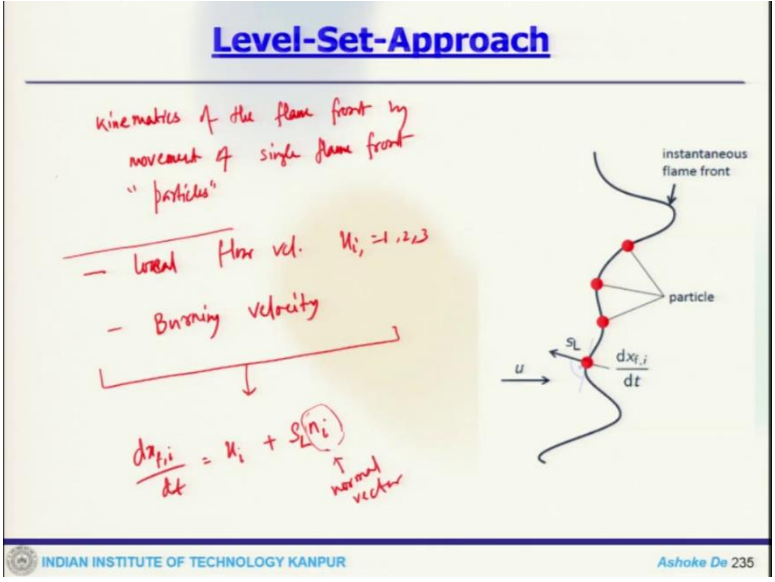

Level-Set-Approach

kinematics of the flame front by movement of single flame front "particles"

- local flow vel. $u_i, =1,2,3$
- Burning velocity

$$\frac{dx_{f,i}}{dt} = u_i + S_L n_i$$

normal vector

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Now, we move to the level set approach or D equation approach. Now here you have an instantaneous flame front. This is our instantaneous flame front and there are so many points, where you can show the kinematics of the flame front can be examined by examining the movement of single flame front particles. So, these movements which are influenced by local flow velocity which is u_i 1, 2, 3 and then burning velocity. So, this movement of these particles they are essentially.

So, in one side is your flame front, you can assume to have so many particles and using that you can basically the kinematics means essentially in this is called level set up approach that means, you try to capture these. I mean propagating flame front. So, by capturing the flame front, you want to model this particular way. So, once we say that the local velocity and all these this will lead to the kinematics equation of the flame front:

$$\frac{dx_{f,i}}{dt} = u_i + S_L n_i$$

Which is nothing but the normal vector.

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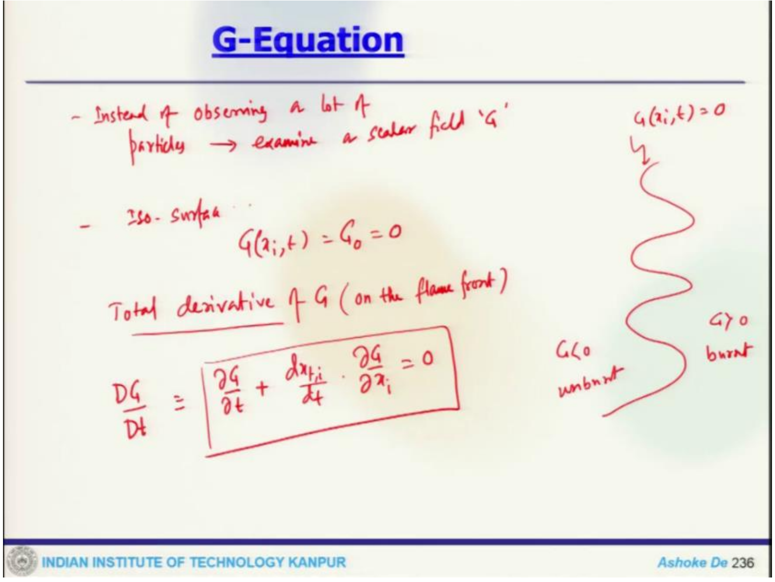

G-Equation

- Instead of observing a lot of particles → examine a scalar field 'G'
- Iso-surface

$G(x_i,t) = G_0 = 0$

Total derivative of G (on the flame front)

$$\frac{DG}{Dt} = \boxed{\frac{\partial G}{\partial t} + \frac{dx_{f,i}}{dt} \cdot \frac{\partial G}{\partial x_i} = 0}$$

So, then we can have the same flame front where G < 0 and G > 0. So, this could be our burnt side, this could be unburnt side, and this is G(x_i,t) is 0. So, another way one can look at, instead of observing a lot of particles, one can examine a scalar field like G. So, the iso surface is defined like, G(x_i,t) is G_0 is 0. So that is the definition of the iso surface. Now, we can find out the total derivative of G. This is on the flame front.

