Premixed Laminar Flame

1 Flame Structure

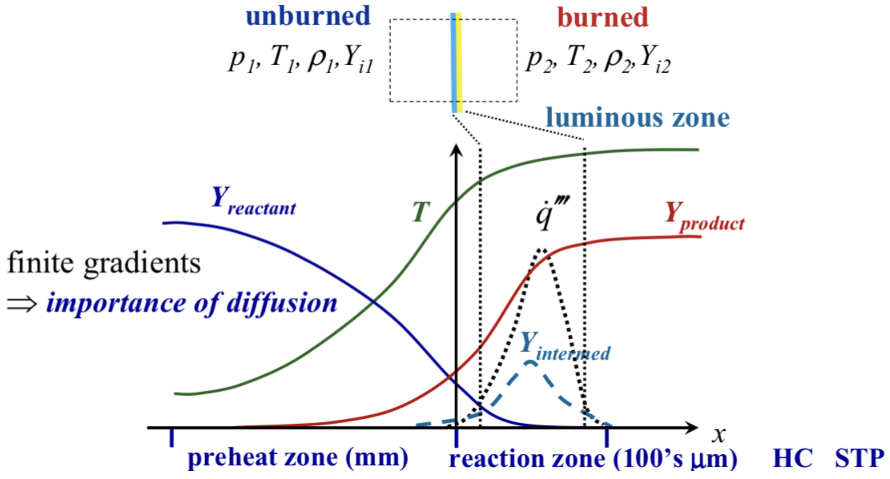


Figure 1: Flame Structure

The structure of a premixed laminar flame can be broadly divided into three regions:

1. **Preheat Zone:** This is the region just ahead of the flame front where the unburned gas mixture is heated by thermal conduction from the hot reaction zone. The temperature increases, but the concentration of the reactants remains relatively constant.

2. **Reaction Zone (Flame Front):** This is where the actual combustion occurs. The temperature is at its highest, and the reactants are converted into products. This is often where light from the flame is primarily produced.

3. **Post-flame Zone:** This is the area beyond the reaction zone, where the combustion products cool down by conduction and radiation.

2 Flame Speed

One of the main goal for the study of premixed laminar flame is determining the wave speed for weak deflagration, which is also called **laminar flame speed**, S_L.

2.1 Governing Equations

To calculate flame speed, we still need to start from basic physics equations. Details could be find in Transport Equation section.

Mass Conservation:

$$\frac{d(\rho u)}{dx} = 0, \dot{m}'' = const \tag{1}$$

Momentum Conservation:

If we assume uniform velocity profile, no viscous dissipation:

$$\frac{d(\rho u u)}{dx} + \frac{dp}{dx} = 0 \tag{2}$$

For the laminar flames, $M_1 << 1$, we assume nearly constant pressure:

$$\frac{d(\rho u u)}{dx}, \frac{dp}{dx} = 0 \tag{3}$$

Ideal Gas Law:

$$p = \rho R T, \frac{\rho T}{\bar{W}} = const \tag{4}$$

Species:

$$\underbrace{\dot{m}''\frac{dY_i}{dx}}_{\text{convection}} = \underbrace{-\frac{dj_{i,x}}{dx}}_{\text{diffusion}} - \underbrace{\bar{W}_i\dot{\omega}_i}_{\text{sink term}} \tag{5}$$

Energy:

$$\underbrace{\dot{m}''c_p\frac{dT}{dx}}_{\text{convection}} = \underbrace{\frac{d}{dx}(k(\frac{dT}{dx}))}_{\text{diffusion heat}} - \underbrace{\sum_i c_{p,i}j_{i,x}\frac{dT}{dx}}_{\text{diffusion species}} - \underbrace{\sum_i h_i\dot{\omega}_i\bar{W}_i}_{\text{sink term}} \tag{6}$$

Based on assumptions and simplifications, we get the Shvab-Zeldovich forms:

$$\frac{d}{dx}[\dot{m}''Y_i - \rho D\frac{dY_i}{dx}] = \bar{W}_i\dot{\omega}_i \tag{7}$$

$$\frac{d}{dx}[\dot{m}''h_{sens} - \rho\alpha\frac{dh_{sens}}{dx}] = -\sum_i \Delta\bar{h}^0_{f,i,T_{ref}}\dot{\omega}_i \tag{8}$$

