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Structure and Dynamics of Combustion Waves in Premixed Gases

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Lecture VII
Flame kernels and quasi-isobaric ignition

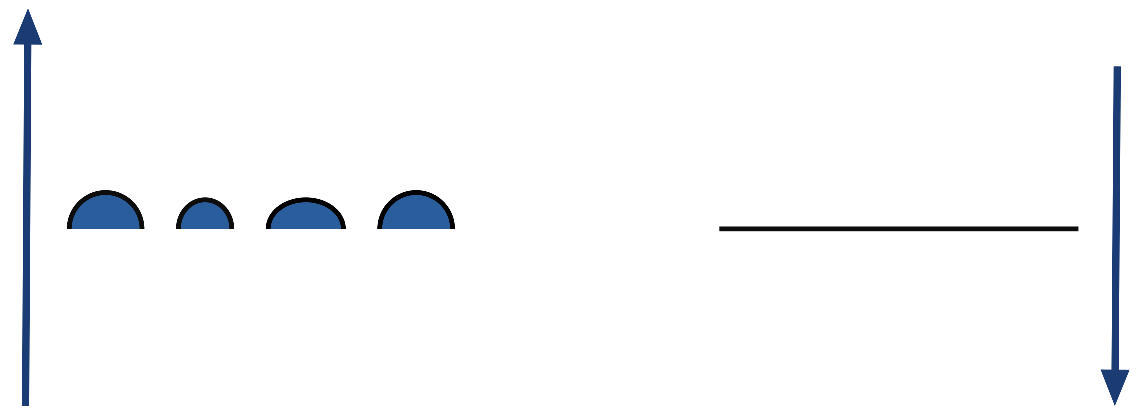
Lecture 7: Flame kernels and quasi-isobaric ignition

VII-I) Introduction

Flammability limits **Critical conditions of ignition**

Some hydrocarbon lean mixtures that are flammable cannot be ignited quasi-isobarically
Some hydrocarbon rich mixtures that are non-flammable can sustain curved flames

Limits for upstream propagation $\neq$ downstream propagation



Ignition in turbulent flows

Princeton experiments (2014) Wu & al.

Turbulence facilitates ignition of hydrocarbon lean mixtures
Turbulence may suppress ignition of hydrocarbon rich mixtures

VII-2) Zeldovich critical radius

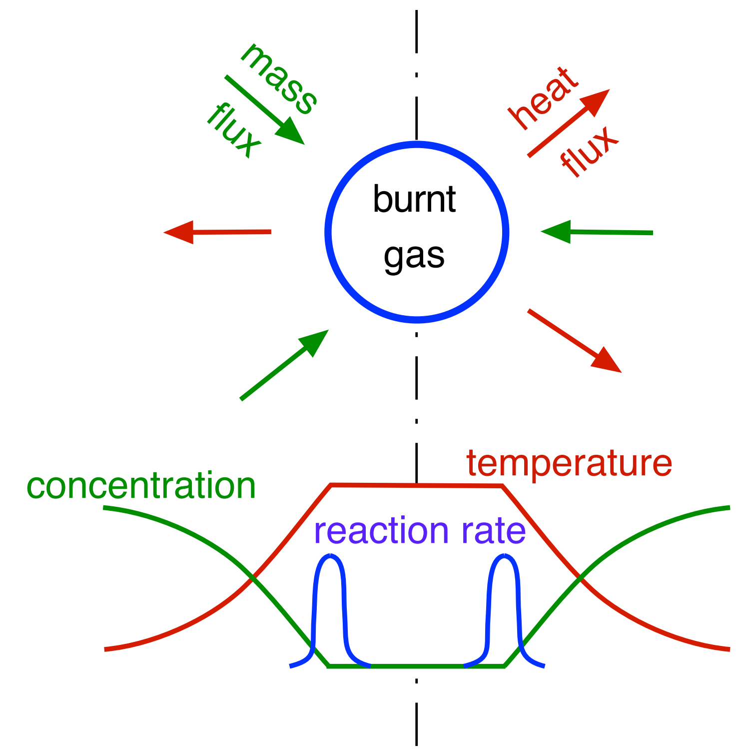
Zeldovich

Flame kernel for a flame far from the flammability limits

Unstable **steady spherical solution** for the one-step model of adiabatic flames

$$\theta \equiv (T - T_u)/(T_b - T_u) \qquad \psi \equiv Y/Y_u \qquad \tau_{rb} \equiv \tau_r(T_b) \qquad c_p(T_b - T_u) = q_R Y_u$$

$$\Delta\theta = \frac{1}{R^2}\frac{\mathrm{d}}{\mathrm{d}R}\left(R^2\frac{\mathrm{d}\theta}{\mathrm{d}R}\right) \qquad \Delta\psi = \frac{1}{R^2}\frac{\mathrm{d}}{\mathrm{d}R}\left(R^2\frac{\mathrm{d}\psi}{\mathrm{d}R}\right)$$