So which we can write:

$$\frac{DG}{Dt} = \frac{dG}{dt} + \frac{dx_{f,i}}{dt} . \frac{\partial G}{\partial x_i} = 0$$

Which is 0. So, this is what you get the total derivative of the G on the flame front. So, now once we look at the kinematic equation. So, that will now this is our instantaneous flame front, which is G(x_i,t) equal to 0.

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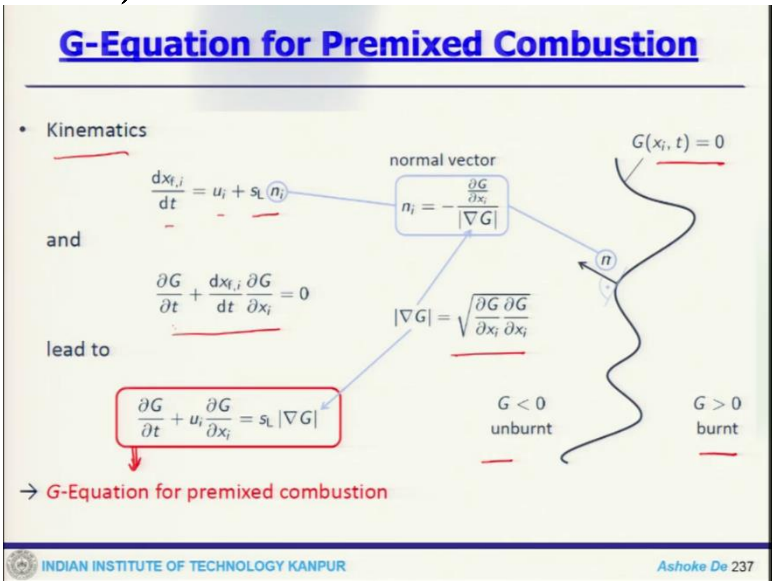

G-Equation for Premixed Combustion

- Kinematics

$$\frac{dx_{f,i}}{dt} = u_i + s_L n_i$$

and

$$\frac{\partial G}{\partial t} + \frac{dx_{f,i}}{dt}\frac{\partial G}{\partial x_i} = 0$$

lead to

$$\boxed{\frac{\partial G}{\partial t} + u_i \frac{\partial G}{\partial x_i} = s_L |\nabla G|}$$

→ G-Equation for premixed combustion

normal vector

$$n_i = -\frac{\frac{\partial G}{\partial x_i}}{|\nabla G|}$$

$$|\nabla G| = \sqrt{\frac{\partial G}{\partial x_i}\frac{\partial G}{\partial x_i}}$$

This is our burnt side, this is unburnt side and this is the normal. So, the normal vector can be calculated as $\frac{\frac{\partial G}{\partial x_i}}{|\nabla G|}$ and now the kinematics of the individual particle can be retained at $u_i + S_L n_i$ and this would be 0. So, using these 2 it leads to:

$$\frac{\partial G}{\partial t} + u_i \frac{\partial G}{\partial x_i} = S_L |\nabla G|$$

Where $|\nabla G|$ is:

$$|\nabla G| = \sqrt{\frac{\partial G}{\partial x_i}\frac{\partial G}{\partial x_i}}$$

So, this is a well-known G equation for premixed combustion where you track the flame front of this turbulent propagating flame.

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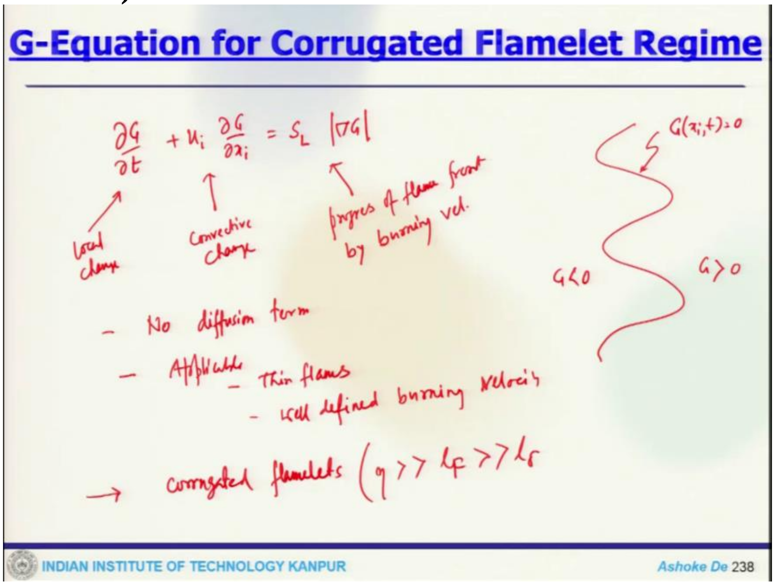

G-Equation for Corrugated Flamelet Regime

$$\frac{\partial G}{\partial t} + u_i \frac{\partial G}{\partial x_i} = S_L |\nabla G|$$

local change

Convective change

progress of flame front by burning vel.