Assume **single-step** chemical reaction:

$$\sum_{i=1}^{n} v_i' M_i \rightarrow \sum_{i=1}^{n} v_i'' M_i \tag{9}$$

Species net production:

$$\dot{\omega}_i \bar{W}_i = (v_i'' - v_i')RR \tag{10}$$

Heat release:

$$\sum_i \Delta \bar{h}^0_{f,i,T_{ref}} \dot{\omega}_i = \Delta h_{R,T_{ref}} RR \tag{11}$$

Here we define two dimensionless parameters:

$$\eta_i = \frac{Y_i}{v_i'' - v_i'}, \eta_T = \frac{h_{sens,T}}{-\Delta h_{R,T_{ref}}} \tag{12}$$

Now we use **unity Lewis number assumption**, two parameters are combined into one, we get single 2nd order ODE:

$$\frac{d}{dx}[\dot{m}''\eta - \rho D \frac{d\eta}{dx}] = -RR\Delta h_{R,T_{ref}} \tag{13}$$

The boundary conditions are listed below:

1. $\eta(x = -\infty) = \eta_{unburned}$
2. $\eta(x = +\infty) = \eta_{burned}$
3. $\frac{d\eta}{dx}|_{-\infty} = 0$
4. $\frac{d\eta}{dx}|_{+\infty} = 0$

Assume average and constant $\bar{c_p}$, the ODE could be expressed as:

$$\rho_1 S_L \bar{c_p} \frac{dT}{dx} - \frac{d}{dx}(k\frac{dT}{dx}) = -\Delta h_{R,T_{ref}} RR \tag{14}$$

Now what we need to do is solve this equation in both preheat region and reaction region, and match them at interface (x=i)

2.2 Flame Speed Model

2.2.1 Preheat Zone

There is no reaction in this zone, so the reaction rate is zero. Integrate once we get:

$$\rho_1 S_L \bar{c_p} T - k\frac{dT}{dx} = const \tag{15}$$

At $x = -\infty$, $\frac{dT}{dx} = 0$, so:

$$\rho_1 S_L \bar{c_p} T - 0 = const \tag{16}$$

Therefore at interface:

$$\rho_1 S_L \bar{c_p}(T_i - T_1) = k\frac{dT}{dx}|_i \tag{17}$$

Which means that the diffusion from interface is used to preheat the oncoming gas.

2.2.2 Reaction Zone

For high activation energy reaction, T_i near T_2. Also, we assume the diffusive flux than convective flux:

$$\frac{d^2T}{dx^2} >> \frac{dT}{dx} \tag{18}$$

So ignore the first derivative in ODE:

$$\begin{aligned}\Delta h_{R,T_{ref}} RR &= \frac{d}{dx}(k\frac{dT}{dx}) \\ &= \frac{dT}{dx}\frac{d}{dT}(k\frac{dT}{dx})\end{aligned} \tag{19}$$

$$\int_i^\infty k\frac{dT}{dx}d(k\frac{dT}{dx}) = \int_{T_i}^{T_2} kRR\Delta h_{R,T_{ref}}\, dT \tag{20}$$

Assume:

$$\theta = k\frac{dT}{dx} \tag{21}$$

Then:

$$\int_i^\infty \theta d\theta = \int_{T_i}^{T_2} kRR\Delta h_{R,T_{ref}}\, dT \tag{22}$$

Which is a derivative of square. Also because 0 gradient at ∞, rearrange:

$$k\frac{dT}{dx}|_i = \sqrt{2\Delta h_{R,T_{ref}}\int_{T_i}^{T_2} kRRdT} \tag{23}$$

2.2.3 Match at Interface

$$\rho_1 S_L \bar{c_p}(T_i - T_1) = \sqrt{2\Delta h_{R,T_{ref}}\int_{T_i}^{T_2} kRRdT} \tag{24}$$

$$S_L = \frac{1}{\rho_1 \bar{c_p}}\frac{1}{(T_i - T_1)}\sqrt{2\bar{k}\Delta h_{R,T_{ref}}\int_{T_i}^{T_2} RRdT} \tag{25}$$

$$S_L = \sqrt{\frac{\bar{k}}{\rho_1 \bar{c}_p} \frac{2\Delta h_{R,T_{ref}}}{\rho_1 \bar{c}_p (T_i - T_1)} \frac{\int_{T_i}^{T_2} RRdT}{(T_i - T_1)}} \tag{26}$$

$$S_L \approx \sqrt{\frac{\bar{k}}{\rho_1 \bar{c}_p} \frac{2\Delta h_{R,T_{ref}}}{\rho_1 \bar{c}_p (T_2 - T_1)} \frac{\int_{T_1}^{T_2} RRdT}{(T_2 - T_1)}} \tag{27}$$

