

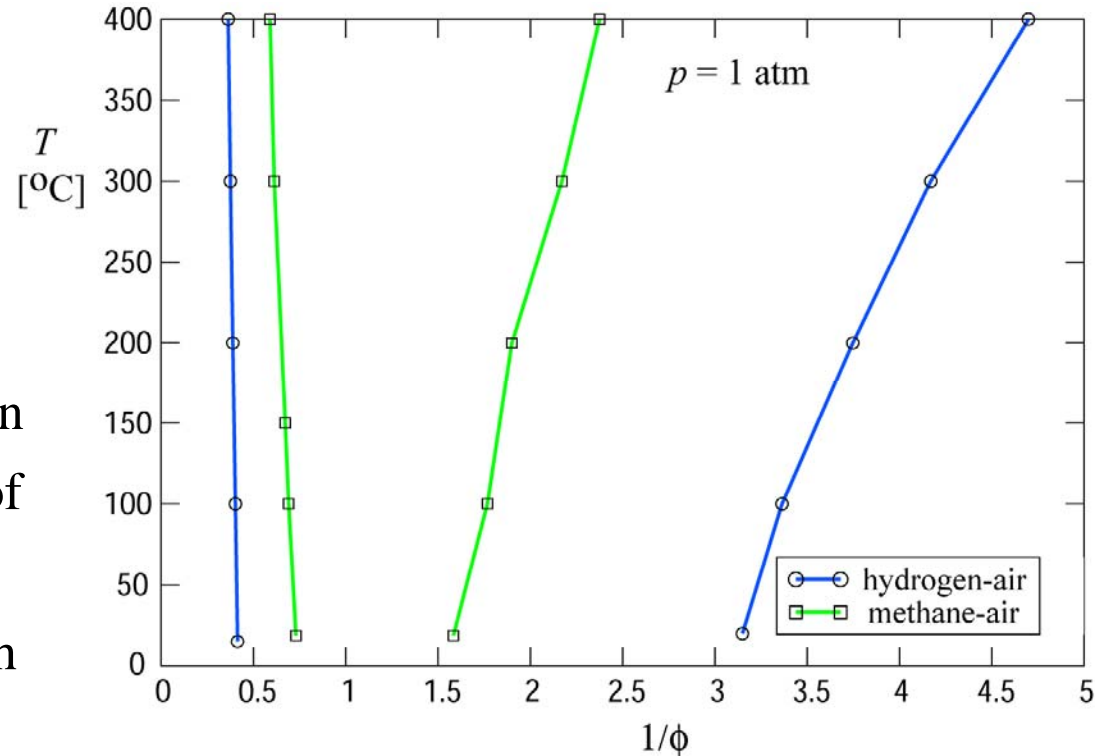
Lecture 7

Flame Extinction and Flamability Limits

Lean and rich flammability limits are a function of temperature and pressure of the original mixture.

Flammability limits of methane and hydrogen for increasing temperatures as a function the air-fuel equivalence ratio.

It is seen, that in particular for lean mixtures, which are on the r.h.s. of this diagram, the flammability limits of hydrogen extract to much larger values than for methane.



This shows that hydrogen leakage may cause safety hazards more readily than, for instance, hydrocarbons which have flammability limits close to those of methane.