- No diffusion term
- Applicable
  - Thin flames
  - well defined burning velocity

→ corrugated flamelets $(\eta \gg l_F \gg l_\delta$

So, now, for this flame front like, where this is G < 0, G > 0 and this is G(x_i,t) which is 0. You say:

$$\frac{\partial G}{\partial t} + u_i \frac{\partial G}{\partial x_i} = S_L |\nabla G|$$

So, this is our local change, this is the convective change and this is the progress of flame front by burning velocity. So, there is no diffusion term involved there and this particular equation is applicable for thin flames and well defined burning velocity and also it can be applied to corrugated flamelets where your flamelets is delta and which is eta is that. So, this particular zone also you can use it.

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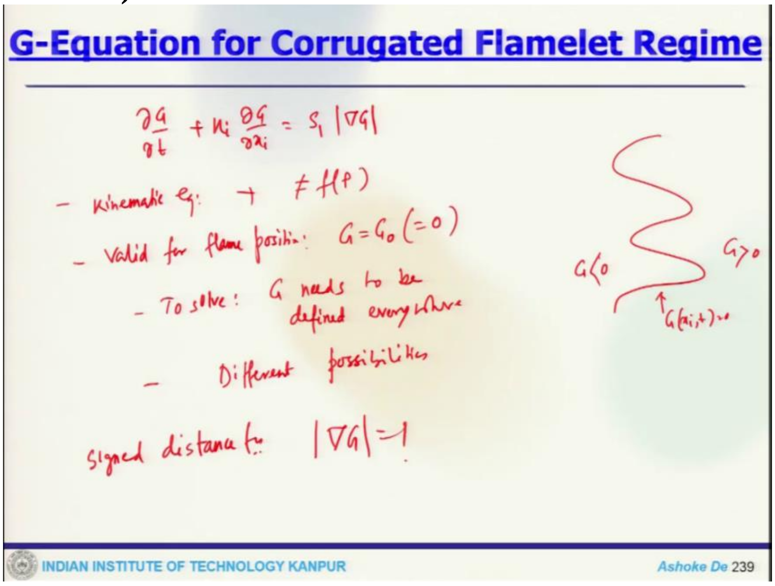

G-Equation for Corrugated Flamelet Regime

$$\frac{\partial G}{\partial t} + u_i \frac{\partial G}{\partial x_i} = S_L |\nabla G|$$

- Kinematic eq. → $\neq f(\rho)$
- Valid for flame position: $G = G_0 (= 0)$
  - To solve: G needs to be defined everywhere
  - Different possibilities

Signed distance fn: $|\nabla G| = 1$

Now, if you look at that flame front, this is my equation from the previous slide. So kinematics, now kinematic equation is no more a function of density. So, this is valid for flame position, where:

$$G = G_0 = 0$$

Now, to solve this G needs to be defined everywhere in the flow field. So, there are different possibilities which are available to define G, For example, one is the very common that is used signed distance function which used ∇G equals to 1.

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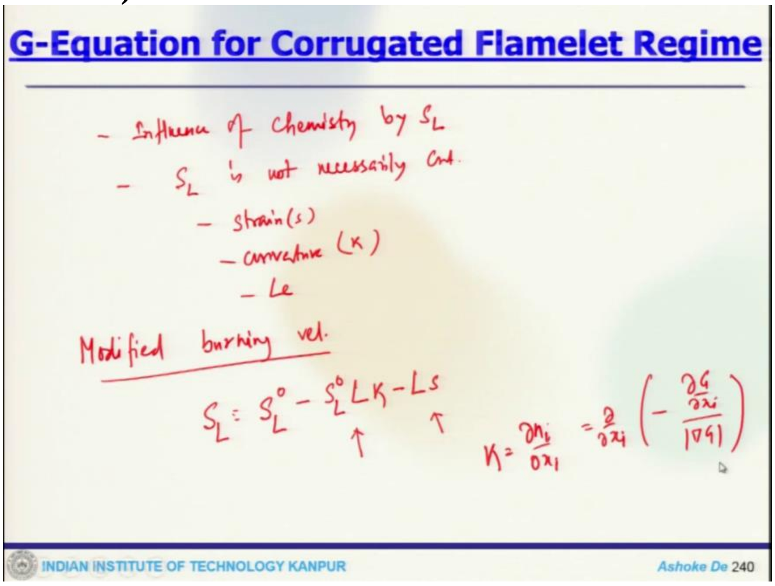