Define v_f as the stoichiometric fuel-oxidizer ratio, then:

$$m\bar{c_p}(T_2 - T_1) = -\frac{\Delta h_{R,T_{ref}}}{v_f} m_f \tag{28}$$

Therefore:

$$\frac{\Delta h_{R,T_{ref}}}{\bar{c_p}(T_2 - T_1)} = \frac{m}{m_f} v_f = \frac{v_f}{Y_f} \tag{29}$$

Finally, we get the flame speed model:

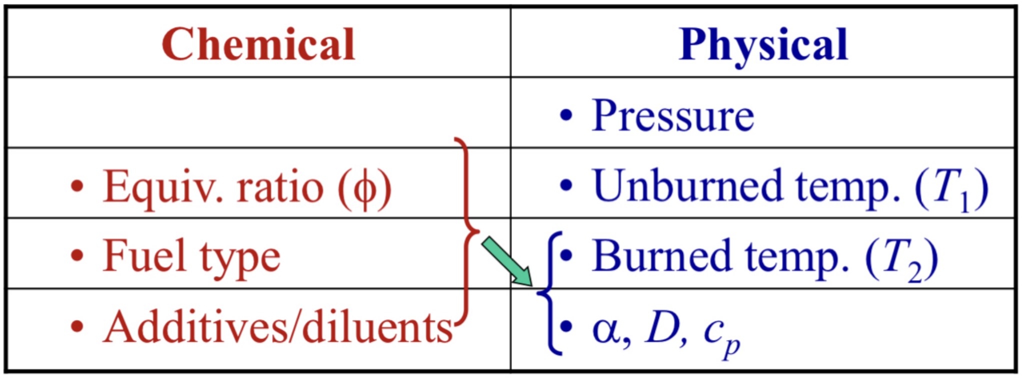
$$S_L = \sqrt{\frac{2v_f}{\rho_1 Y_{f,1}} \bar{\alpha} R\bar{R}R} \propto \sqrt{\bar{\alpha} R\bar{R}R} \tag{30}$$

Here:

1. $\bar{\alpha}$: average thermal diffusivity of energy and species from reaction zone into unburned gas, with the unit as m^2/s. $\bar{\alpha} = \frac{\bar{k}}{\rho c_p}$.
2. $R\bar{R}$: reaction rate, or rate of radical production, with the unit as $\frac{density}{s}$
3. v_f: stoichiometric fuel-oxidizer ratio

2.3 Flame Speed Dependence

After we get the flame model, we want to predict how premixed flame parameters will be influenced by changes in chemical and physical properties of the reactants:



Chemical	**Physical**
	• Pressure
• Equiv. ratio (φ)	• Unburned temp. (T_1)
• Fuel type	• Burned temp. (T_2)
• Additives/diluents	• α, D, c_p

Figure 2: Common Parameters

2.3.1 Scaling Law

For the reaction rate, recall the Arrhenius Rate Law:

$$RR = A'\rho^n (Y_f)^a (Y_{ox})^b e^{-E_a/RT} \tag{31}$$

Here, a and b are the fuel and oxidizer coefficients, and:

$$n = a + b \tag{32}$$

For the thermal diffusivity:

$$\alpha = \frac{k}{\rho_1 c_p} \tag{33}$$

Based on the kinetic theory,

$$k \propto (T/\bar{W})^m, m \approx 0.5 - 0.8 \tag{34}$$

$$\rho_1 = \frac{p}{RT_1} = \frac{p\bar{W}}{\bar{R}T_1} \propto \frac{p}{T_1}\bar{W} \tag{35}$$

$$c_p = \bar{c_p}/\bar{W} \tag{36}$$

Combine all of them:

$$\alpha \propto \frac{T_1 \bar{T}^m}{p\bar{c_p}} \frac{1}{\bar{W}^m} \tag{37}$$

2.3.2 Pressure Dependence

Include all the terms including pressure:

$$S_L \propto \sqrt{\alpha RR/\rho_1} \tag{38}$$

Notice that $p \propto \rho$:

$$S_L \propto \sqrt{\frac{1}{p} p^n \frac{1}{p}} \propto p^{\frac{n-2}{2}} \tag{39}$$