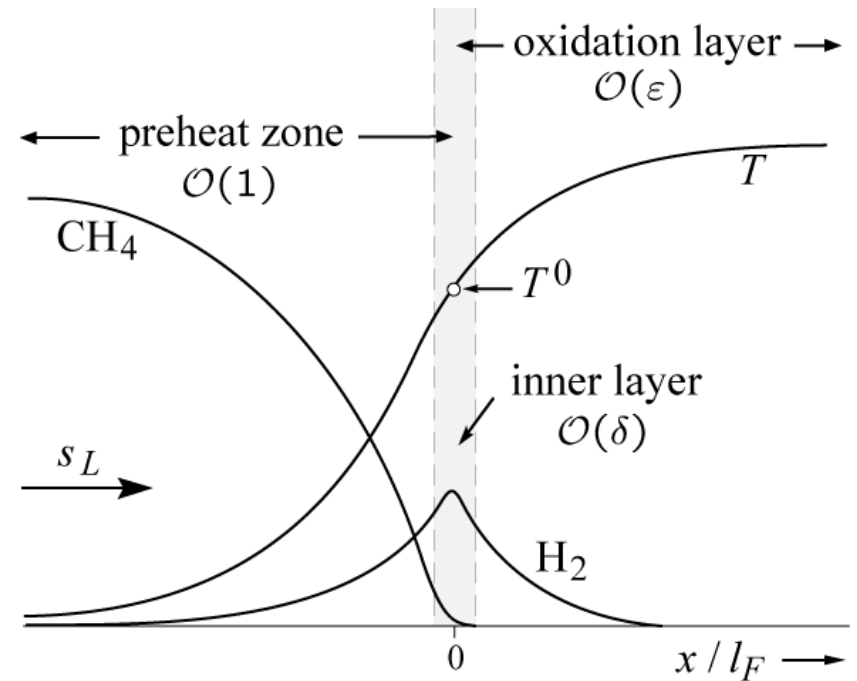
Lean Flammability Limits of Hydrocarbon Flames

Definition:

Flammability is the ability of an ignited mixture to enable flame propagation without further heat addition.

This requires that a sufficient amount of fuel is available to reach a temperature, that, in view of the flame structure should exceed the inner layer temperature T^0 .

Le Chatelier in 1891 was the first to point towards a criterion that relates the flammability limit to the thermodynamic properties of the fuel mixture.



In 1898 Le Chatelier and Boudouard investigated experimental data and wrote:

The flammability limit of most hydrocarbons corresponds to a heat of combustion close to 12.5 kcal.

This is essentially Le Chatelier's famous *mixing rule*.

It determines an adiabatic flame temperature and should be valid for mixtures of hydrocarbons with inerts, too.

The equation

$$s_L = Y_{F_u}^m A(T^0) \frac{T_u}{T^0} \left(\frac{T_b - T^0}{T_b - T_u} \right)^n$$

now shows that the burning velocity vanishes if the adiabatic flame temperature is equal to the inner layer temperature.

A lower theoretical limit for the lean flammability limit is therefore given by

$$T_b = T^0$$

In view of this criterion the adiabatic flame temperature identified by Le Chatelier and Boudouard corresponds to the inner layer temperature and thus describes a chemical rather than a thermodynamic property.

As the lean flammability limit is approached, the burning velocity drops sharply, but shows a finite value at the limiting point. Egerton and Thabet and Powling report a value of 5 cm/s at atmospheric pressure using flat flame burners.

Experimental data for the lean flammability limit are always influenced by external disturbances, such as radiative heat loss or flame stretch.

Radiation heat loss will be discussed in the next section.

We note that flame extinction occurs at a finite value of the burning velocity.

$T_b = T^0$ may be used to calculate the limiting fuel mass fraction $(Y_{F,u})_{l.l.}$ as a quantity that determines the flammability limit.

At the flammability limit it is accurate enough to assume complete combustion and to determine T_b as a function of $Y_{F,u}$ and T_u (Lecture 2):

$$T_b - T_u = \frac{Q_{\text{ref}} Y_{F,u}}{c_p \nu'_F W_F}$$

Then, with $T_b = T^0$, one obtains

$$(Y_{F,u})_{l.l.} = \frac{(T^0 - T_u) c_p \nu'_F W_F}{Q_{\text{ref}}}$$

$(Y_{F,u})_{l.l.}$ decreases linearly with increasing T_u .

Extinction of a Plane Flame by Volumetric Heat Loss

An additional influence that affects the stability of flames is volumetric heat loss.

In order to analyze this effect we will compare the one-step model with a large activation energy and unity Lewis number and the four-step model.

We will assume that the volumetric heat loss is proportional to the temperature difference $T - T_u$ and write

$$\dot{q}_R = -\alpha(T - T_u)$$

α is a heat loss coefficient.