G-Equation for Corrugated Flamelet Regime

- Influence of Chemistry by S_L
- S_L is not necessarily Cnt.
  - strain(s)
  - curvature (κ)
  - Le

Modified burning vel.

$$S_L = S_L^0 - S_L^0 L\kappa - Ls$$

$$\kappa = \frac{\partial n_i}{\partial x_i} = \frac{\partial}{\partial x_i}\left(-\frac{\frac{\partial G}{\partial x_i}}{|\nabla G|}\right)$$

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Now, we see the other thing like what is the influence of the chemistry by S_L. Now, S_L is not necessarily constant, but it is influenced by strain, curvature, which is κ and Lewis number. So, then one can write down these modified burning velocity using this impact. So, modified burning velocity is written as:

$$S_L = S_L^0 - S_L^0 L\kappa - LS$$

Where, this is the influence of curvature, this is influence of strain. So now, the κ is defined as:

$$\kappa = \frac{\partial n_i}{\partial x_i} = \frac{\partial}{\partial x_i}\left(-\frac{\frac{\partial G}{\partial x_i}}{|\nabla G|}\right)$$

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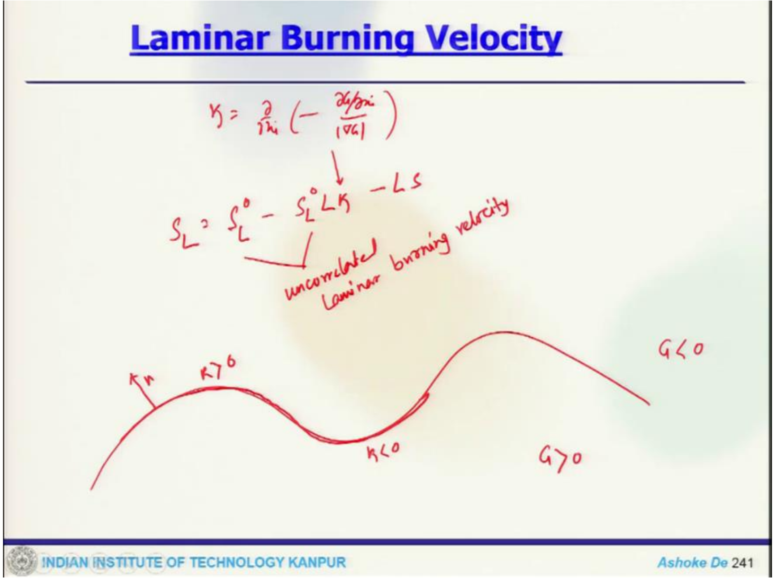

Laminar Burning Velocity

$$\kappa = \frac{\partial}{\partial x_i}\left(-\frac{\partial G/\partial x_i}{|\nabla G|}\right)$$

$$S_L = \underbrace{S_L^0}_{\text{uncorrelated Laminar burning velocity}} - S_L^0 L\kappa - Ls$$

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So if you look at this, which is G > 0 and G < 0, this is a position where one needs to this position κ is 0, this is curvature where κ is high because κ is defined as:

$$\kappa = \frac{\partial}{\partial x_i}\left(-\frac{\frac{\partial G}{\partial x_i}}{|\nabla G|}\right)$$

So for S$_L$, there are 2 terms, $S_L^0 - S_L^0 L\kappa - LS$. This is how the kappa is modelled and these 2 terms one can think about these are uncorrelated laminar burning velocity. So, one can think in that way.

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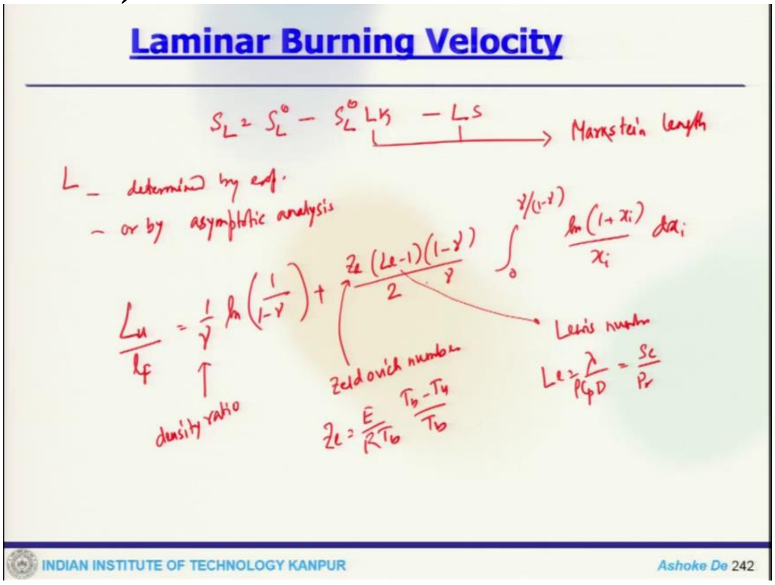

Laminar Burning Velocity

$$S_L = S_L^0 - \underbrace{S_L^0 L\kappa - LS}\rightarrow \text{Marnstein length}$$

L – determined by exp.

