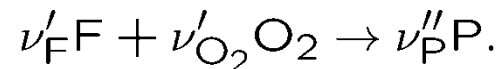


# Lecture 5

## 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
- Prerequisite: Single one-step reaction



- 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

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

- The most important feature in is the Arrhenius type temperature dependence
- The activation energy  $E$  is assumed to be large
- Both the activation energy  $E$  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

## Schematic Flame Structure

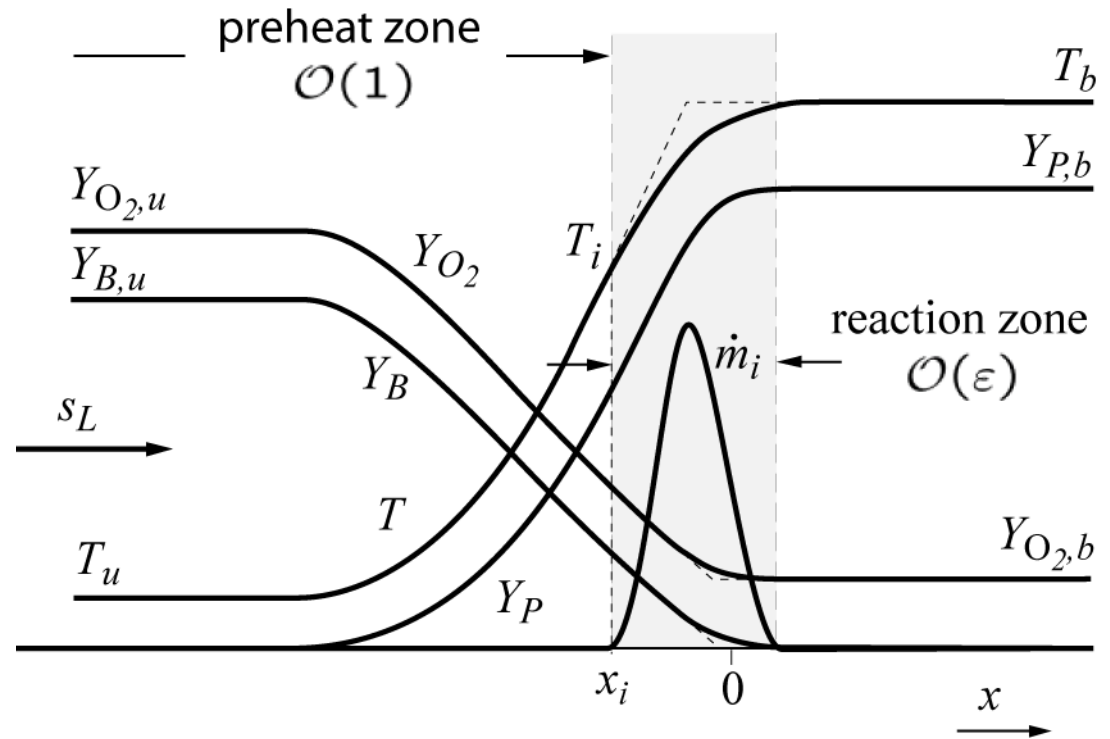
• Reaction is assumed to be irreversible

→ Reaction rate must vanish in burnt gas

• Therefore one of the reactants must be entirely depleted:

- Fuel for lean flames
- Oxidizer for rich flames
- Both for stoichiometric flames

• This leads to the condition in the burnt gas:  $Y_{F,b} \cdot Y_{O_2,b} = 0$ .



- Combustion of 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

$$\dot{j}_i = -\rho D_i \text{grad} Y_i, \quad D_i = D_{i,N_2},$$

where Lewis number is unity

- The species balance equation

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

is considered for 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

$$\rho \frac{DT}{Dt} = \frac{1}{c_p} \frac{Dp}{Dt} + \text{div} \left( \frac{\lambda}{c_p} \text{grad} T \right) + \sum_{l=1}^r \frac{Q_l}{c_p} \omega_l + \frac{\dot{q}_R}{c_p}.$$

using  $\rho u = \rho_u s_L$  yields

$$\rho_u s_L \frac{dT}{dx} = \frac{d}{dx} \left( \frac{\lambda}{c_p} \frac{dT}{dx} \right) - \frac{Q}{c_p} \omega.$$

- These can be combined with the species equations in the coupling functions

$$Y_F = -\frac{\nu'_F W_F c_p}{Q} (T - T_b) + Y_{F,b}$$

$$Y_{O_2} = -\frac{\nu'_{O_2} W_{O_2} c_p}{Q} (T - T_b) + Y_{O_2,b}$$

- 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

$$\rho = \text{const}$$

- 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 as  $\rho u = \rho_u S_L$ ,