One-dimensional temperature equation for a steady state premixed flame

$$\rho_u s_L \frac{dT}{dx} = \frac{d}{dx} \left(\frac{\lambda}{c_p} \frac{dT}{dx} \right) + \frac{(\Delta H)}{c_p} \omega - \frac{\alpha (T - T_u)}{c_p}$$

In terms of the non-dimensional quantities defined

$$X_i = \frac{Y_i W_{\text{CH}_4}}{Y_{\text{CH}_4 u} W_i}, \quad x_i = \frac{X_i}{\text{Le}_i},$$

$$T^* = \frac{T - T_u}{T_b - T_u}, \quad x^* = \rho_u s_L \int_0^x \frac{c_p}{\lambda} dx,$$

$$\omega^* = \frac{\lambda W_{\text{CH}_4} \omega_l}{c_p Y_{\text{CH}_4 u} (\rho v)_u^2}$$

this may be written (with the asterisks removed)

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

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M is the burning velocity of the plane flame with heat loss normalized by the reference burning velocity $s_{L,\text{ref}}$ of a plane flame without heat loss

$$M = \frac{s_L}{s_{L,\text{ref}}}$$

The non-dimensional heat loss parameter is defined

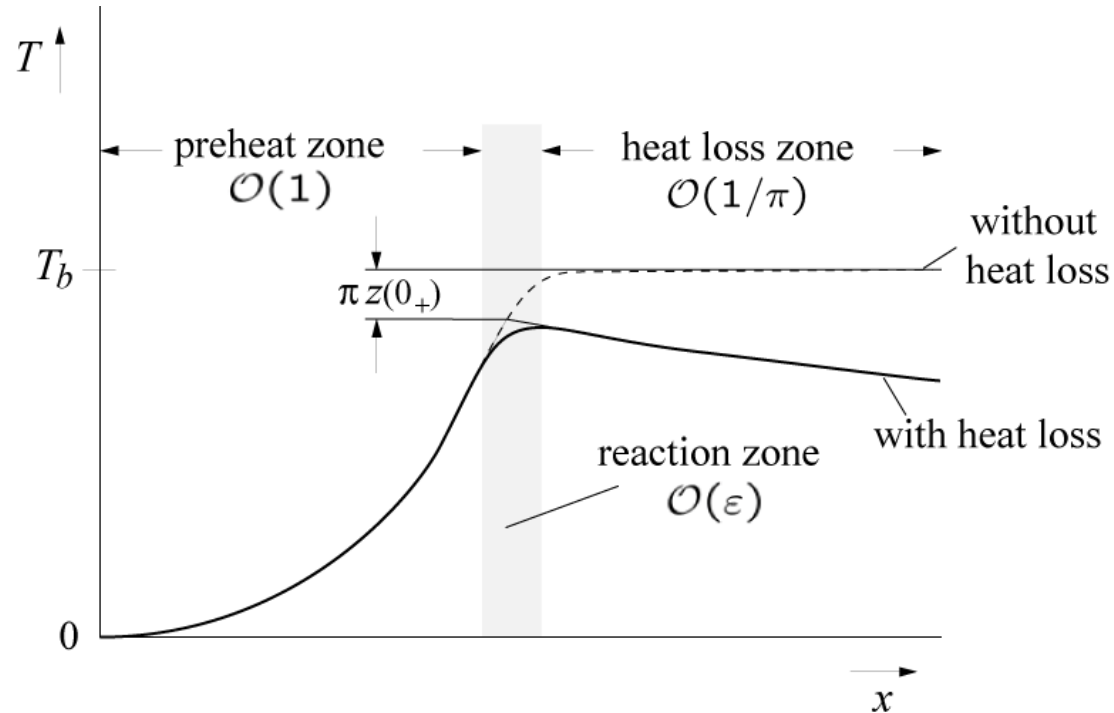
$$\pi = \frac{\lambda \alpha}{\rho_u^2 s_{L,\text{ref}}^2 c_p^2}$$

It will be assumed constant with λ evaluated at $T = T^0$.

It should be noted here that π increases rapidly as $s_{L,\text{ref}}$ decreases.

Heat loss has a strong influence close to the flammability limit when $s_{L,\text{ref}}$ is small.

Structure of a premixed flame with heat loss



Solution of

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

We will treat π as a small expansion parameter and expand the temperature as

$$T = T^0(1 + \pi z)$$

T^0 is the leading order temperature for $\pi \rightarrow 0$.

The reaction term ω in

$$\rho_u s_L \frac{dT}{dx} = \frac{d}{dx} \left(\frac{\lambda}{c_p} \frac{dT}{dx} \right) + \frac{(\Delta H)}{c_p} \omega - \frac{\alpha (T - T_u)}{c_p}$$

can be eliminated by coupling it with the equation for the fuel mass fraction.