For most hydrocarbons, $n \leq 2$, so **flame speed decreases as pressure increases.** However, for hydrogen, flame speed decreases as pressure increases for lean mixture, flame speed increases as pressure increases for rich mixture.

2.3.3 Temperature Dependence

Include all the terms including temperature:

$$S_L \propto \sqrt{\alpha RR/\rho_1} \propto \sqrt{T_1 T_2^m e^{-E_a/RT_2}/(1/T_1)} \propto T_1 T_2^{m/2} e^{-E_a/2RT_2} \tag{40}$$

From the formula, we can observe that the flame speed increases with the increase of unburned temperature T_1. This effect is mostly preheating, and it will also increase the final temperature T_2. Although $m \approx 0.5 - 0.8$, the final temperature dependence is determined by the exponential term, so flame speed will increase with the increase of T_2, without changing T_1.

2.3.4 Gas Properties

Now we include the terms which have the nonchemical properties ($\bar{W}, \bar{c_p}$) (Here we do not consider the density):

$$S_L \propto \sqrt{\alpha RR/\rho_1} \propto \sqrt{\frac{1}{\bar{c_p}\bar{W}^m}}, m \approx 0.5 - 0.8 \tag{41}$$

Which means light gases increase flame speed. The faster the mean molecular speed, the more diffusion.

2.3.5 Equivalence Ratio

For hydrogen-air combustion, the maximum flame speed occurs at $\phi = 1.7 - 1.9$ and the maximum flame temperature occurs at $\phi = 1.2 - 1.3$. With high equivalence ratio, there are more hydrogen molecules, which will make the flow lighter and move faster, also help the diffusion.

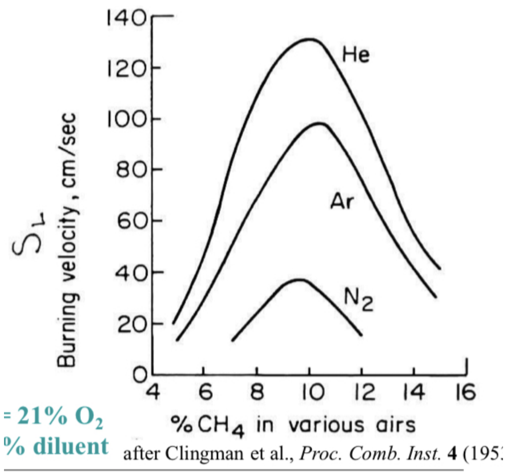
For CH4-air combustion, the maximum flame speed occurs at $\phi = 1.1 - 1.2$ and the maximum flame temperature occurs at $\phi = 1.05$. For H-C fuels, the primary influence of equivalence ratio is on adiabatic flame temperature, so two peak values are nearly the same.

2.3.6 Diluents

Adding diluents will also affect the flame speed. In this example, we assume:

$$Air = 21\% O_2 + 79\% diluent \tag{42}$$

And the result is shown below:



after Clingman et al., *Proc. Comb. Inst.* **4** (195

Figure 3: Diluents

First, He has the lowest molar mass (4 kg/mole, Ar: 40 kg/mole, N2: 28 kg/mole), so its diffusivity is the largest and it has largest flame speed. This effect is much larger than the c_p effect. Even though the molar mass of Ar is larger than N2, but it has lower c_p value because of single atom structure and higher adiabatic temperature. So it has faster flame speed.