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

$$\rho u s_L \frac{dT}{dx} = \frac{d}{dx} \left( \frac{\lambda}{c_p} \frac{dT}{dx} \right) - \frac{Q}{c_p} \omega$$

- Zeldovich and Frank-Kamenetzki used the following assumptions introducing the ignition temperature  $T_i$ :
  1. In the preheat zone,  $T \leq T_i$ , no reactions take place, therefore  $\omega = 0$
  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,  $T \leq T_i$  and  $\omega = 0$  the temperature equation can be integrated
- Considering the boundary condition

$$\left. \frac{dT}{dx} \right|_{x \rightarrow -\infty} = 0 \quad \text{and} \quad T \Big|_{x \rightarrow -\infty} = T_u$$

we achieve for the first derivative

$$\frac{dT}{dx} = \frac{c_p \rho_u s_L}{\lambda} (T - T_u).$$

- With the second assumption the temperature equation can be integrated once, if the temperature  $T$  is introduced as an **independent** variable
- One substitutes the heat conduction term with

$$\frac{d}{dx} \left( \frac{\lambda dT}{c_p dx} \right) = \frac{dT}{dx} \frac{d}{dT} \left( \frac{\lambda dT}{c_p dx} \right) = \frac{c_p}{\lambda} \frac{1}{2} \frac{d}{dT} \left( \frac{\lambda dT}{c_p dx} \right)^2$$

- After multiplication with  $\lambda/c_p$  it follows

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

- With the boundary conditions at  $x = \infty$

$$\left. \frac{dT}{dx} \right|_{x \rightarrow +\infty} = 0 \quad \text{and} \quad T \Big|_{x \rightarrow +\infty} = T_b$$

- This equation can be integrated once to yield

$$\frac{dT}{dx} = \sqrt{2 \frac{(-\Delta H)}{\lambda^2} \int_T^{T_b} \lambda \omega(T) dT}$$

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

$$\frac{dT}{dx} = \frac{c_p \rho_u s_L}{\lambda} (T - T_u).$$

and the reaction zone

$$\frac{dT}{dx} = \sqrt{2 \frac{(-\Delta H)}{\lambda^2} \int_T^{T_b} \lambda \omega(T) dT}.$$

- This yields an equation for the burning velocity

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

- An analysis of the integral in closed form is only possible, if further simplifications are introduced
- Expanding the term in the exponent in

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

in a series in  $T$  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

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

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

- 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

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

and

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

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

the reaction rate can be written as

$$\omega = B \rho_b^2 \frac{c_p \mathcal{R} T_b^2}{(-\Delta H) E} \exp \left( -\frac{E}{\mathcal{R} T_b} \right) \left[ - \left( \frac{\nu'_F Y_{O_2,b}}{M_{O_2}} + \frac{\nu'_{O_2} Y_{F,b}}{M_F} \right) \Theta + \frac{\nu'_{O_2} \nu'_F c_p \mathcal{R} T_b^2}{(-\Delta H) E} \Theta^2 \right] \exp \Theta$$



- Integration yields

$$\begin{aligned}
 \int_{T_i}^{T_b} \lambda \omega dT &= \lambda_b \frac{\mathcal{R}T_b^2}{E} \int_{\Theta_i}^0 w(\Theta) d\Theta \\
 &= \frac{\lambda_b B \rho_b^2 c_p \mathcal{R}^2 T_b^4}{(-\Delta H) E} \exp\left(-\frac{E}{\mathcal{R}T_b}\right) \left[ \left( \frac{\nu'_F Y_{O_2,b}}{M_{O_2}} + \frac{\nu'_{O_2} Y_{F,b}}{M_F} \right) (1 + (\Theta_i - 1) \exp \Theta_i) \right. \\
 &\quad \left. + 2 \frac{\nu'_{O_2} \nu'_F c_p \mathcal{R} T_b^2}{(-\Delta H) E} \left( 1 - \left( 1 - \Theta_i + \frac{\Theta_i^2}{2} \right) \exp \Theta_i \right) \right]
 \end{aligned}$$

- 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,  $\Theta_i$  is substituted by  $\Theta_u$ , 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 below the temperature  $T_i$ , the integral

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

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

- On the other hand, on the left hand side of

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

$T_i$  is replaced by  $T_b$  and  $\lambda_i$  by  $\lambda_b$

- This implies the concept that the reaction zone is so thin, that the preheat zone stretches until  $T_b$  and that  $T_i$  is hardly distinguishable from  $T_b$
- The equation above then reads