No flow

$$-D_T\frac{1}{R^2}\frac{\mathrm{d}}{\mathrm{d}R}\left(R^2\frac{\mathrm{d}\theta}{\mathrm{d}R}\right) = D\frac{1}{R^2}\frac{\mathrm{d}}{\mathrm{d}R}\left(R^2\frac{\mathrm{d}\psi}{\mathrm{d}R}\right) = \frac{\psi}{\tau_{rb}}\mathrm{e}^{-\beta(1-\theta)}$$

$$R \leqslant R_f: \quad \theta = \theta_f, \quad \psi = 0; \qquad R \to \infty: \quad \theta = 0, \quad \psi = 1$$

Flame temperature

$$\mathrm{Le} \neq 1 \;\Rightarrow\; T_f \neq T_b$$

$$D_T\frac{\mathrm{d}}{\mathrm{d}R}\left(R^2\frac{\mathrm{d}\theta}{\mathrm{d}R}\right) + D\frac{\mathrm{d}}{\mathrm{d}R}\left(R^2\frac{\mathrm{d}\psi}{\mathrm{d}R}\right) = 0 \qquad \text{(conservation energy)}$$

$$\mathrm{Le} \equiv D_T/D$$

$$\mathrm{Le} < 1 \Rightarrow T_f > T_b$$

$$\mathrm{Le} > 1 \Rightarrow T_f < T_b$$

double integration from $R = 0$ to $R = \infty$

$$D_T\theta = D(1 - \psi) \quad \Rightarrow \quad \theta_f = 1/\mathrm{Le}$$

Unstable **steady spherical solution** for the one-step model of adiabatic flames

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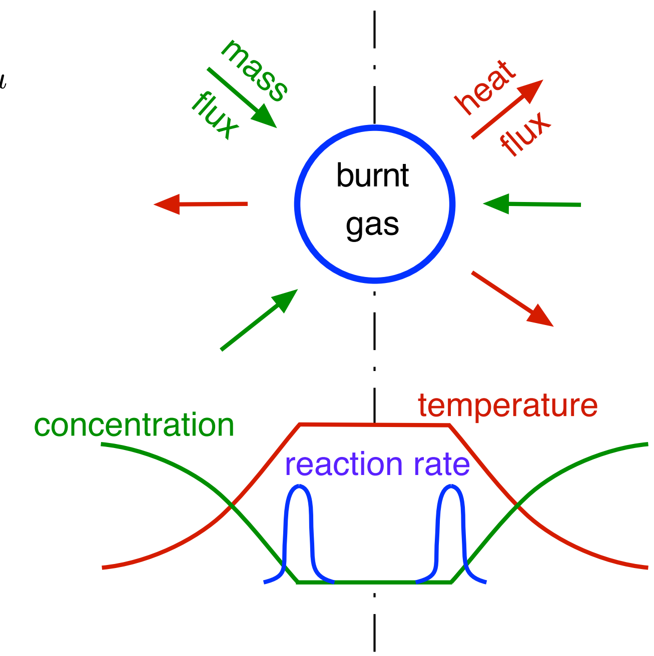
$$-D_T \frac{1}{R^2}\frac{\mathrm{d}}{\mathrm{d}R}\left(R^2 \frac{\mathrm{d}\theta}{\mathrm{d}R}\right) = D \frac{1}{R^2}\frac{\mathrm{d}}{\mathrm{d}R}\left(R^2 \frac{\mathrm{d}\psi}{\mathrm{d}R}\right) = \frac{\psi}{\tau_{rb}} \mathrm{e}^{-\beta(1-\theta)}$$

$$R \leqslant R_f: \quad \theta = \theta_f, \quad \psi = 0; \qquad R \to \infty: \quad \theta = 0, \quad \psi = 1$$



Asymptotic analysis $\beta \gg 1$

Thin reaction zone $\beta \to \infty$ thickness $\ll$ flame radius R_f

$$x \equiv R - R_f, \quad |x| \ll R_f: -D_T \frac{\mathrm{d}^2\theta}{\mathrm{d}x^2} = D \frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = \frac{\psi}{\tau_{rb}} \mathrm{e}^{-\beta(1-\theta)}$$

$$\eta \equiv \beta(x/R_f) = O(1), \qquad \eta \in [-\infty, +\infty] \qquad \psi \equiv \mathrm{Le}(\theta_f - \theta) \qquad \psi \mathrm{e}^{-\beta(1-\theta)} = \mathrm{e}^{\beta(\theta_f-1)}(\mathrm{Le}/\beta)\Theta \mathrm{e}^{-\Theta}$$

$$\Theta \equiv \beta(\theta_f - \theta) = O(1) \qquad \Theta \in [0, \infty] \qquad \frac{\mathrm{d}^2\Theta}{\mathrm{d}\eta^2} = \frac{R_f^2}{D_T}\frac{\mathrm{e}^{\beta(\theta_f-1)}}{\beta^2 \tau_{rb}} \mathrm{Le}\, \Theta \mathrm{e}^{-\Theta}$$

Inner variables

$$\times \frac{\mathrm{d}\Theta}{\mathrm{d}\eta} + \int_0^\Theta \mathrm{d}\Theta \quad \Rightarrow \quad \beta \to \infty: \quad -\lim_{\Theta\to\infty} D_T \frac{\mathrm{d}\theta}{\mathrm{d}R} = \mathrm{e}^{\beta(\theta_f-1)/2}\sqrt{2\,\mathrm{Le}\frac{D_T}{\beta^2 \tau_{rb}}}$$