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

In non-dimensional form one then obtains the enthalpy

$$h = T + Y - 1$$

governed by the equation

$$M \frac{dh}{dx} = \frac{d^2h}{dx^2} - \pi T$$

This equation may be integrated across the thin reaction zone from $x = -\infty$ to $x = 0_+$.

This leads to

$$Mh(0_+) = \left. \frac{dh}{dx} \right|_{0_+} - \pi \int_{-\infty}^{0_+} T^0 dx$$

since at $x \rightarrow -\infty$ the enthalpy and its gradient vanishes.

Introducing $T = T^0(1 + \pi z)$ into $h = T + Y - 1$ at $x = 0_+$, where $T^0 = 1$ and $Y = 0$ one obtains

$$h(0_+) = \pi z(0_+)$$

The integral over the preheat zone in

$$Mh(0_+) = \left. \frac{dh}{dx} \right|_{0_+} - \pi \int_{-\infty}^{0_+} T^0 dx$$

may be evaluated by integrating the temperature equation to leading order

$$M \frac{dT^0}{dx} = \frac{d^2 T^0}{dx^2}$$

leading to

$$T^0 = \exp(Mx) \quad \text{for } x < 0$$

The downstream enthalpy gradient at the flame front is equal to the downstream temperature gradient since $Y = 0$ for $x \geq 0$.

It can be evaluated by realizing that the heat loss region behind the $h(0_+) = \pi z(0_+)$ order π^{-1} .

This suggests the introduction of a contracted coordinate $\tilde{x} = \pi x$

into the downstream temperature equation

$$M \frac{dT}{d\tilde{x}} = \pi \frac{d^2T}{d\tilde{x}^2} - T \quad x > 0$$

In the limit $\pi \rightarrow 0$ the heat conduction term can now be neglected and with $T^0(0_+) = 1$ one obtains to leading order

$$\left. \frac{dh}{dx} \right|_{0_+} = \left. \frac{dT}{dx} \right|_{0_+} = -\frac{\pi}{M}$$

With

$$h(0_+) = \pi z(0_+)$$

and

$$T^0 = \exp(Mx) \quad \text{for } x < 0$$

inserted into

$$\left. \frac{dh}{dx} \right|_{0_+} = \left. \frac{dT}{dx} \right|_{0_+} = -\frac{\pi}{M}$$

the flame temperature perturbation is

$$z(0_+) = -\frac{2}{M^2}$$

Since for a one step flame with a large activation energy the burning velocity depends on the flame temperature as

$$s_L^2 \sim \exp\left(-\frac{E}{RT_b}\right),$$

a perturbation of the temperature at $x = 0_+$ behind the reaction zone will lead in terms of the dimensional temperature to

$$M = \exp\left\{-\frac{E}{2R}\left(\frac{1}{T(0_+)} - \frac{1}{T^0}\right)\right\}$$

Using the expansion

$$T = T^0(1 + \pi z)$$

in terms of the non-dimensional temperature one obtains with $Ze = \frac{E(T_b - T_u)}{\mathcal{R}T_b^2}$

$$M^2 = \exp(\pi Ze z(0_+))$$

When this is combined with

$$z(0_+) = -\frac{2}{M^2}$$

one obtains

$$M^2 \ln M^2 = -2\pi Ze.$$

A similar analysis may be performed for the four-step asymptotic analysis of methane flames. Then

$$s_L^2 = \frac{8}{15} \frac{k_1^2}{k_{11}} \frac{1}{q^4 X_{\text{H}_2\text{O}}} \frac{Y_{\text{CH}_4,u}}{W_{\text{CH}_4}} \frac{\lambda_0}{c_{p0}} \left(\frac{\text{Le}_{\text{O}_2}^5 \text{Le}_{\text{H}_2}^3 K_{\text{IV}}(T^0)}{\text{Le}_{\text{CH}_4} 2^5 (1 + \alpha_0)^3} \right)^{1/2} \frac{T_u^2}{T_0^2} \frac{(T_b - T^0)^4}{(T_b - T_u)^4}$$

and therefore

$$s_L^2 \sim (T_b - T^0)^4$$

With $\varepsilon z_0 = \frac{T_b - T^0}{T_b - T_u}$ and $Ze = \frac{E(T_b - T_u)}{RT_b^2} = \frac{4}{\varepsilon z_0}$

since

$$T_b = (T_b - T^0) = 1/(\varepsilon z_0) = Ze/4$$

one obtains to leading order

$$M^2 = \frac{(T_b - T^0 + T_b \pi z(0_+))^4}{(T_b - T^0)^4} = \left(1 + \frac{\pi Ze z(0_+)}{4}\right)^4$$

