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Lectures on
Dynamics of Combustion Waves
in Premixed Gases

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Lecture VII
Flame kernels and quasi-isobaric ignition

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Lecture 7: **Flame kernels and quasi-isobaric ignition**

7-1. Introduction

7-2. Zeldovich critical radius

7-3. Critical radius near the flammability limits

7-4. Dynamics of slowly expanding flames

7-5. Quasi-steady dynamic of thin flames

Semi-phenomenological model

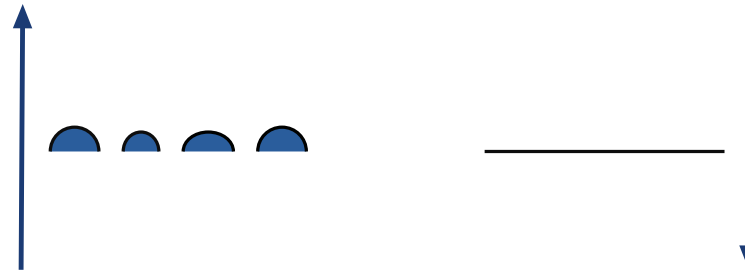
Opened-tip Bunsen flames

VII-I) Introduction

Flammability limits \times **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

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

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

No flow

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

$$R \leq R_f : \quad \theta = \theta_f, \quad \psi = 0; \quad R \rightarrow \infty : \quad \theta = 0, \quad \psi = 1$$

Flame temperature

$$Le \neq 1 \Rightarrow T_f \neq T_b$$

$$D_T \frac{d}{dR} \left(R^2 \frac{d\theta}{dR} \right) + D \frac{d}{dR} \left(R^2 \frac{d\psi}{dR} \right) = 0$$

(conservation energy)

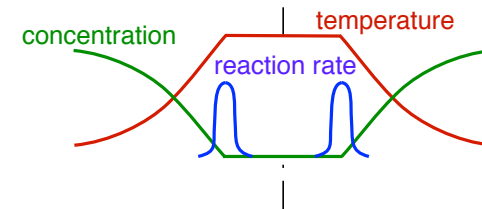
double integration from $R = 0$ to $R = \infty$

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

$$Le \equiv D_T/D$$

$$Le < 1 \Rightarrow T_f > T_b$$

$$Le > 1 \Rightarrow T_f < T_b$$

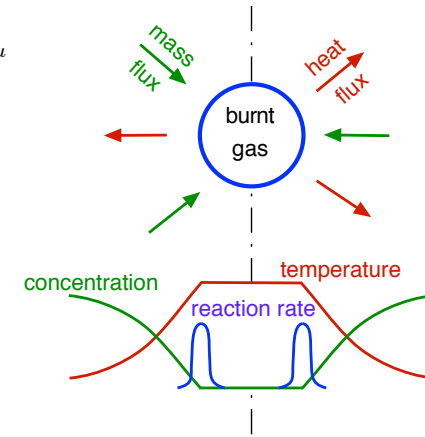


P.Clavin VII Unstable **steady spherical solution** for the one-step model of adiabatic flames

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

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

$$R \leq R_f: \quad \theta = \theta_f, \quad \psi = 0; \quad R \rightarrow \infty: \quad \theta = 0, \quad \psi = 1$$



Asymptotic analysis $\beta \gg 1$

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

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

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

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

Inner variables

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

External zones

$$\frac{d}{dR} \left(R^2 \frac{d\theta}{dR} \right) = 0 \quad R \geq R_f: \quad \theta = \frac{1}{\text{Le}} \frac{R_f}{R}, \quad R = R_f: \quad D_T \frac{d\theta}{dR} = -\frac{1}{\text{Le}} \frac{D_T}{R_f} \quad R < R_f: \quad \theta = \theta_f$$

$$R^2 \frac{d\theta}{dR} = \text{cst.} \quad R = R_f: \quad \theta = \theta_f = 1/\text{Le}$$

Radius of the kernel

matching $\Rightarrow \frac{1}{\text{Le}} \frac{D_T}{R_f} = e^{\frac{\beta}{2}(\frac{1}{\text{Le}}-1)} \sqrt{\text{Le} \frac{D_T}{\tau_b}} \Leftrightarrow \frac{R_f}{d_L} = \text{Le}^{-3/2} e^{\frac{\beta}{2}(1-\frac{1}{\text{Le}})}$

