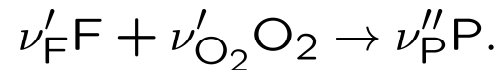# Lecture 5

The Thermal Flame Theory

In 1938 Zeldovich and Frank-Kamenetzki develops the classical example of an asymptotic description of the structure of a premixed flame

Presequisite: single one-step reaction

$$\nu'_F F + \nu'_{O_2} O_2 \rightarrow \nu''_P P.$$

We will assume that reaction rate is first order with respect to fuel and to oxygen

$$\omega = B \frac{\rho Y_F}{W_F} \frac{\rho Y_{O_2}}{W_{O_2}} \exp\left(\frac{-E}{\mathcal{R}T}\right)$$

Alternative forms, in particular a rate which is first order with respect to the fuel only, may also be considered.

We will show that this case will be contained as a limit for lean flames in the expression above.

The most important feature in
$$\omega = B \frac{\rho Y_F}{W_F} \frac{\rho Y_{O_2}}{W_{O_2}} \exp\left(\frac{-E}{\mathcal{R}T}\right)$$

is the Arrhenius type temperature dependence.

The activation energy E is assumed to be large.
Both the activation energy and the frequency factor B are adjustable parameters and cannot be deduced from elementary kinetic data.

The one-step model has widely been used in descriptions of flame stability, where it essentially serves as model that produces a thin flame with a strong temperature sensitivity.

In this lecture we will derive an explicit expression for the burning velocity.

This is to be compared in Lecture 7 to results derived from a four-step reduced mechanism for methane-air flames.
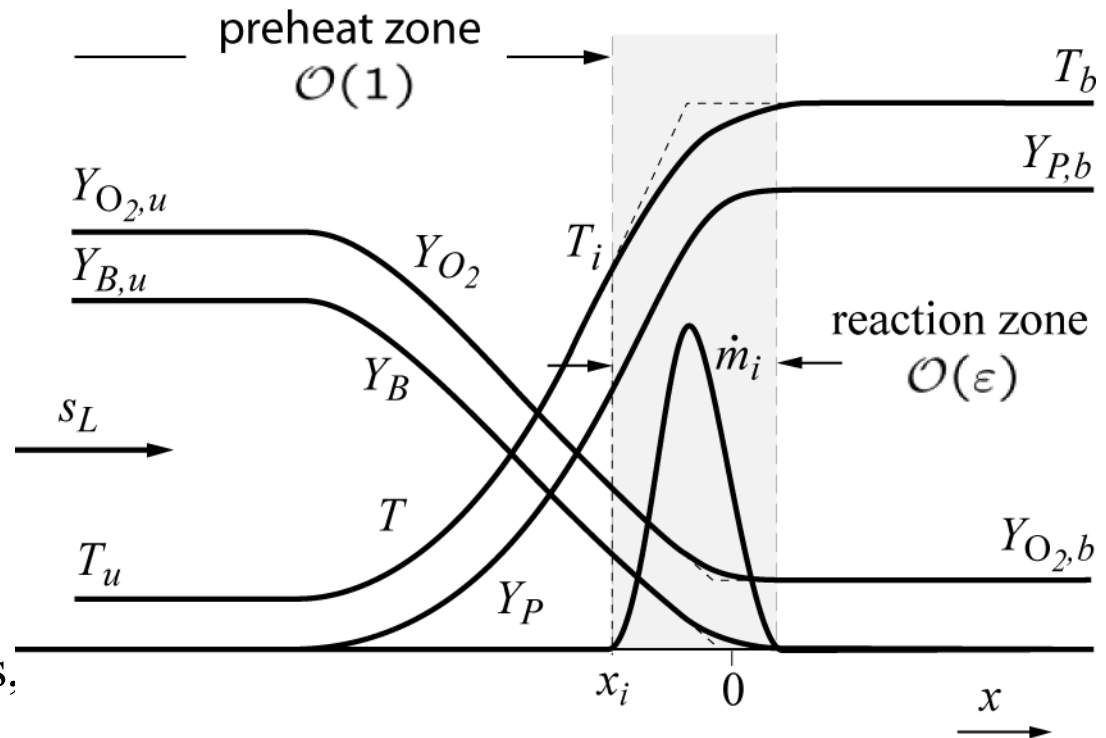
Flame structure schematically

Since the reaction is assumed to be irreversible, the reaction rate must vanish in the burnt gas.

