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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**

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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

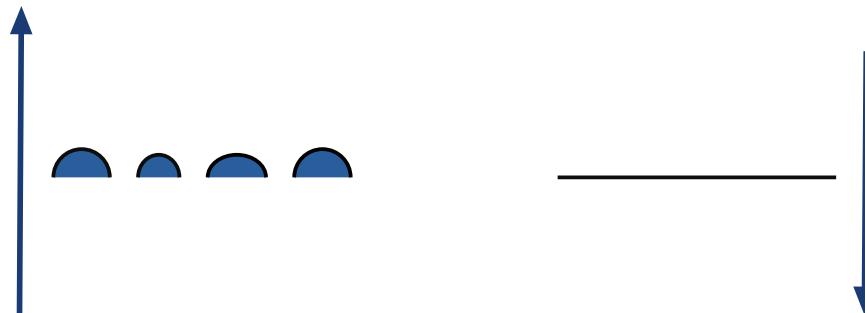
7-4. Dynamics of slowly expanding flames

# 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

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# VII-2) Zeldovich critical radius



Flame kernel for a flame far from the flammability limits

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

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

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

No flow

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

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

Flame temperature

$$\text{Le} \neq 1 \Rightarrow T_f \neq T_b$$

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

(conservation energy)

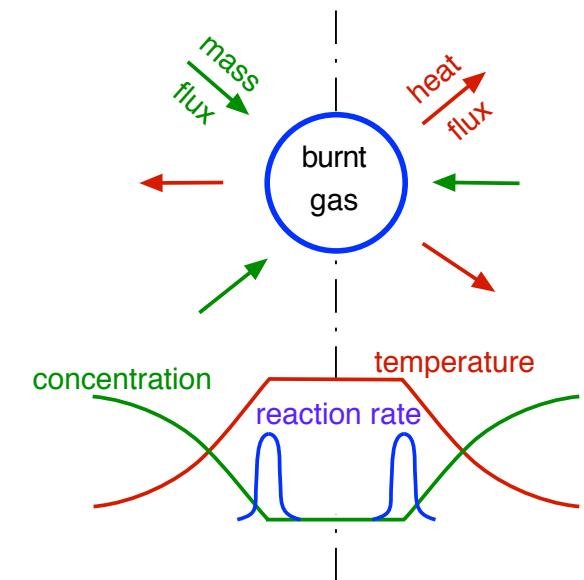
double integration from  $R = 0$  to  $R = \infty$

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

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

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

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



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

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

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

Asymptotic analysis  $\beta \gg 1$

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

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

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

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

Inner variables

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

**External zones**

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

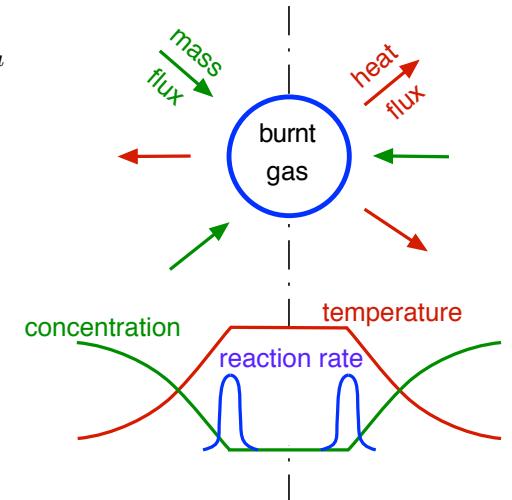
$$R^2 \frac{d\theta}{dR} = \text{cst.} \quad R = R_f : \theta = \theta_f = 1/\text{Le}$$

**Radius of the kernel**

matching

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

$$\text{Le} < 1 : R_f \ll d_L \quad \text{Le} > 1 : R_f \gg d_L$$



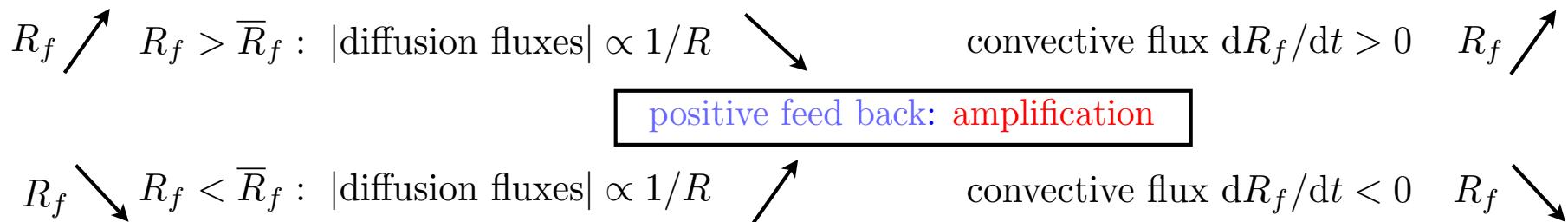
## Instability ? (adiabatic condition)