Le < 1 : $R_f \ll d_L$ Le > 1 : $R_f \gg d_L$

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

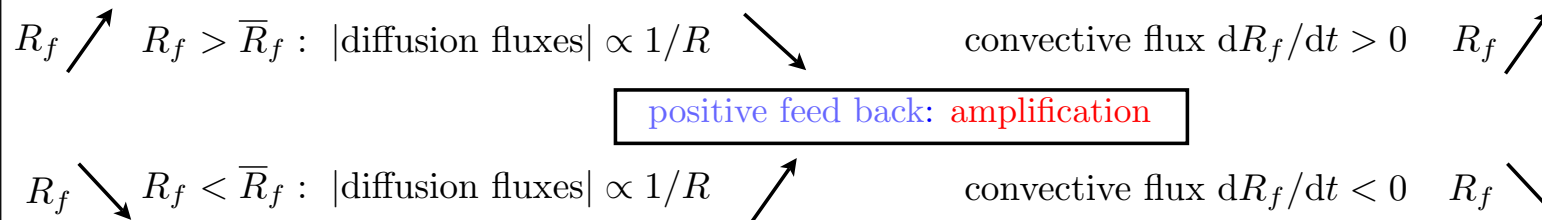
Instability ? (adiabatic condition)

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

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

heat flux towards the preheated zone

convection should be added to restore equilibrium



Quasi-isobaric ignition as a nucleation problem

$$\text{Le} < 1 : \bar{R}_f \ll d_L \quad \text{Le} > 1 : \bar{R}_f \gg d_L$$

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

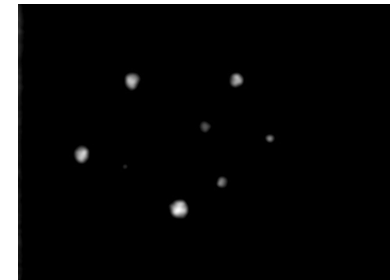
$$D_{C_n H_m} < D_{O_2} \approx D_T, \quad \text{Le} \approx D_{O_2}/D_{C_n H_m} > 1$$

Stability analyses

Stabilization in the presence of heat loss for $\text{Le} < 1$ (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

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

$$R \leq R_f : \quad \theta = \theta_f, \quad \psi = 0; \quad R \rightarrow \infty : \quad \theta = 0, \quad \psi = 1 \quad \begin{cases} T > T^* : \quad \dot{W} = \frac{\rho_b}{\rho_u} \frac{\psi^2}{\tau_{rb}} [e^{-\beta(1-\theta)} - e^{-\varepsilon}] \\ T < T^* : \quad \dot{W} = 0 \end{cases}$$

$$\frac{1}{\tau_{rb}} \equiv \frac{1}{\tau^*} e^{\frac{E}{k_B} \left(\frac{1}{T^*} - \frac{1}{T_b} \right)} = \frac{B_{4f}}{B_{5f}} B_{1f} e^{-\frac{E}{k_B T_b} c_{O_2u}^*}$$

$$\varepsilon \equiv \beta \frac{(T_b - T^*)}{(T_b - T_u)} > 0 \quad \beta \equiv \frac{E}{k_B T_b} \left(1 - \frac{T_u}{T_b} \right) \gg 1 \quad \begin{cases} \varepsilon = O(1) : \text{near to flammability limits } (\varepsilon = 0 : \text{quenching } \dot{W} = 0) \\ \varepsilon \gg 1, e^{-\varepsilon} \approx 0 : \text{far from flammability limits} \end{cases}$$

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

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

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

$$\psi = Le(\theta_f - \theta)$$

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

$$\theta^* \leq \theta < \theta_f$$

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

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

$\theta^* = 1 - \varepsilon/\beta$
 $\dot{w} = 0$

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

$$\left(\frac{d\theta}{d\zeta}\right)^2 = \frac{Le^2}{2} e^{\beta(\theta_f - 1)} \int_{\theta^* = 1 - \varepsilon/\beta}^{\theta_f} \beta^3 (\theta_f - \theta)^2 \left\{ e^{\beta(\theta - \theta_f)} - e^{-\varepsilon - \beta(\theta_f - 1)} \right\} d\theta \quad \text{at the exit of the reaction layer (entrance of the preheated zone)}$$