External zones

$$\frac{\mathrm{d}}{\mathrm{d}R}\left(R^2 \frac{\mathrm{d}\theta}{\mathrm{d}R}\right) = 0 \qquad R^2 \frac{\mathrm{d}\theta}{\mathrm{d}R} = \text{cst.}$$

$$R \geqslant R_f: \quad \theta = \frac{1}{\mathrm{Le}}\frac{R_f}{R}, \qquad R = R_f: \quad D_T \frac{\mathrm{d}\theta}{\mathrm{d}R} = -\frac{1}{\mathrm{Le}}\frac{D_T}{R_f} \qquad R < R_f: \theta = \theta_f$$

$$R = R_f: \quad \theta = \theta_f = 1/\mathrm{Le}$$

Radius of the kernel

matching $\Rightarrow$

$$\frac{1}{\mathrm{Le}}\frac{D_T}{R_f} = \mathrm{e}^{\frac{\beta}{2}\left(\frac{1}{\mathrm{Le}}-1\right)}\sqrt{\mathrm{Le}\frac{D_T}{\tau_b}} \Leftrightarrow \frac{R_f}{d_L} = \mathrm{Le}^{-3/2}\mathrm{e}^{\frac{\beta}{2}\left(1-\frac{1}{\mathrm{Le}}\right)},$$

$$\tau_b \equiv \beta^2 \tau_{rb}/2, \qquad d_L \equiv \sqrt{D_T \tau_b} \ (\mathrm{Le}=1)$$

$$\mathrm{Le} < 1: \ R_f \ll d_L \qquad \mathrm{Le} > 1: \ R_f \gg d_L$$

Instability ? (adiabatic condition)

$$\theta = \theta_f R_f / R \qquad \theta_f = 1/\mathrm{Le} = \mathrm{cst.}$$ preheated zone at rest

$$\mathrm{d}\theta/\mathrm{d}R|_{R=R_f} = -\theta_f / R_f$$

heat flux towards the preheated zone

convection should be added to restore equilibrium

$R_f \nearrow$ $R_f > \overline{R}_f$: $|\text{diffusion fluxes}| \propto 1/R$ $\searrow$ convective flux $\mathrm{d}R_f/\mathrm{d}t > 0$ $R_f \nearrow$

positive feed back: amplification

$R_f \searrow$ $R_f < \overline{R}_f$: $|\text{diffusion fluxes}| \propto 1/R$ $\nearrow$ convective flux $\mathrm{d}R_f/\mathrm{d}t < 0$ $R_f \searrow$

Quasi-isobaric ignition as a nucleation problem

$$\mathrm{Le} < 1 : \ \overline{R}_f \ll d_L \qquad \mathrm{Le} > 1 : \ \overline{R}_f \gg d_L$$

Lean hydrocarbon mixtures $\mathrm{Le} > 1$ **are difficult to ignite** $(R_f > d_L)$

$$D_{C_nH_m} < D_{O_2} \approx D_T, \quad \mathrm{Le} \approx D_{O_2}/D_{C_nH_m} > 1$$

Stability analyses

Stabilization in the presence of heat loss for $\mathrm{Le} < 1$ (Buckmaster, Joulin, Ronney 1990)

Flame balls in micro-gravity experiments (Ronney 1985-2004) (Deshaies Joulin 1984)
lean hydrogen mixtures, diameter $= 2 - 15$ mm

Extension of the Zeldovich analysis to a constant energy source

VII -3) Critical radius near the flammability limits

(He Clavin 1993-94)

model of lecture VI p. 6, 7

$$-D_T \frac{1}{R^2}\frac{\mathrm{d}}{\mathrm{d}R}\left(R^2\frac{\mathrm{d}\theta}{\mathrm{d}R}\right) = D\frac{1}{R^2}\frac{\mathrm{d}}{\mathrm{d}R}\left(R^2\frac{\mathrm{d}\psi}{\mathrm{d}R}\right) = \dot{W}$$

$$\begin{cases} T > T^*: & \dot{W} = \dfrac{\rho_b}{\rho_u}\dfrac{\psi^2}{\tau_{rb}}[\mathrm{e}^{-\beta(1-\theta)} - \mathrm{e}^{-\varepsilon}] \\ T < T^*: & \dot{W} = 0 \end{cases}$$

$$R \leqslant R_f: \quad \theta = \theta_f, \quad \psi = 0; \qquad R \to \infty: \quad \theta = 0, \quad \psi = 1$$

$$\frac{1}{\tau_{rb}} \equiv \frac{1}{\tau^*}\mathrm{e}^{\frac{E}{k_B}\left(\frac{1}{T^*}-\frac{1}{T_b}\right)} = \frac{B_{4f}}{B_{5f}}B_{1f}\mathrm{e}^{-\frac{E}{k_B T_b}}c^*_{O_2 u}$$

$$\varepsilon \equiv \beta\frac{(T_b - T^*)}{(T_b - T_u)} > 0 \qquad \beta \equiv \frac{E}{k_B T_b}\left(1 - \frac{T_u}{T_b}\right) \gg 1$$

$$\begin{cases} \varepsilon = O(1): \text{ near to flammability limits } (\varepsilon = 0: \text{ quenching } \dot{W} = 0) \\ \varepsilon \gg 1, \ \mathrm{e}^{-\varepsilon} \approx 0: \text{ far from flammability limits} \end{cases}$$