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

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

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 ( $R_f > d_L$ )**

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

## 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



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# Critical radius near the flammability limits

(He Clavin 1993-94)

chemical-kinetics data:  $T^*$  crossover temperature  $\theta^* \equiv (T^* - T_u)/(T_b - T_u)$   
composition:  $T_b$  associated with the heat release  $T_b - T_u = q/c_p$   
flame temperature of a spherical flame:  $T_f$ ,  $\theta_f \equiv (T_f - T_u)/(T_b - T_u) = 1/\text{Le}$

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

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

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

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

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

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

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

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

$$\begin{aligned} \theta^* \leq \theta < \theta_f \\ \theta^* \equiv \frac{T^* - T_u}{T_b - T_u} = 1 - \frac{\varepsilon}{\beta} \end{aligned}$$

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

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

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

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

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

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

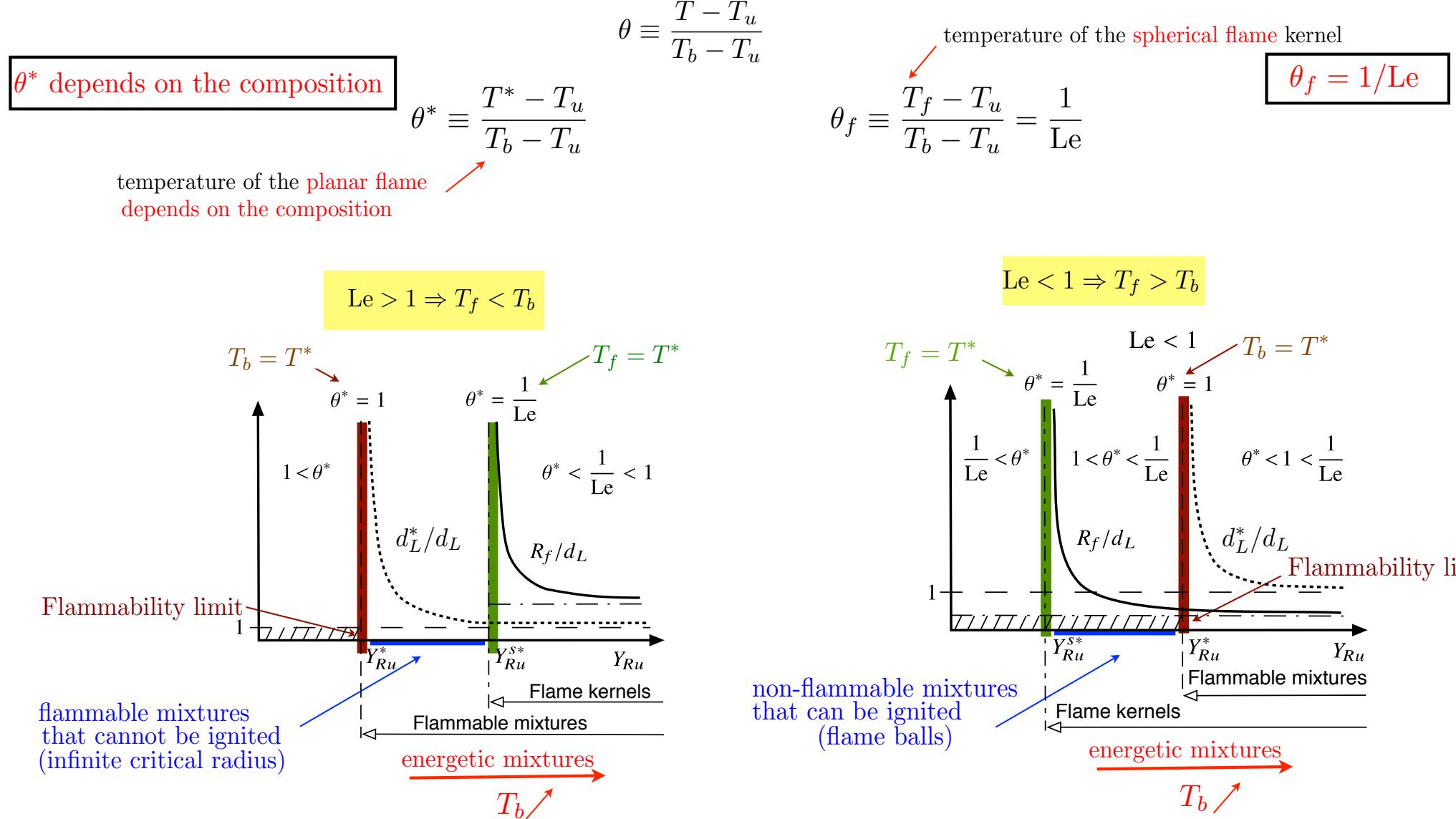
$d_L$  for  $\varepsilon \gg 1$ ,  $Le = 1$ , 2<sup>nd</sup> reaction order