If this is now combined with $z(0_+) = -\frac{2}{M^2}$

one obtains

$$M^2 \left(1 - M^{1/2}\right) = \pi Ze$$

instead of

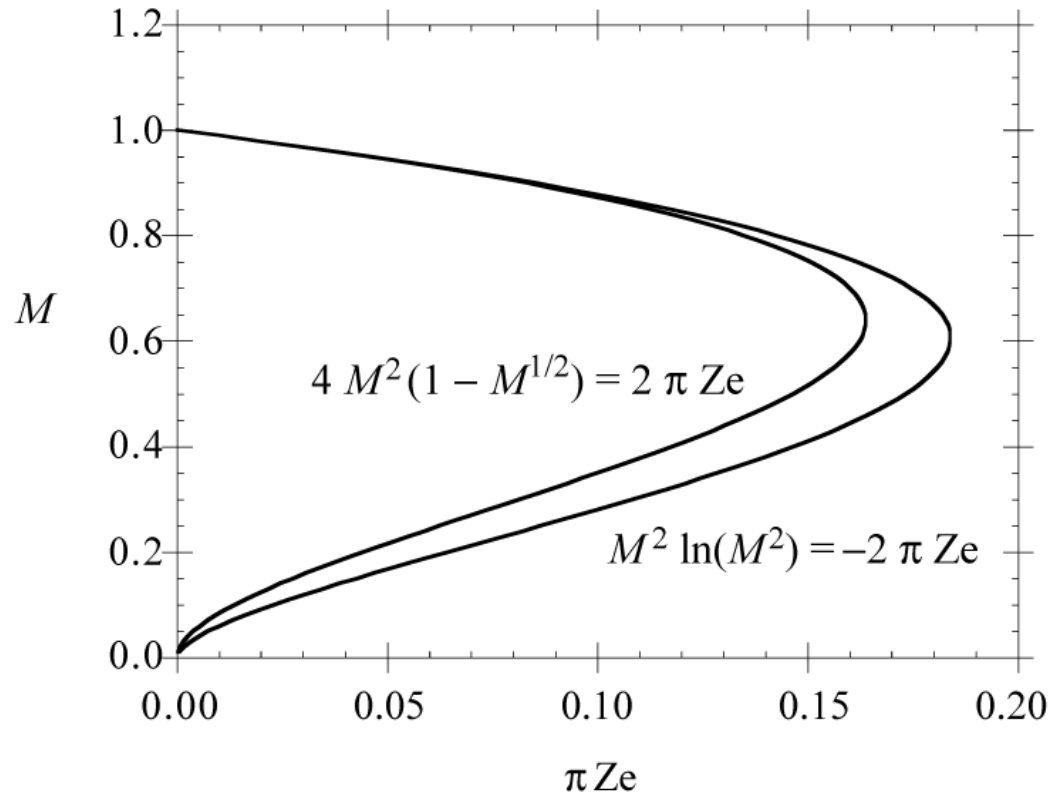
$$M^2 \ln M^2 = -2\pi Ze.$$

Both equations show a qualitatively and even quantitatively very similar behavior.

Only the upper branch of these curves represents a stable solution.

It shows a decrease of the burning velocity as the heat loss parameter π increases.

There is a maximum value for πZe for each of these curves beyond which no solution exists.



At these maximum value heat loss extinguishes the flame.

The non-dimensional burning rates at which this happens are very close to each other: $M_{ex} = 0.61$ for the one step kinetics and $M_{ex} = 0.64$ for the four-step kinetics.

This is surprising because the kinetics for both cases are fundamentally different.

This supports the previous conclusion that the one-step large activation energy model is a good approximation for the temperature sensitivity of hydrocarbon flames.