Thin reaction zone $\beta \to \infty$ (non-dimensional form $\zeta = x/d_L$, d_L for $\varepsilon \gg 1$, $\mathrm{Le} = 1$, 2^{nd}reaction order)

$$-\mathrm{d}^2\theta/\mathrm{d}\zeta^2 = \dot{\mathrm{w}}(\theta,\psi), \quad (1/\mathrm{Le})\mathrm{d}^2\psi/\mathrm{d}\zeta^2 = \dot{\mathrm{w}}(\theta,\psi) \qquad \theta = \theta_f: \psi = 0$$

$$\frac{D_T}{d_L^2} = 4\frac{\rho_b}{\rho_u}\frac{1}{\beta^3\tau_{rb}}$$

$$\psi = \mathrm{Le}(\theta_f - \theta)$$

$$\begin{cases} T > T^*: & \dot{\mathrm{w}} = (\beta^3/4)\mathrm{Le}^2\mathrm{e}^{\beta(\theta_f-1)}\left\{(\theta_f-\theta)^2\left[\mathrm{e}^{\beta(\theta-\theta_f)} - \mathrm{e}^{-\varepsilon-\beta(\theta_f-1)}\right]\right\} \\ T < T^*: & \dot{\mathrm{w}} = 0 \end{cases}$$

$$\theta^* \leqslant \theta < \theta_f$$

$$\theta^* \equiv \frac{T^* - T_u}{T_b - T_u} = 1 - \frac{\varepsilon}{\beta}$$

$$\times\frac{\mathrm{d}\theta}{\mathrm{d}\zeta} \Rightarrow \left(\frac{\mathrm{d}\theta}{\mathrm{d}\zeta}\right)^2 = \frac{\mathrm{Le}^2}{2}\mathrm{e}^{\beta(\theta_f-1)}\int_{\substack{\theta^*=1-\varepsilon/\beta \\ \dot{\mathrm{w}}=0}}^{\theta_f}\beta^3(\theta_f-\theta)^2\left\{\mathrm{e}^{\beta(\theta-\theta_f)} - \mathrm{e}^{-\varepsilon-\beta(\theta_f-1)}\right\}\mathrm{d}\theta$$

at the exit of the reaction layer (entrance of the preheated zone)

$$\left(\frac{\mathrm{d}\theta}{\mathrm{d}\zeta}\right)^2 = \frac{\mathrm{Le}^2}{2}\mathrm{e}^{\beta(\theta_f-1)} \int_{\theta^*=1-\varepsilon/\beta}^{\theta_f} \beta^3(\theta_f-\theta)^2 \left\{\mathrm{e}^{\beta(\theta-\theta_f)} - \mathrm{e}^{-\varepsilon-\beta(\theta_f-1)}\right\} \mathrm{d}\theta$$

at the exit of the reaction layer (entrance of the preheated zone)

$$\Theta = \beta(\theta_f - \theta) \in [0, \Theta_f] \qquad \Theta_f \equiv \beta\left(\frac{T_f - T^*}{T_b - T_u}\right) = \beta(\theta_f - \theta^*) = \varepsilon + \beta(\theta_f - 1) \geqslant 0$$

$$\mathrm{d}\theta = -\beta \mathrm{d}\Theta$$

measure of the distance from the flammability limit: $\Theta_f \in [0, \infty]$

$$(\mathrm{d}\theta/\mathrm{d}\zeta)^2 = \mathrm{Le}^2 \mathrm{e}^{\beta(\theta_f-1)} J(\Theta_f) \qquad J(\Theta_f) \equiv \frac{1}{2}\int_0^{\Theta_f} \Theta^2(\mathrm{e}^{-\Theta} - \mathrm{e}^{-\Theta_f})\mathrm{d}\Theta \in [0,1]$$

$$J(\Theta_f) = 1 - \mathrm{e}^{-\Theta_f}\left(1 + \Theta_f + \frac{\Theta_f^2}{2!} + \frac{\Theta_f^3}{3!}\right) \qquad \begin{cases} \Theta_f \gg 1: & J \approx 1 \\ 0 \leqslant \Theta_f \ll 1: & J \approx \Theta_f^4/(4!) \end{cases}$$

Preheated zone and matching

flame temperature of the spherical flame

$$R \geqslant R_f: \quad \frac{\mathrm{d}\theta}{\mathrm{dR}} = -\theta_f \frac{R_f}{R^2}, \quad \boxed{\theta_f = \frac{1}{\mathrm{Le}}}$$

d_L for $\varepsilon \gg 1,\ \mathrm{Le} = 1,\ 2^{nd}$ reaction order

$$\beta \to \infty: \quad \boxed{\frac{d_L}{R_f} = \mathrm{Le}^2 \mathrm{e}^{\frac{\beta}{2}\left(\frac{1}{\mathrm{Le}}-1\right)} \sqrt{J(\Theta_f)}}$$

$$T_f \to T^* \Rightarrow R_f/d_L \to \infty$$

$$\Theta_f \to 0$$

T_b is determined by the composition of the mixture Y_{Ru} (mass fraction of the limiting component)