Therefore one of the reactants must be entirely depleted: the fuel in the case of lean flames, the oxidizer for rich flames and both for stoichiometric flames.

This leads to the condition in the burnt gas:

$$Y_{F,b} \cdot Y_{O_2,b} = 0.$$

The combustion of the reactants in the reaction zone leads to an increase in temperature and therefore an increase of the reaction rate.

In the asymptotic analysis to be developed, the large temperature dependence of the reaction rate, expressed by the large activation energy will play a crucial role.

Let us assume at first that the diffusion flux can be written as

$$\boldsymbol{j}_i = -\rho D_i \, \mathbf{grad} Y_i, \quad D_i = D_{i,\mathsf{N}_2},$$

where Lewis number is unity.

The species balance equation

$$\rho \frac{DY_i}{Dt} = \frac{1}{\text{Le}_i} \mathbf{div}\left(\frac{\lambda}{c_p}\mathbf{grad}Y_i\right) + W_i \sum_{l=1}^{r} \nu_{il}\omega_l.$$

now is considered for the mass fractions of fuel and oxygen

Fuel

$$\rho_u s_L \frac{dY_F}{dx} = \frac{d}{dx}\left(\frac{\lambda}{c_p}\frac{dY_F}{dx}\right) - \nu'_F W_F \omega$$

Oxygen

$$\rho_u s_L \frac{dY_{O_2}}{dx} = \frac{d}{dx}\left(\frac{\lambda}{c_p}\frac{dY_{O_2}}{dx}\right) - \nu'_{O_2} W_{O_2} \omega.$$

The temperature equation

$$\rho\frac{\mathrm{D}T}{\mathrm{D}t} = \frac{1}{c_p}\frac{\mathrm{D}p}{\mathrm{D}t} + \mathbf{div}\left(\frac{\lambda}{c_p}\,\mathbf{grad}T\right) + \sum_{l=1}^{r}\frac{Q_l}{c_p}\omega_l + \frac{\dot{q}_R}{c_p}.$$

using $\rho\,u = \rho_u\,s_L$ yields

$$\rho_u s_L\frac{\mathrm{d}T}{\mathrm{d}x} = \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\lambda}{c_p}\frac{\mathrm{d}T}{\mathrm{d}x}\right) - \frac{Q}{c_p}\omega.$$

These can be combined with the species equations in the form

$$Y_\mathsf{F} = -\frac{\nu'_\mathsf{F}W_\mathsf{F}c_p}{Q}\left(T - T_b\right) + Y_{\mathsf{F},b}$$

$$Y_{\mathsf{O}_2} = -\frac{\nu'_{\mathsf{O}_2}W_{\mathsf{O}_2}c_p}{Q}\left(T - T_b\right) + Y_{\mathsf{O}_2,b}$$

Here Q and c_p have been assumed constant for simplicity.

In the small Mach number limit from the momentum equation one obtains the solution

$$p = \text{const.}$$

With the aid of the thermal equation of state the fuel and oxidizer mass fractions, the density , the thermal conductivity as well as the reaction rate can be expressed as a function of temperature.

Again one obtains the solution of the continuity equation. $\rho u = \rho_u s_L,$

The only differential equation remaining describes the temperature profiles in x-direction.

$$\rho_u s_L \frac{\mathrm{d}T}{\mathrm{d}x} = \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\lambda}{c_p}\frac{\mathrm{d}T}{\mathrm{d}x}\right) - \frac{Q}{c_p}\omega$$

Zeldovich and Frank-Kamenetzki introduce the following assumptions introducing the ignition temperature T_i:

1. in the preheat zone, $T \leq T_i$, no reactions take place, therefore $\omega=0$ is assumed.

2. in the reaction zone $T \geq T_i$, the convective term in the temperature equation can be neglected compared to the diffusion and the reaction term.

In the preheat zone, $T \leq T_i$, with $\omega = 0$ the temperature equation can be integrated Considering the boundary condition

$$\frac{\mathrm{d}T}{\mathrm{d}x}\Big|_{x \to -\infty} = 0 \quad \text{and} \quad T\Big|_{x \to -\infty} = T_u$$

we achieve for the first derivative

$$\frac{\mathrm{d}T}{\mathrm{d}x} = \frac{c_p \, \rho_u s_L}{\lambda}(T - T_u).$$

With the second assumption the temperature equation can be integrated for a first time, if the temperature T is introduced as an independent variable.