– or by asymptotic analysis

$$\frac{L_u}{l_F} = \frac{1}{\gamma}\ln\left(\frac{1}{1-\gamma}\right) + \frac{Ze(Le-1)(1-\gamma)}{2\gamma}\int_0^{\gamma/(1-\gamma)}\frac{\ln(1+x_i)}{x_i}dx_i$$

density ratio

Zeldovich number

$$Ze = \frac{E}{RT_b}\frac{T_b-T_u}{T_b}$$

Lewis number

$$Le = \frac{\lambda}{\rho C_p D} = \frac{Sc}{Pr}$$

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Now, the other terms which you have an S$_L$ equals to:

$$S_L = S_L^0 - S_L^0 L\kappa - LS$$

This L which is known as Markstein length. So that, L can be the determined by experiment or by asymptotic analysis. So the correlation which one can use is that:

$$\frac{L_u}{l_F} = \frac{1}{\gamma}ln\left(\frac{1}{1-\gamma}\right) + \frac{Ze(Le-1)(1-\gamma)}{2\gamma}\int_0^{\gamma/_{1-\gamma}}\frac{\ln(1+x_i)}{x_i}dx_i$$

So, this guy is nothing but density ratio and this is Zeldovich number which is:

$$Ze = \frac{E}{RT_b}\frac{T_b - T_u}{T_b}$$

It is Lewis number which is:

$$Le = \frac{\lambda}{\rho C_p D} = \frac{Sc}{Pr}$$

So, these are the different terms which contain air. So, now using this, so we got:

$$S_L = S_L^0 - S_L^0 L\kappa - LS$$

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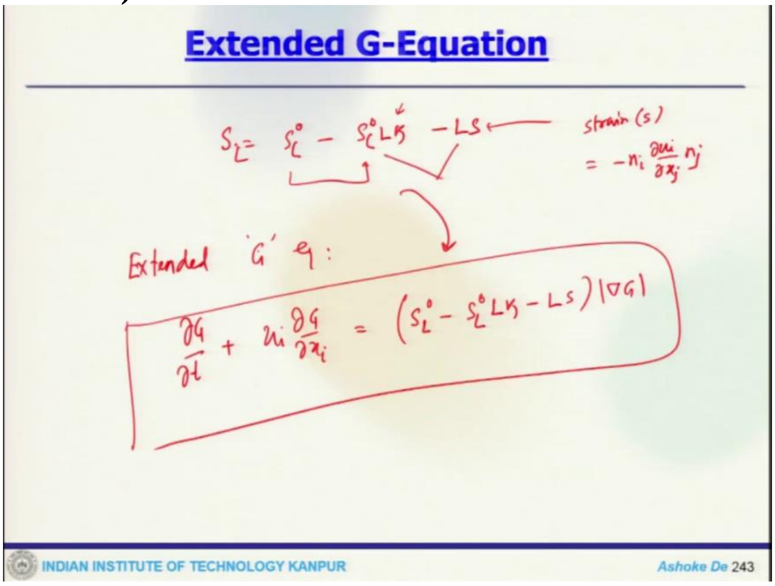

Extended G-Equation

$S_L = S_L^0 - S_L^0 L\kappa - LS \leftarrow$ strain (s) $= -n_i \frac{\partial u_i}{\partial x_j} n_j$

Extended 'G' eq:

$$\boxed{\frac{\partial G}{\partial t} + u_i \frac{\partial G}{\partial x_i} = (S_L^0 - S_L^0 L\kappa - LS)|\nabla G|}$$

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So these 2 terms are uncorrelated, these are maximum length, this is curvature and S, which is strain, which is defined as:

$$S = -n_i \frac{\partial u_i}{\partial x_j} n_j$$

Now using this expression the extended G equation one can write, which will look like:

$$\frac{\partial G}{\partial t} + x_i \frac{\partial G}{\partial x_i} = (S_L^0 - S_L^0 L\kappa - LS)|\nabla G|$$

So, this is what your extended looks like because we use an expression of modified burning velocity. So, this is slowly if you see, we start with that simple expression for S_L, then we incorporate the effect of curvature and strain and all these and then slowly so, that goes to the more like and realistic situation, where due to turbulence, you will have all these effect. Now look at corrugated flamelet in thin reaction zone. Now, so the previous examination which was limited to corrugated flamelets.