T^* is determined by the chemical kinetics Y_{Ru}

$$\theta \equiv \frac{T - T_u}{T_b - T_u}$$

θ^* depends on the composition

$$\theta^* \equiv \frac{T^* - T_u}{T_b - T_u}$$

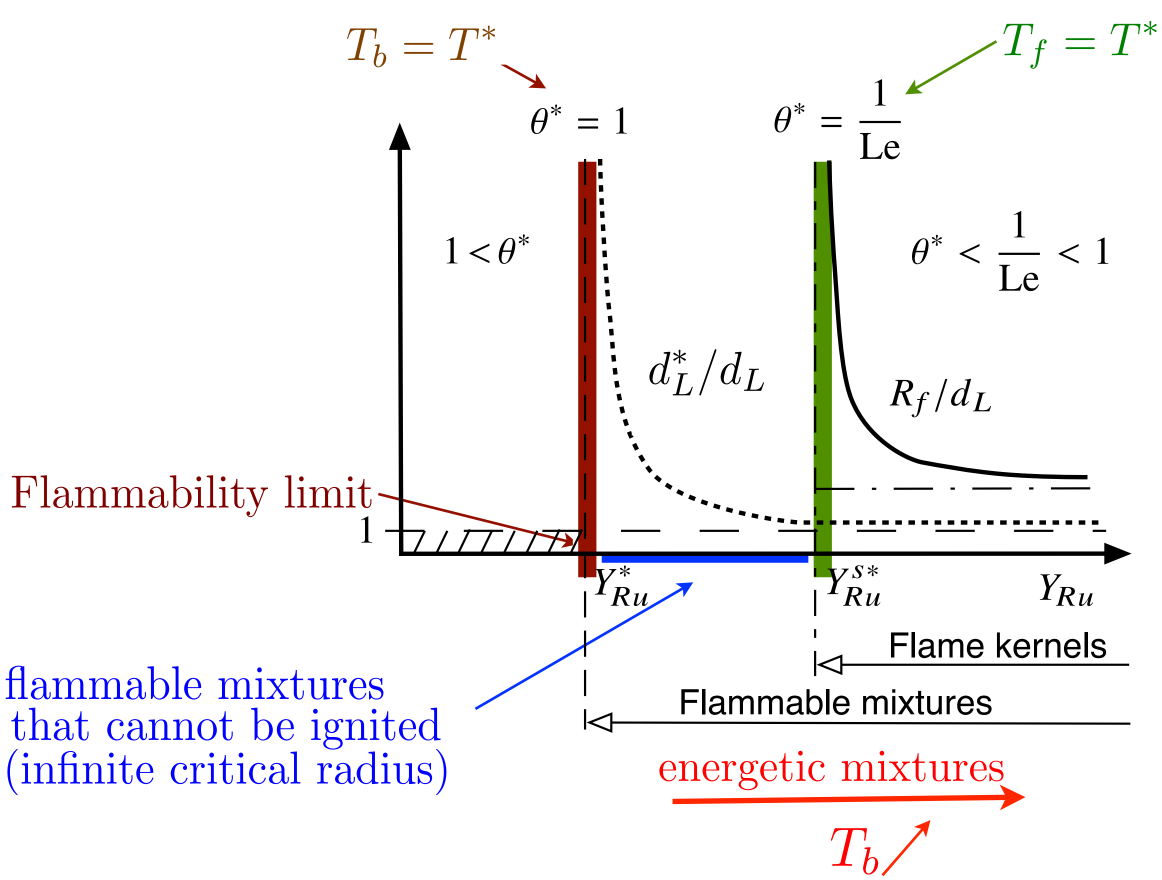
temperature of the planar flame depends on the composition