One substitutes the heat conduction term with

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\lambda}{c_p}\frac{\mathrm{d}T}{\mathrm{d}x}\right) = \frac{\mathrm{d}T}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}T}\left(\frac{\lambda}{c_p}\frac{\mathrm{d}T}{\mathrm{d}x}\right) = \frac{c_p}{\lambda}\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}T}\left(\frac{\lambda}{c_p}\frac{\mathrm{d}T}{\mathrm{d}x}\right)^2$$

After multiplication with λ/c_p it follows

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}T}\left(\frac{\lambda}{c_p}\frac{\mathrm{d}T}{\mathrm{d}x}\right)^2 = -\frac{(-\Delta H)\lambda}{c_p^2}\,\omega(T)$$

With the boundary conditions at x = ∞

$$\frac{\mathrm{d}T}{\mathrm{d}x}\Big|_{x\to+\infty} = 0 \quad \text{and} \quad T\Big|_{x\to+\infty} = T_b$$

this equation can be integrated for a first time

$$\frac{\mathrm{d}T}{\mathrm{d}x} = \sqrt{2\frac{(-\Delta H)}{\lambda^2}\int_T^{T_b}\lambda\,\omega(T)\,\mathrm{d}T}$$

Now at the position x_i for $T = T_i$ Zeldovich and Frank-Kamenetzki equalize the derivatives of the preheat zone,

$$\frac{\mathrm{d}T}{\mathrm{d}x} = \frac{c_p\,\rho_u s_L}{\lambda}(T - T_u).$$

and the reaction zone,

$$\frac{\mathrm{d}T}{\mathrm{d}x} = \sqrt{2\frac{(-\Delta H)}{\lambda^2}\int_T^{T_b}\lambda\,\omega(T)\,\mathrm{d}T}.$$

This yields an equation for the burning velocity

$$\frac{c_p\rho_u s_L}{\lambda_i}(T_i - T_u) = \sqrt{2\frac{(-\Delta H)}{\lambda_i^2}\int_{T_i}^{T_b}\lambda\,\omega(T)\,\mathrm{d}T}.$$

An analysis of the integral in closed form is only possible, if further simplifying assumptions are introduced.

Expanding the term in the exponent

$$\omega = B \frac{\rho Y_\mathsf{F}}{W_\mathsf{F}} \frac{\rho Y_{\mathsf{O}_2}}{W_{\mathsf{O}_2}} \exp\left(\frac{-E}{\mathcal{R}T}\right)$$

in a series around T_b and neglecting higher order terms, one obtains

$$-\frac{E}{\mathcal{R}T} = -\frac{E}{\mathcal{R}T_b} + \frac{E(T - T_b)}{\mathcal{R}T_b^2}.$$

Since in the reaction zone T and T_b are only slightly different, it is meaningful to introduce the dimensionless temperature

$$\ominus = \frac{E(T - T_b)}{\mathcal{R}T_b^2},$$

which stays of the order $\mathcal{O}(1)$ for large $\ominus = \dfrac{E}{\mathcal{R}T_b^2}.$

In the reaction zone for $T \approx T_b$ in first approximation the material properties are also constant

$$\rho = \rho_b, \ \lambda = \lambda_b$$

Considering

$$Y_{\mathsf{F},b} \cdot Y_{\mathsf{O}_2,b} = 0$$

and

$$\rho_u s_L \frac{\mathsf{d} Y_{\mathsf{F}}}{\mathsf{d} x} = \frac{\mathsf{d}}{\mathsf{d} x}\left(\frac{\lambda}{c_p}\frac{\mathsf{d} Y_{\mathsf{F}}}{\mathsf{d} x}\right) - \nu'_{\mathsf{F}} W_{\mathsf{F}}\, \omega$$

$$\rho_u s_L \frac{\mathsf{d} Y_{\mathsf{O}_2}}{\mathsf{d} x} = \frac{\mathsf{d}}{\mathsf{d} x}\left(\frac{\lambda}{c_p}\frac{\mathsf{d} Y_{\mathsf{O}_2}}{\mathsf{d} x}\right) - \nu'_{\mathsf{O}_2} W_{\mathsf{O}_2}\, \omega.$$