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

with

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

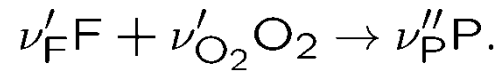
- The contribution of the individual terms in  $S$  depends strongly on the equivalence ratio  $\phi$ 
  - In very lean or very fat mixtures, respectively,  $Y_{O_2,b}$  or  $Y_{F,b}$  are large, while both vanish for stoichiometric mixtures
  - Therefore in stoichiometric mixtures, the last term is predominant

- It follows

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

- 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 exponential term is expanded. Material properties are set constant and are 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 set equal to  $T_b$

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



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 presented here shows that a reaction of 1st order is conform with a very fat or very lean mixture, for which the abundant component 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  $Le = \alpha/D = 1$  and

$$\rho_u s_L = \sqrt{2 \frac{B \rho_b^2 \lambda_b \mathcal{R}^2 T_b^4}{c_p (T_b - T_u)^2 E^2} \exp\left(-\frac{E}{\mathcal{R} T_b}\right) S}$$
$$S = \frac{\nu'_F Y_{O_2,b}}{M_{O_2}} + \frac{\nu'_{O_2} Y_{F,b}}{M_F} + \frac{2 \nu'_{O_2} \nu'_F c_p \mathcal{R} T_b^2}{(-\Delta H) E}.$$

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

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

while the chemical time is given by

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

- The square of the Zeldovich number, defined by

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

appears



- 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  $\rho_u/\rho_b$ , would be calculated from the reaction rate, for example for very lean flames  $\phi \gg 1$  as the inverse of

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

- 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

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

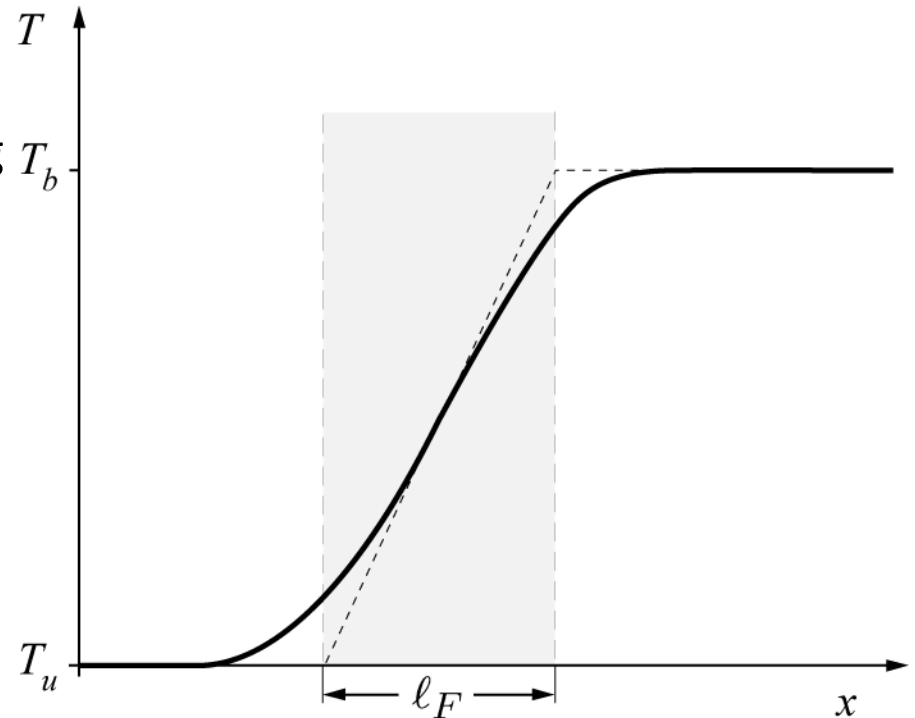
- This is the time, which the flame front requires, to propagate the distance of the thickness of the flame
- The comparison between  $s_L = \sqrt{D/t_c}$  and  $\ell_F = \frac{D}{s_L} = \frac{\lambda_b}{c_p \rho_u s_L}$  up to  $t_F = \frac{\ell_F}{s_L}$

shows, 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  

$$\frac{dT}{dx} = \frac{c_p \rho_u s_L}{\lambda} (T - T_u).$$

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

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

- Below, we will introduce a normalized coordinate

$$x^* = \rho_u s_L \int_0^x \frac{c_p}{\lambda} dx$$

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

$$\frac{dT}{dx} = \frac{d^2T}{dx^2} + \omega$$

- This suggests

$$\rho_u s_L \int_0^{\ell_F} \frac{\lambda}{c_p} dx = 1.$$

- 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 from a cold wall, for which a flame extinguishes
- An estimation is  $d = c \ell_F$ ,  $c = 5 \div 6$