temperature of the spherical flame kernel

$$\theta_f \equiv \frac{T_f - T_u}{T_b - T_u} = \frac{1}{\text{Le}}$$

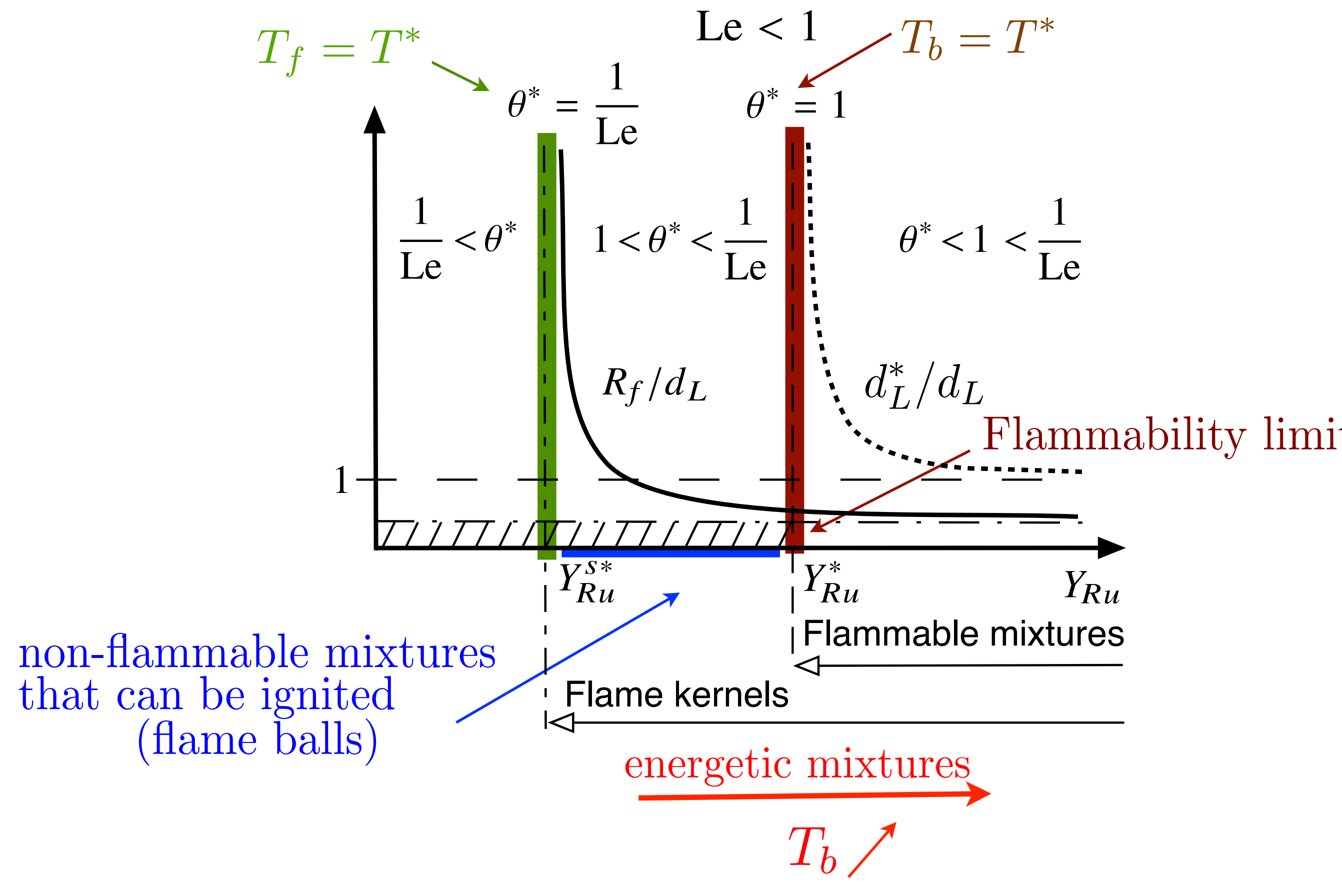
$\theta_f = 1/\text{Le}$

$\text{Le} > 1 \Rightarrow T_f < T_b$

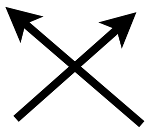


$\text{Le} > 1$: Heavy hydrocarbon lean mixtures
Hydrogen rich mixtures

$\text{Le} < 1 \Rightarrow T_f > T_b$



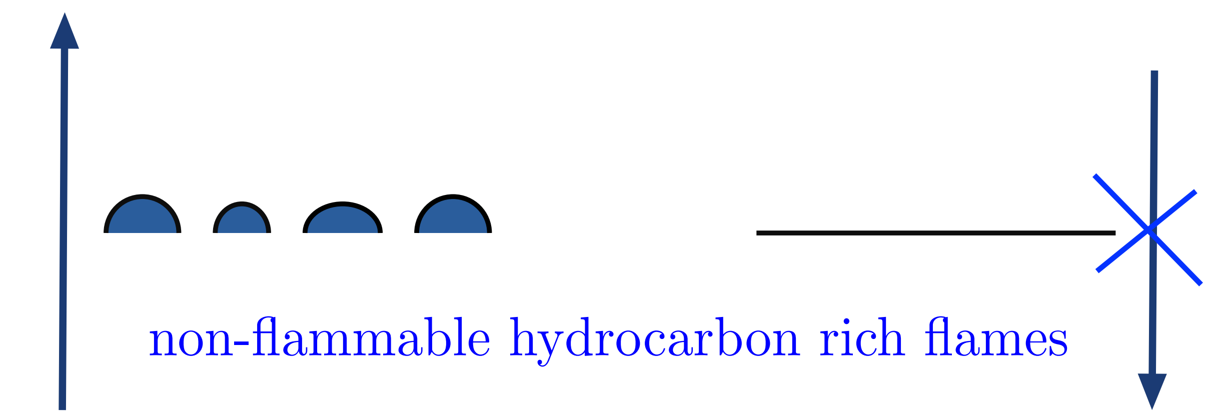
$\text{Le} < 1$: Heavy hydrocarbon rich mixtures
Hydrogen lean mixtures

Flammability limits  Critical conditions of ignition

Some hydrocarbon lean mixtures that are flammable cannot be ignited quasi-isobarically

Some hydrocarbon rich mixtures that are non-flammable can sustain curved flames

Limits for upstream propagation $\neq$ downstream propagation



Buoyancy promoted curved flames

Ignition in turbulent flows

Princeton experiments (2014) Wu & al.