the reaction rate can be written as

$$\omega = B\rho_b^2 \frac{c_p \mathcal{R} T_b^2}{(-\Delta H)E}\exp\left(-\frac{E}{\mathcal{R} T_b}\right)\left[-\left(\frac{\nu'_{\mathsf{F}} Y_{\mathsf{O}_2,b}}{M_{\mathsf{O}_2}} + \frac{\nu'_{\mathsf{O}_2} Y_{\mathsf{F},b}}{M_{\mathsf{F}}}\right)\Theta + \frac{\nu'_{\mathsf{O}_2}\nu'_{\mathsf{F}} c_p \mathcal{R} T_b^2}{(-\Delta H)E}\Theta^2\right]\exp\Theta$$

Integration yields

$$\int\limits_{T_i}^{T_b} \lambda\,\omega\,\mathrm{d}T = \lambda_b \frac{\mathcal{R}T_b^2}{E} \int\limits_{\Theta_i}^{0} w(\Theta)\,d\Theta$$

$$= \frac{\lambda_b B \rho_b^2 c_p \mathcal{R}^2 T_b^4}{(-\Delta H)E} \exp\left(-\frac{E}{\mathcal{R}T_b}\right)\left[\left(\frac{\nu_F' Y_{O_2,b}}{M_{O_2}} + \frac{\nu_{O_2}' Y_{F,b}}{M_F}\right)(1 + (\Theta_i - 1)\exp\Theta_i)\right.$$

$$\left. + 2\frac{\nu_{O_2}' \nu_F' c_p \mathcal{R} T_b^2}{(-\Delta H)E}\left(1 - \left(1 - \Theta_i + \frac{\Theta_i^2}{2}\right)\exp\Theta_i\right)\right]$$

Now a consideration is introduced which is obvious only for an asymptotic expansion for large activation energy and the matching process to adjust the solutions from the preheat zone and the reaction zone.

In the integral Θ_i is substituted by Θ_u, which may be interpreted as the assumption that the solution of the reaction zone is valid far into the preheat zone.

That is equivalent with the physical conception that underneath the temperature T_i the integral

$$\int_{T_i}^{T_b} \lambda\,\omega\,\mathrm{d}T = \lambda_b \frac{\mathcal{R}T_b^2}{E} \int_{\Theta_i}^{0} w(\Theta)\,d\Theta$$

is negligible because of the strong dependence of the reaction rate on temperature for which reason it makes no difference whether integration is performed between T_i and T_b or T_u and T_b.

Since Θ_u takes large negative values for large activation energies, in all terms containing $\exp\Theta_u$, Θ_u will finally be replaced by $-\infty$, so that they disappear.

On the other hand on the left side of

$$\frac{c_p\,\rho_u s_L}{\lambda_i}(T_i - T_u) = \sqrt{2\frac{(-\Delta H)}{\lambda_i^2}\int\limits_{T_i}^{T_b}\lambda\,\omega(T)\,\mathrm{d}T}$$

T_i is replaced by T_b and λ_i by λb .

This implies the concept that the reaction zone is so thin, that the preheat zone is stretching till T_b and that T_i is hardly distinguishable from T_b.

The Equation above reads

$$\rho_u s_L = \sqrt{2\frac{B\rho_b^2\lambda_b\mathcal{R}^2 T_b^4}{c_p(T_b - T_u)^2 E^2}\exp\left(-\frac{E}{\mathcal{R}T_b}\right)S}$$

$$S \quad = \frac{\nu'_\mathsf{F} Y_{\mathsf{O}_2,b}}{M_{\mathsf{O}_2}} + \frac{\nu'_{\mathsf{O}_2} Y_{\mathsf{F},b}}{M_\mathsf{F}} + \frac{2\,\nu'_{\mathsf{O}_2}\nu'_\mathsf{F} c_p \mathcal{R} T_b^2}{(-\Delta H)E}.$$

The contribution of the individual terms in S depends strongly on the equivalence ratio $\phi = 1/\lambda$:

In very lean or very fat mixtures respectively $Y_{O_2,b}$ or $Y_{F,b}$ are large, while both vanish for stoichiometric mixtures.