3 Flame Thickness

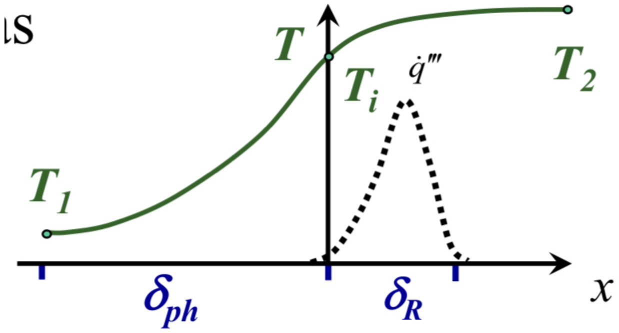


Figure 4: Flame Thickness

We define the thickness of flame as preheat and reactions:

$$\delta_f = \delta_{ph} + \delta_R \tag{43}$$

Recall the governing equation, now approximate T_i by T_2:

$$\rho_1 S_L \bar{c_p}(T_2 - T_1) = k\frac{dT}{dx}|_i \approx k\frac{T_2 - T_1}{\delta_f} \tag{44}$$

Therefore:

$$\delta_f = \frac{k}{\rho_1 \bar{c_p}}\frac{1}{S_L} = \frac{\alpha}{S_L} \propto \sqrt{\alpha \tau_{chem}} \tag{45}$$

3.1 Zeldovich Number

Assume stepwise linear T profiles:

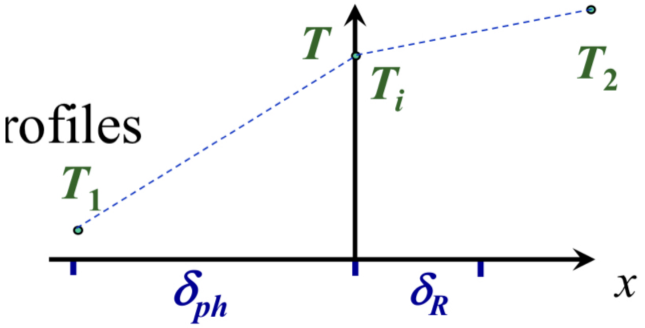


Figure 5: Linear Temperature Profile

To match two regions' profiles:

$$k\frac{T_i - T_1}{\delta_{ph}} = k\frac{T_2 - T_i}{\delta_R} \tag{46}$$

$$\frac{\delta_R}{\delta_p h} = \frac{T_2 - T_i}{T_i - T_1} \approx \frac{T_2 - T_i}{T_2 - T_1} \tag{47}$$

Based on the definition of the reaction rate:

$$\frac{d}{dT}RR(T_2) = \frac{RR(T_2) - RR(T_i)}{T_2 - T_i} \approx \frac{RR(T_2)}{T_2 - T_i} \tag{48}$$

Also based on the Arrhenius Rate Law:

$$RR(T_2) = Ce^{-E_a/RT_2} \tag{49}$$

$$\frac{d}{dT}RR(T_2) = \frac{d}{dT}(-E_a/RT_2)Ce^{-E_a/RT_2} = \frac{E_a}{RT_2^2}RR(T_2) \tag{50}$$

Therefore:

$$T_2 - T_i = \frac{RR(T_2)}{(E_a/RT_2^2)RR(T_2)} = \frac{1}{E_a/RT_2^2} \tag{51}$$

$$\frac{\delta_R}{\delta_{PH}} = \frac{RT_2^2/E_a}{T_2 - T_1} = \frac{1}{Ze} \tag{52}$$

This equation shows that with high activation energy and heat release, the reaction zones will be thin.

3.2 Flame Thickness Dependence

3.2.1 Pressure

$$\delta_f = \frac{\alpha}{S_L} = \sqrt{\frac{\alpha \rho_1}{RR}} \tag{53}$$

Include all the pressure terms:

$$\delta_f \propto \sqrt{\frac{\frac{1}{p}p}{p^n}} = p^{-n/2} \tag{54}$$

For most hydrocarbon, $n \leq 2$, so flame thickness decrease with the increase of pressure.

3.2.2 Final Temperature

Include all the temperature terms:

$$\delta_f \propto \sqrt{\frac{T_1 T_2^m (\frac{1}{T_1})}{e^{-E_a/RT_2}}} = T_2^{m/2} e^{\frac{E_a/R}{2T_2}} \tag{55}$$

So the flame is thinner when T_2 is higher.

3.2.3 Gas Properties

Only include α:

$$\delta_f \propto \sqrt{\frac{1}{\bar{c_p} \bar{W}^m}} \tag{56}$$

The dependence is the same as flame speed.