Turbulence facilitates ignition of hydrocarbon lean mixtures

Turbulence may suppress ignition of hydrocarbon rich mixtures

simplest explanation:

Turbulent diffusion coefficients are all equal $\Leftrightarrow \begin{cases} \mathrm{Le} > 1 \\ \mathrm{Le} < 1 \end{cases} \rightarrow \mathrm{Le} = 1$

laminar **turbulent**

VII-4) Dynamics of slowly expanding flame kernels

Quasi-steady preheated zone of flame kernel ?

preheated zone in the reference frame attached to $R_f(t)$ $\qquad \dot{R}_f \equiv \dfrac{\mathrm{d}R_f}{\mathrm{d}t}$

$$\cancel{\frac{\partial \theta}{\partial t}} - \dot{R}_f \frac{\partial \theta}{\partial R} - D_T \frac{1}{R^2}\frac{\partial}{\partial R}\left(R^2 \frac{\partial \theta}{\partial R}\right) = 0$$

quasi-steady state ? $\boxed{t_{relax} \equiv \dfrac{R^2}{D_T} \ll t_{evol} \equiv \dfrac{R_f}{\dot{R}_f}}$ $\quad R \ll \sqrt{D_T t_{evol}}$, not valid at **large distance**

The evolution of spherical flame kernel cannot be quasi-steady at large distance

exact solution of the heat equation with a point energy source $\quad \partial T/\partial t = D_T \Delta T \quad$ point source, $R=0,\ t>0:\ \dot{Q}(t)$

$$T(R,t) - T_u = \int_0^t \frac{\dot{Q}(t-\tau)}{\rho c_p} \frac{\exp(-R^2/4D_T\tau)}{(4\pi D_T \tau)^{3/2}} \mathrm{d}\tau$$

$\dot{Q} = \text{cst.} \qquad X' \equiv R/\sqrt{4D_T\tau} \qquad \mathrm{d}X' = -2D_T R \dfrac{\mathrm{d}\tau}{(4D_T\tau)^{3/2}}$

$$T - T_u = \frac{1}{4\pi D_T}\frac{\dot{Q}}{\rho c_p}\frac{1}{R}\frac{2}{\sqrt{\pi}}\int_{R/\sqrt{4D_T t}}^{\infty} \mathrm{d}X' \mathrm{e}^{-X'^2}$$

relax time toward $(T-T_u) \propto 1/R$ increases with R like R^2/D_T

$R^2/(4D_T t) \to 0$

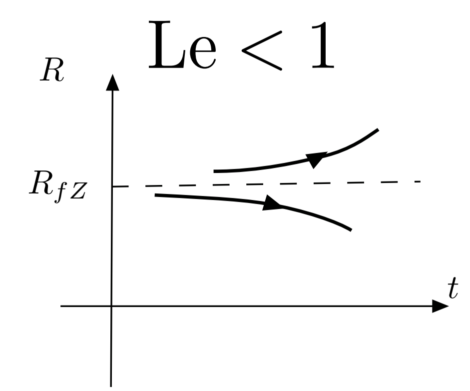
For Le < 1 and near to **the Zeldovich radius** the **slow** evolution of flame kernels is governed by the diffusion at **large** distance

$$\tau \equiv t/t_{ref} \qquad \sqrt{t_{ref}} \equiv \frac{\beta(1-\mathrm{Le}^{1/2})}{\mathrm{Le}} \frac{R_{fZ}}{(4\pi D_T)^{1/2}} \qquad \mathrm{r}_f \equiv R_f/R_{fZ}$$

Joulin's equation (Joulin 1985)

$$\frac{\beta}{2}\left(\theta_f - \frac{1}{\mathrm{Le}}\right) = -\int_0^{\tau} \frac{\mathrm{d}\tau'}{\tau'^{1/2}} \dot{\mathrm{r}}_f(\tau-\tau')$$

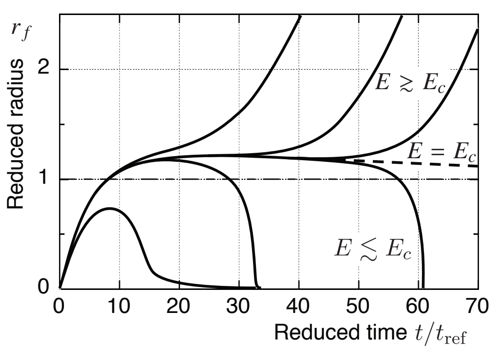
$$\frac{1}{\mathrm{r}_f} = \exp\left[-\int_0^{\tau} \frac{\mathrm{d}\tau'}{\tau'^{1/2}} \dot{\mathrm{r}}_f(\tau-\tau')\right]$$



The structure and the dynamics of flame kernels $\neq$ planar flames even for $R_f \gg d_L$ $(\theta \approx \theta_f/R)$

Extension to a short pulse of an energy source (Joulin 1985)

Extension to the proximity of flammability limits + heat loss (Clavin 2015)



Dynamical quenching of flame kernels in **nonflammable mixtures** for Le < 1 (Clavin 2016)

$$\frac{1}{\sqrt{\mathrm{r}_f}} + H_b \mathrm{r}_f^2 = 1 - I(\tau) \quad \text{where} \quad I(\tau) \equiv \int_0^{\tau} \frac{\mathrm{d}\tau'}{\tau'^{1/2}} \dot{\mathrm{r}}_f(\tau-\tau')$$

Self-extinguished flames in micro-gravity experiments of lean methane-air mixtures (Ronney 1985-1990)

VII-5) Quasi-steady dynamics of thin flames ?

thin flames: flame thickness $(\approx D_T/\dot{R}_f) \ll R_f$

quasi-steady preheated zone $(R > R_f)$

evolution time $\gg$ diffusion time on the flame thickness

$$x \equiv (R - R_f) \qquad \frac{\partial\theta}{\partial t} - \left[\dot{R}_f + 2\frac{D_T}{R}\right]\frac{\mathrm{d}\theta}{\mathrm{d}x} - D_T\frac{\mathrm{d}^2\theta}{\mathrm{d}x^2} = 0$$

$$\frac{\dot{R}_f}{R_f} \ll \frac{D_T}{(D_T/\dot{R}_f)^2} \Leftrightarrow \boxed{R_f\dot{R}_f \gg D_T}$$

moving frame $\quad \Delta\theta$

also negligible !