Therefore in stoichiometric mixtures the last term is predominant. It holds

$$
S = \begin{cases}
\dfrac{\nu'_F Y_{O_2,b}}{M_{O_2}} & \text{für} \quad \phi \ll 1, \\[2em]
\dfrac{2\,\nu'_{O_2}\nu'_F c_p \mathcal{R} T_b^2}{(-\Delta H)E} & \text{für} \quad \phi = 1, \\[2em]
\dfrac{\nu'_{O_2} Y_{F,b}}{M_F} & \text{für} \quad \phi \gg 1.
\end{cases}
$$

Finally the assumptions introduced should be summarized:

1. In the preheat zone the reaction rate is neglected.

2. In the reaction zone the convective term is neglected

3. The reaction rate is approximated by an expansion around T_b, only the expo-nential term is expanded. Material properties are set constant and evaluated at T_b

4. The integration over the reaction zone leads to an expression that correspond to an integral between the limits $T = -\infty$ and $T = T_b$.

5. Using the solution from the preheat zone the ign. temperature T_i is equalized to T_b.

Originally the thermal flame theory of Zeldovich and Frank-Kamenetzki was not derived for reaction rates in the form of

$$\nu_F' F + \nu_{O_2}' O_2 \rightarrow \nu_P'' P.$$
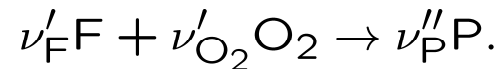
being of 1st order both for the fuel and the oxidizer.

Rather several solutions were derived for the reaction rate of 0th, 1st and 2nd order.

The comparison with the result resented here shows that a reaction of 1st order is conform with a very fat or very lean mixture, for which the component in-deficit governs the conversion rate.

In contrast the stoichiometric mixture relates to a reaction of 2nd order, since here both components are rate determining.

Flame Thickness and Flame Time

Previously we have identified the burning velocity s_L as an eigenvalue of the problem, which results from the solution of the one-dimensional balance equations.

Under the assumption of a one step reaction, in which only a chemical time scale has been introduced, and with the assumption of Le $= a /D =1$, with

$$\rho_u s_L = \sqrt{2\frac{B\rho_b^2\lambda_b\mathcal{R}^2T_b^4}{c_p(T_b - T_u)^2 E^2} \exp\left(-\frac{E}{\mathcal{R}T_b}\right) S}$$

$$S = \frac{\nu'_{\mathsf{F}}Y_{\mathsf{O_2},b}}{M_{\mathsf{O_2}}} + \frac{\nu'_{\mathsf{O_2}}Y_{\mathsf{F},b}}{M_{\mathsf{F}}} + \frac{2\,\nu'_{\mathsf{O_2}}\nu'_{\mathsf{F}}c_p\mathcal{R}T_b^2}{(-\Delta H)E}.$$

one obtains a relation for s_L. which combines the parameters diffusivity and chemical time as

$$s_L = \sqrt{D/t_c}$$

Here the thermal diffusivity D determined with $\rho = \rho_u$ and $\lambda = \lambda_b$ is defined as

$$D = \frac{\lambda_b}{\rho_u c_{\mathsf{p}}}$$

while the chemical time is given by

$$t_c = \frac{\rho_u E^2 (T_b - T_u)^2}{2B\rho_b^2 (\mathcal{R}T_b^2)^2 S} \exp\left(\frac{E}{\mathcal{R}T_b}\right)$$

Here the Zeldovich number, defined by

$$\mathsf{Ze} = \frac{E(T_b - T_u)}{\mathcal{R}T_b^2}$$

appears squared.

Since Ze is of the order of 10, the chemical time t_c is by two orders of magnitude larger than a chemical time, which, irrespective of the density ratio ρ_u/ρ_b, would be calculated from the reaction rate for example for very lean flames $\phi \gg 1$ as the reciprocal of

$$B\frac{\rho Y_{O_2}}{M_{O_2}}\exp(\frac{-E}{\mathcal{R}T}) \quad \text{bei} \quad T = T_b,\ \rho = \rho_b,\ Y_{O_2} = Y_{O_2,b}$$

Obviously t_c is no time, which is solely determined by chemistry.

t_c incorporates the structure of the flame also. This will become apparent, if from dimensional arguments one defines the flame thickness as

$$\ell_F = \frac{D}{s_L} = \frac{\lambda_b}{c_p \rho_u s_L}$$

Then one can further introduce the flame time

$$t_F = \frac{\ell_F}{s_L}$$

This is the time, which the flame front requires, to propagate the distance of the thickness of the flame.