$$\beta \rightarrow \infty : \boxed{\frac{d_L}{R_f} = Le^2 e^{\frac{\beta}{2}(\frac{1}{Le} - 1)} \sqrt{J(\Theta_f)}}$$

$$\begin{array}{l} T_f \rightarrow T^* \Rightarrow R_f/d_L \rightarrow \infty \\ \Theta_f \rightarrow 0 \end{array}$$

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

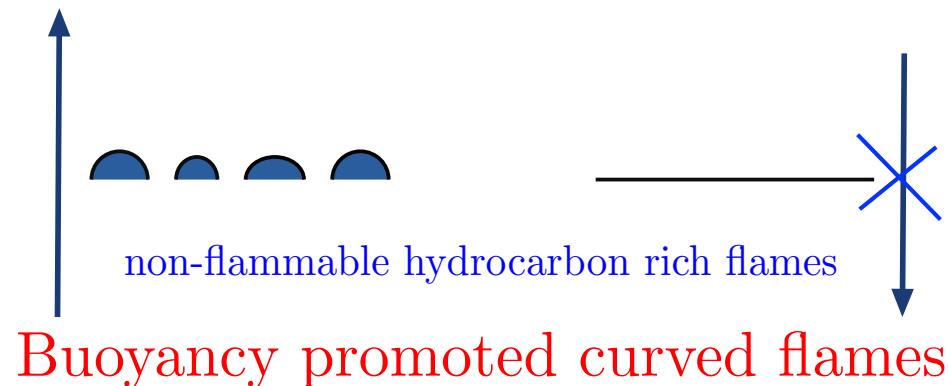
$T^*$  is determined by the chemical kinetics  $Y_{Ru}$



# 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

simplest explanation:  
 Turbulent diffusion coefficients are all equal  $\Leftrightarrow$    
 |  
 12

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# 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 ?       $t_{relax} \equiv \frac{R^2}{D_T} \ll t_{evol} \equiv \frac{R_f}{\dot{R}_f}$        $R \ll \sqrt{D_T t_{evol}}$ , 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     $\partial T / \partial t = D_T \Delta T$     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

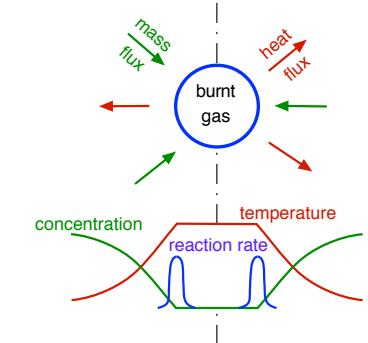
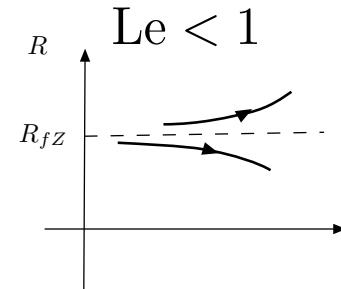
$$\text{Zeldovich radius } R_{fZ}/d_L = e^{\beta(\text{Le}-1)/2\text{Le}}$$

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

Joulin's equation (Joulin 1985)

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

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

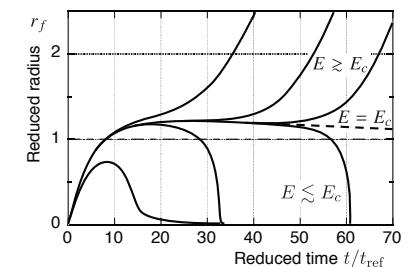


The structure and the dynamics of flame kernels  $\neq$  planar flames even for  $R_f \gg d_L$  ( $\theta \approx \theta_f/R$ )

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)