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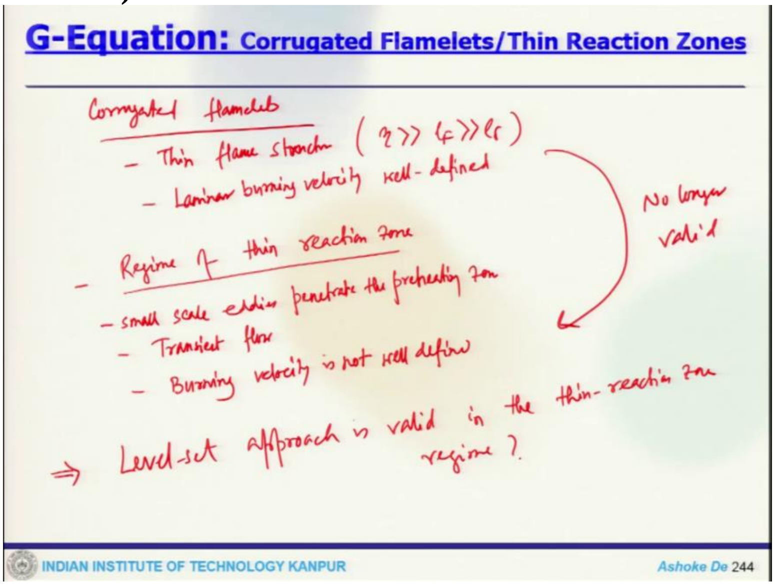

G-Equation: Corrugated Flamelets/Thin Reaction Zones

Corrugated flamelets

- Thin flame structure $(\eta \gg l_F \gg l_\delta)$
  - Laminar burning velocity well-defined

No longer valid

- Regime of thin reaction zone
  - small scale eddies penetrate the preheating zone
  - Transient flow
  - Burning velocity is not well defined

$\Rightarrow$ Level-set approach is valid in the thin-reaction zone regime ?

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So, that means in the corrugated flamelets you have thin flame structure which is $\eta \gg l_F \gg l_\delta$ and laminar burning velocity well defined. So, what we get the regime of thin reaction zone, which is like where your small scale eddies penetrate the preheating zone. You will have transient flow and burning velocity is not well defined. So, that means these things are no longer valid.

So, the problem that one encounter does that means this level set approach is valid in the thin reaction zone regime. So, that is a bigger question to answer. So what happens we can see if we go to thin reaction zone regime. So this is is ignition point, reaction zone, heat zone, that is typical.

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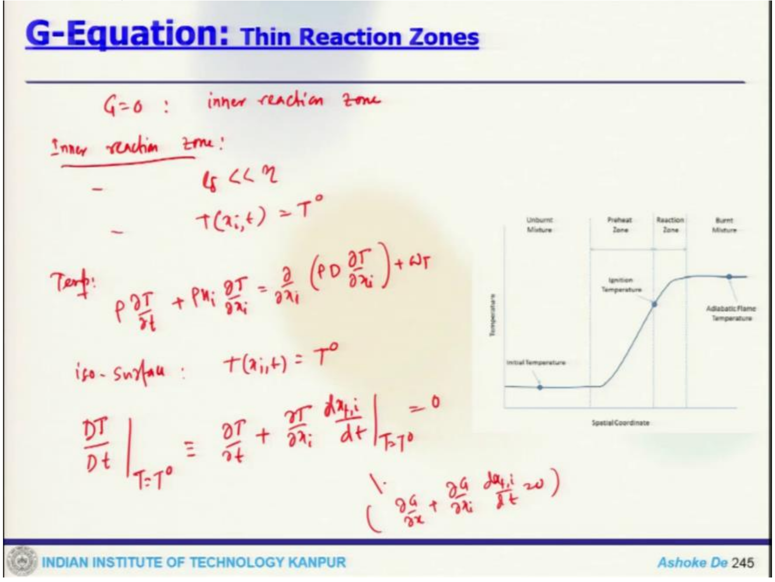

G-Equation: Thin Reaction Zones

$G=0$: inner reaction zone

Inner reaction zone:

- $l_\delta << \eta$
- $T(x_i;t) = T^0$

Temp:

$$\rho \frac{\partial T}{\partial t} + \rho u_i \frac{\partial T}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\rho D \frac{\partial T}{\partial x_i}\right) + \omega_T$$

iso-surface : $T(x_i,t) = T^0$

$$\left.\frac{DT}{Dt}\right|_{T=T^0} \equiv \left.\frac{\partial T}{\partial t} + \frac{\partial T}{\partial x_i}\frac{dx_{f,i}}{dt}\right|_{T=T^0} = 0$$

$$\because \left(\frac{\partial G}{\partial x} + \frac{\partial G}{\partial x_i}\frac{dx_{f,i}}{dt} = 0 \right)$$

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So, here the G_0 is the surface which is represented by inner reaction zone. We do that in the inner reaction zone, what we have, which is thin compared to small scale eddies that means my l_δ will be smaller than η so that we can describe our temperature as T^0. So our temperature equation will take the shape of:

$$\rho\frac{\partial T}{\partial t} + \rho u_i\frac{\partial T}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\rho D\frac{\partial T}{\partial x_i}\right) + w_T$$

Now one can look at the iso surface of temperature which is:

$$T(x_i, t) = T^0$$

Then we can write:

$$\left|\frac{DT}{Dt}\right|_{T=T^0} = \frac{\partial T}{\partial t} + \frac{\partial T}{\partial x_i}\left|\frac{dx_i}{dt}\right|_{T=T^0} = 0$$

So, which essentially is sort of an, what can think about:

$$\frac{\partial G}{\partial x} + \frac{\partial G}{\partial x_i}\frac{dx_i}{dt} = 0$$

It is a similar kind of expression one can look at it like what we obtained earlier.

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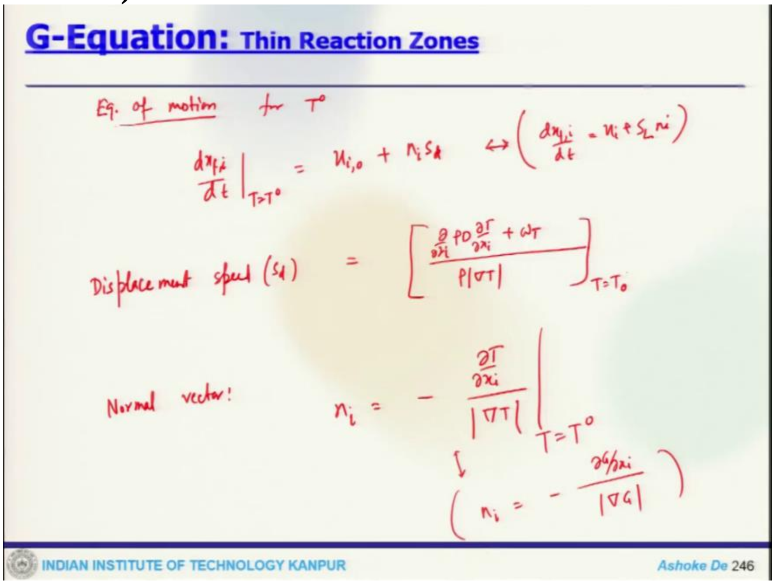

G-Equation: Thin Reaction Zones

Eq. of motion for T^0

$$\left.\frac{dx_{f,i}}{dt}\right|_{T=T^0} = u_{i,0} + n_i s_d \leftrightarrow \left(\frac{dx_{f,i}}{dt} = u_i + S_L n_i\right)$$

Displacement speed (s_d) $= \left[\frac{\frac{\partial}{\partial x_i}\rho D\frac{\partial T}{\partial x_i} + \omega_T}{\rho|\nabla T|}\right]_{T=T_0}$

Normal vector: $n_i = -\left.\frac{\frac{\partial T}{\partial x_i}}{|\nabla T|}\right|_{T=T^0}$

$$\downarrow$$

$$\left(n_i = -\frac{\partial G/\partial x_i}{|\nabla G|}\right)$$

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Now we write the equation of motion. So the equation of motion for T^0:

$$\left|\frac{dx_i}{dt}\right|_{T=T^0} = u_{i,0} + n_i s_d$$

Which was in similar expression, which is written for level set approach equals to $u_i + s_L n_i$. Here, we bring in the displacement speed. Now, this displacement speed which is defined as:

$$S_d = \left[\frac{\frac{\partial}{\partial x_i}\rho D \frac{\partial T}{\partial x_i} + w_T}{\rho|\nabla T|}\right]_{T=T_0}$$

Now similarly you can find out the normal vector. So, that is defined as:

$$n_i = \left|-\frac{\frac{\partial T}{\partial x_i}}{|\nabla T|}\right|_{T=T_0}$$

So, which is a similarity one can see that n_i equals to $-\frac{\frac{\partial G}{\partial x_i}}{|\nabla G|}$. This is how we define it for that thing.