3.2.4 Equivalence Ratio

If the flame is propagating fast, the reaction zone will be thin. Therefore, the minimum δ_f is roughly at ϕ where S_L maximum.

4 Flame Structure Analysis

4.1 H_2 Flame Structure

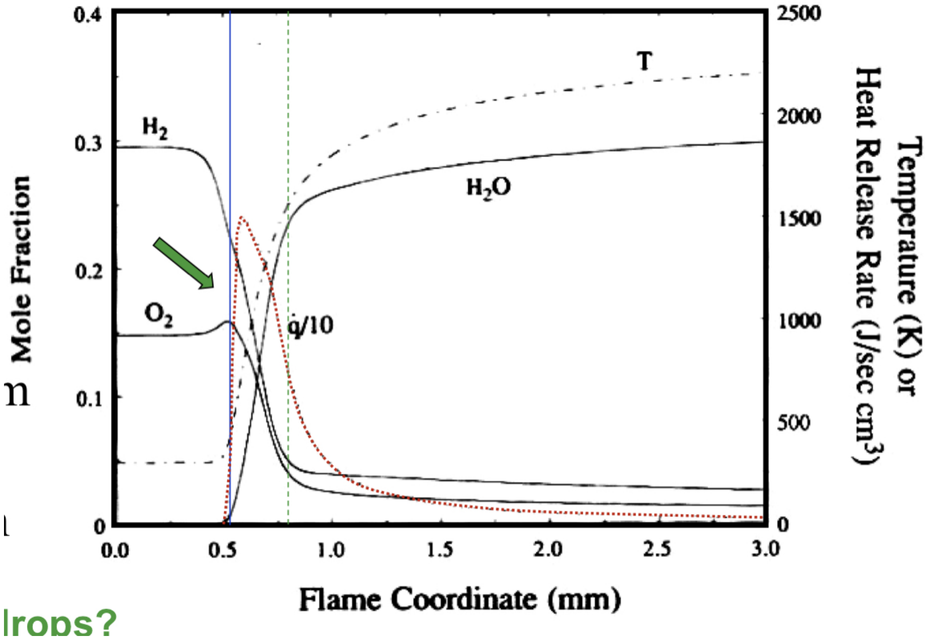


Figure 6: H2 Flame Structure (1)

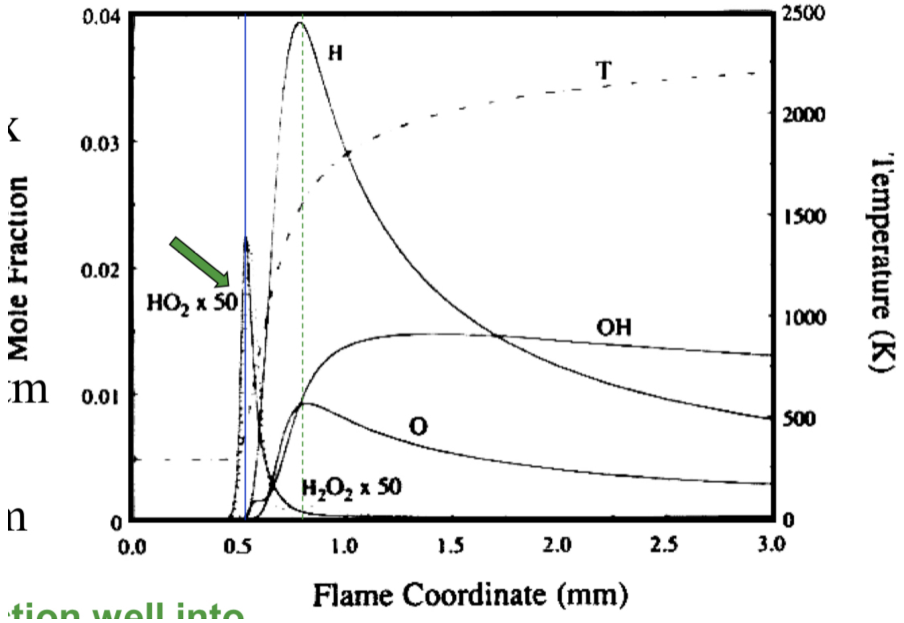


Figure 7: H2 Flame Structure (2)

Remarks:

1. **Why O2 has a small increase at the beginning?** Hydrogen is diffusing much faster than oxygen, which will increase the mole fraction of oxygen.