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

$d\theta = -\beta d\Theta$ measure of the distance from the flammability limit: $\Theta_f \in [0, \infty]$

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

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

Preheated zone and matching

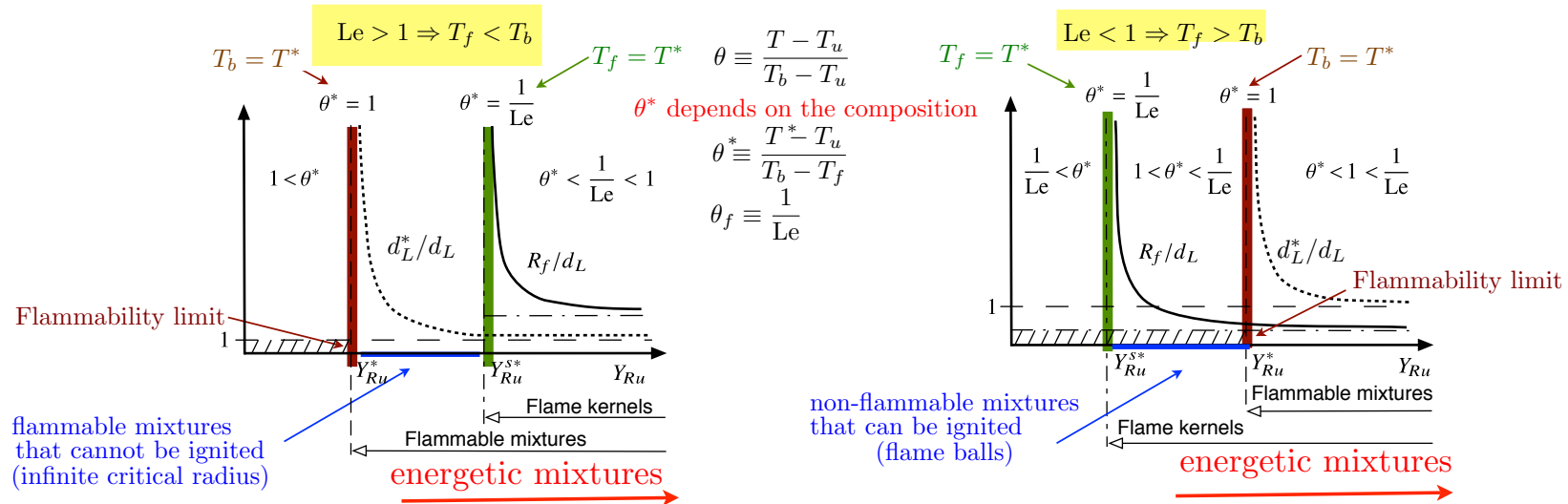
flame temperature of the spherical flame

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

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

$$\beta \rightarrow \infty : \frac{d_L}{R_f} = Le^2 e^{\frac{\beta}{2}(\frac{1}{Le} - 1)} \sqrt{J(\Theta_f)} \quad \begin{cases} T_f \rightarrow T^* \Rightarrow R_f/d_L \rightarrow \infty \\ \Theta_f \rightarrow 0 \end{cases}$$

T_b is determined by the composition of the mixture Y_{Ru} , T_f by Le and T^* by the chemical kinetics



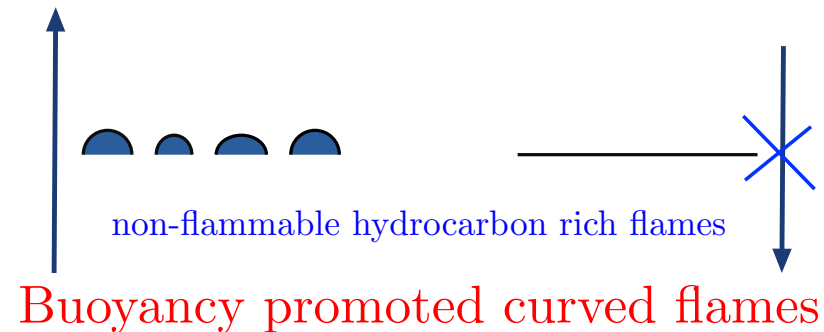
Heavy hydrocarbon lean mixtures

Heavy hydrocarbon rich mixtures

Flammability limits \times 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

simplest explanation:

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

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 $R_f(t)$ $\dot{R}_f \equiv \frac{dR_f}{dt}$

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

quasi-steady state ?

$$t_{relax} \equiv \frac{R^2}{D_T} \ll t_{evol} \equiv \frac{R_f}{\dot{R}_f}$$

not valid in flame kernel at **large radius**

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

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

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

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

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

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

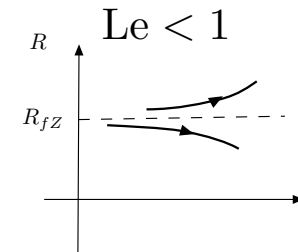
For $\text{Le} < 1$ and near to the Zeldovich radius the slow evolution of flame kernels is governed by the diffusion at large distance

$$\tau \equiv t/t_{ref} \quad \sqrt{t_{ref}} \equiv \frac{\beta(1 - \text{Le}^{1/2})}{\text{Le}} \frac{R_{fZ}}{(4\pi D_T)^{1/2}} \quad r_f \equiv R_f/R_{fZ}$$

Joulin's equation (Joulin 1985)

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

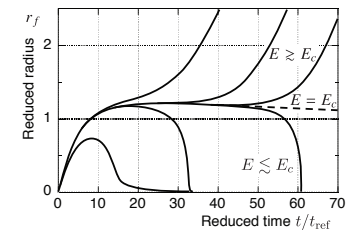
$$\frac{1}{r_f} = \exp \left[- \int_0^\tau \frac{d\tau'}{\tau'^{1/2}} \dot{r}_f(\tau - \tau') \right]$$



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 $\text{Le} < 1$ (Clavin 2016)

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

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

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

$\xrightarrow{\text{moving frame}}$ $\xrightarrow{\Delta \theta}$ $\xrightarrow{\text{also negligible !}}$

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

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

Semi-phenomenological model

$$- \left[\dot{R}_f + 2 \frac{D_T}{R} \right] \frac{d\theta}{dx} - D_T \frac{d^2 \theta}{dx^2} = 0 \quad + \text{asymptotic analysis } \beta \rightarrow \infty$$

$$- \left[\dot{R}_f + 2 \frac{D}{R} \right] \frac{d\psi}{dx} - D \frac{d^2 \psi}{dx^2} = 0 \quad \text{thin reaction zone } \Rightarrow F(\dot{R}_f, R_f) = 0$$

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, Jomaas, Law (2009)

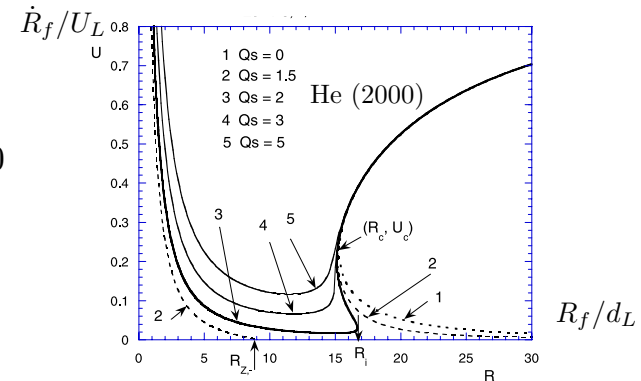


Figure 4. Variation of the flame velocity obtained from equation (12) with different values of the heat power as a function of the flame radius.

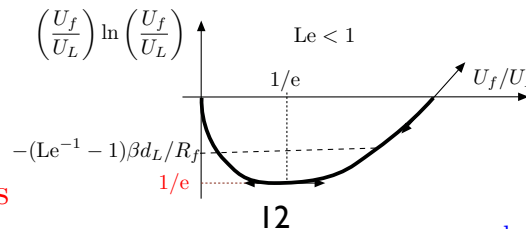
Steady converging flames. Opened-tip Bunsen flames $Le < 1$

Frankel Sivashinsky (1984)

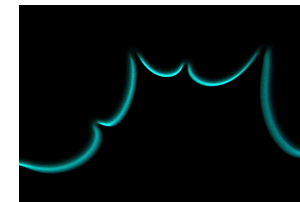
$$U_f = -\dot{R}_f > 0 \quad d_L/\dot{R}_f = O(1/\beta)$$

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

no solution below a minimum radius



rich propane-air flame



heavy hydrocarbon rich flame Almarcha Quinard (2015)