Quasi-steady state approx valid only when $\dfrac{\dot{R}_f - U_L}{U_L} \ll 1,\ d \approx d_L,\ \dfrac{R_f}{d_L} \gg 1,$

Semi-phenomenological model

$$-\left[\dot{R}_f + 2\frac{D_T}{R}\right]\frac{\mathrm{d}\theta}{\mathrm{d}x} - D_T\frac{\mathrm{d}^2\theta}{\mathrm{d}x^2} = 0$$

$$-\left[\dot{R}_f + 2\frac{D}{R}\right]\frac{\mathrm{d}\psi}{\mathrm{d}x} - D\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = 0$$

+ asymptotic analysis $\beta \to \infty$

thin reaction zone $\Rightarrow F(\dot{R}_f, R_f) = 0$

numerical results for a constant heat source

extension of the Deshaies Joulin analysis (1983) by He (2000)

numerical results of He (2000) extended to $R_f\dot{R}_f \approx D_T$!

qualitative agreements with the experiments by Kelley et al. (2009)

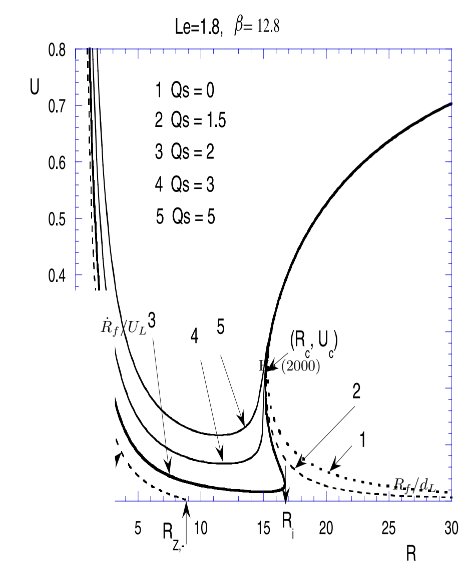


Figure 4. Variation of the flame velocity obtained from equation (12) with different values of the heat power as a function of the flame radius.

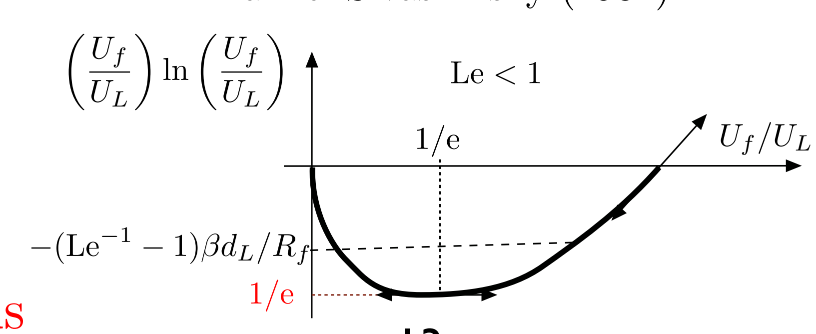
Steady converging flames. Opened-tip Bunsen flames Le < 1

Frankel Sivashinsky (1984)

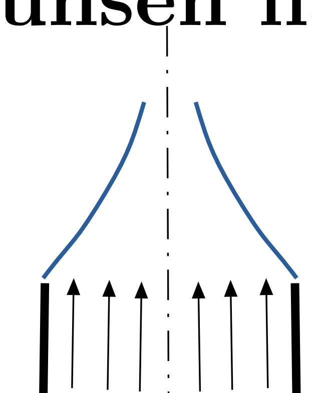
$U_f = -\dot{R}_f > 0 \qquad d_L/\dot{R}_f = O(1/\beta)$

$$\left(\frac{U_f}{U_L}\right)\ln\left(\frac{U_f}{U_L}\right) = -\left(\frac{1}{\mathrm{Le}} - 1\right)\beta\frac{d_L}{R_f}$$

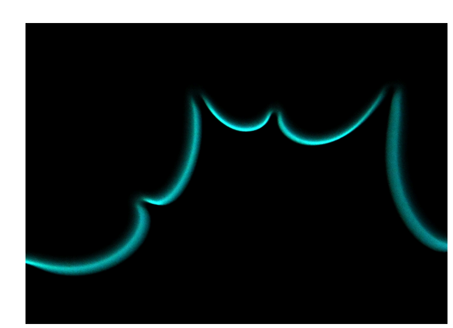
no solution below a minimum radius



rich propane-air flame



heavy hydrocarbon rich flame



Almarcha Quinard (2015)