2. **When O2 starts to drop?** When heat release starts.
3. Peak H production well into heat release zone.

4.2 CH_4 Flame Structure

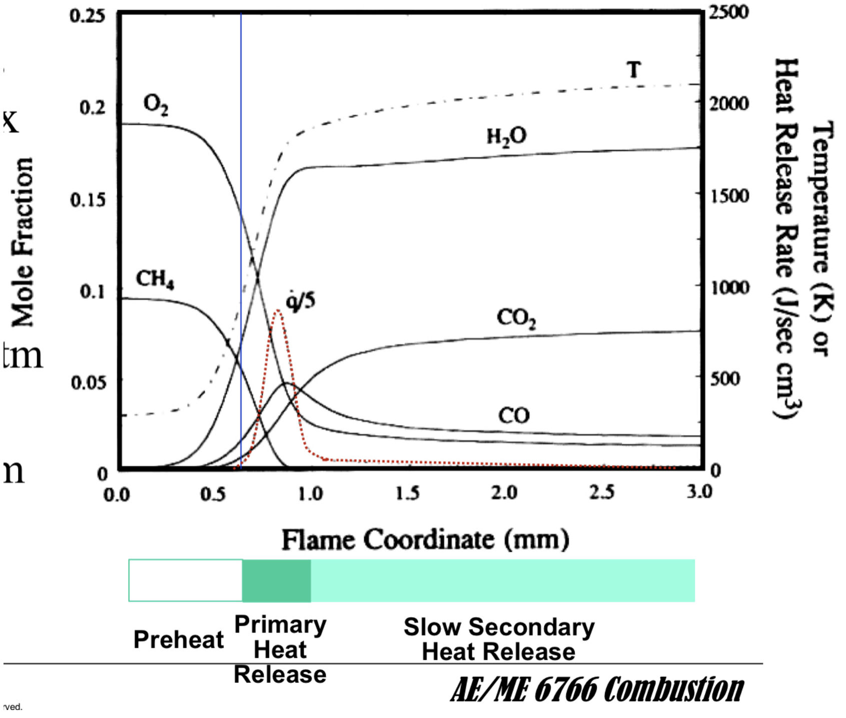


Figure 8: CH4 Flame Structure (1)

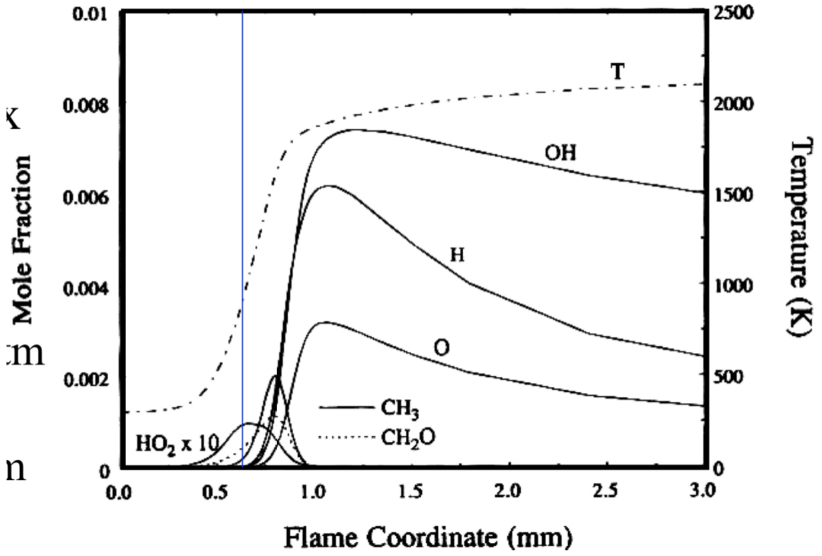


Figure 9: CH4 Flame Structure (2)

Some remarks:

1. The first step in the CH_4 mechanism is the formation of CH_3 and production of H atoms. So species such as CH_3, CH_2O, HCO and CH are produced and destroyed in a narrow interval of great heat release
2. The sequence of the mechanism is $CH_4 \rightarrow CO \rightarrow CO_2$, so the peak destruction of CH_4 must coincide with the peak of production of CO