The comparison between $s_L = \sqrt{D/t_c}$ and $\ell_F = \dfrac{D}{s_L} = \dfrac{\lambda_b}{c_\mathrm{p}\rho_u s_L}$ up to $t_F = \dfrac{\ell_F}{s_L}$

show, that t_c is equal to the flame time.

$$t_c = \frac{D}{s_L^2} = \frac{\ell_F}{s_L} = t_F$$

The flame thickness can be descriptively constructed from the temperature profile.

If one attaches a tangent to the turning point of the temperature profile and determines the intersection with the horizontal line at T_u and T_b, at the abscissa the flame length can be taken.

If one substitutes in

$$\frac{\mathrm{d}T}{\mathrm{d}x} = \frac{c_p\,\rho_u s_L}{\lambda}(T - T_u).$$

the left side by $(T_b - T_u)/\ell_F$ and evaluates the right side at $T=T_b$, one obtains in accordance with

$$\ell_F = \frac{D}{s_L} = \frac{\lambda_b}{c_p \rho_u s_L}$$

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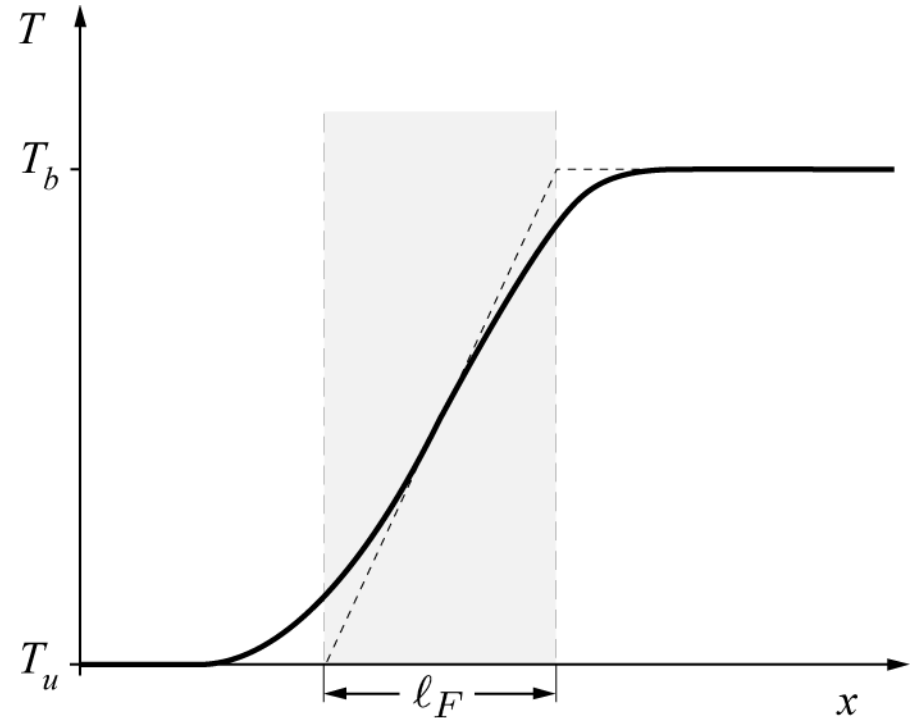
Below we will introduce a normalized coordinate

$$x^* = \rho_u s_L \int\limits_0^x \frac{c_p}{\lambda} \mathsf{d}x$$

which eliminates all properties from the temperature equation, as will be shown with

$$\frac{\mathsf{d}T}{\mathsf{d}x} = \frac{\mathsf{d}^2 T}{\mathsf{d}x^2} + \omega$$

This suggests

$$\rho_u s_L \int\limits_0^{\ell_F} \frac{\lambda}{c_p} \mathsf{d}x = 1.$$

Assuming

$$\lambda/c_p = (\lambda/c_p)_{T^0}$$

where T^0 is the inner layer temperature to be defined in Lecture 6, one obtains a more suitable definition for the flame length

$$\ell_F = \frac{(\lambda/c_p)_{T^0}}{(\rho s_L)_u}.$$

Since the reaction zone was assumed to be thin, the flame thickness hence describes the thickness of the preheat zone of the flame structure.

The flame thickness is a measure for the quenching distance d of a flame.

This is the distance, for whom a flame extinguishes, if it encounters a cold wall. There is the estimation

$$d = c\,\ell_F, \quad c = 5 \div 6$$