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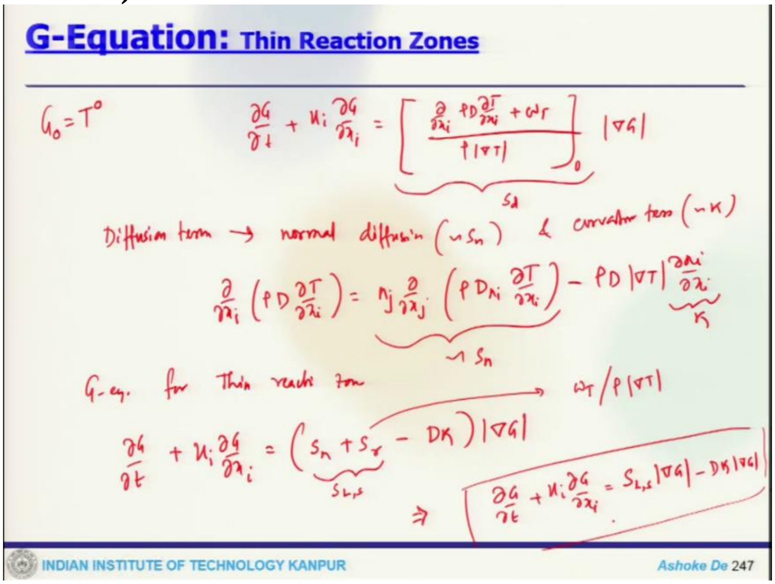

G-Equation: Thin Reaction Zones

$G_0 = T^0$

$$\frac{\partial G}{\partial t} + u_i \frac{\partial G}{\partial x_i} = \underbrace{\left[\frac{\frac{\partial}{\partial x_i}\rho D\frac{\partial T}{\partial x_i} + \omega_T}{\rho|\nabla T|}\right]_0}_{S_d} |\nabla G|$$

Diffusion term → normal diffusion $(\sim S_n)$ & curvature term $(\sim \kappa)$

$$\frac{\partial}{\partial x_i}\left(\rho D \frac{\partial T}{\partial x_i}\right) = \underbrace{n_j \frac{\partial}{\partial x_j}\left(\rho D_{x_i} \frac{\partial T}{\partial x_i}\right)}_{\sim S_n} - \rho D|\nabla T|\underbrace{\frac{\partial n_i}{\partial x_i}}_{\kappa}$$

G-eq. for Thin reaction zone

$\omega_T/\rho|\nabla T|$

$$\frac{\partial G}{\partial t} + u_i \frac{\partial G}{\partial x_i} = (\underbrace{S_n + S_r}_{S_{L,s}} - D\kappa)|\nabla G|$$

$$\Rightarrow \boxed{\frac{\partial G}{\partial t} + u_i \frac{\partial G}{\partial x_i} = S_{L,s}|\nabla G| - D\kappa|\nabla G|}$$

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So, now we can use this $G_0 = T^0$, we write that:

$$\frac{\partial G}{\partial t} + u_i \frac{\partial G}{\partial x_i} = \left[\frac{\frac{\partial}{\partial x_i}\rho D \frac{\partial T}{\partial x_i} + w_T}{\rho|\nabla T|}\right]_0 |\nabla G|$$

And this guy is nothing but our displacement speed. Now, the diffusion term, which is a normal diffusion and curvature term, will be invoked. So, we will have diffusion term which is normal diffusion that is S$_n$ and curvature term which is order of κ. So, there we get:

$$\frac{\partial}{\partial x_i}\left(\rho D \frac{\partial T}{\partial x_i}\right) = n_j \frac{\partial}{\partial x_j}\left(\rho D_{x_i} \frac{\partial T}{\partial x_i}\right) - \rho D|\nabla T|\frac{\partial n_i}{\partial x_i}$$

So, this is nothing but my κ and this is the term which is nothing but my normal diffusion. Now, if I put everything together and write down the equation for this, so, the G equation for this thin reaction zone, we get:

$$\frac{\partial G}{\partial t} + u_i \frac{\partial G}{\partial x_i} = (S_n + S_r - D_\kappa)|\nabla G|$$

This collectively you can think about is a less than this. One can write:

$$\frac{\partial G}{\partial t} + u_i \frac{\partial G}{\partial x_i} = S_{L,s}|\nabla G| - D_\kappa|\nabla G|$$

So, that is the equation you get here S_r is ${}^{w_T}/_{\rho|\nabla T|}$. So, this is what you get for the G equation in the thin reaction zone. Now, we will stop here today. And we will see how we can come up with a 1 G equation, which can be applied to both the regime. We will continue the discussion in the next lecture.