

Tsinghua-Princeton-CI Summer School
July 14-20, 2019

**Structure and Dynamics
of
Combustion Waves in Premixed Gases**

Paul Clavin
Aix-Marseille Université
ECM & CNRS (IRPHE)

**Lecture V
Thermo-diffusive phenomena**

Copyright 2019 by Paul Clavin
This material is not to be sold, reproduced or distributed
without permission of the owner, Paul Clavin

Lecture 5: Thermo-diffusive phenomena

5-1. Flame stretch and Markstein numbers

Passive interfaces

One-step flame model

The second Markstein number

5-2. Thermo-diffusive instabilities

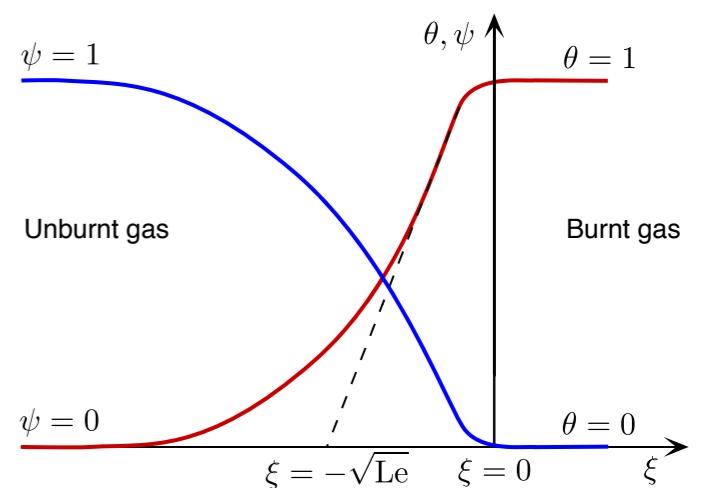
Planar flames for $\text{Le} \neq 1$

Jump conditions across the reaction layer

Linear equations and linear analysis

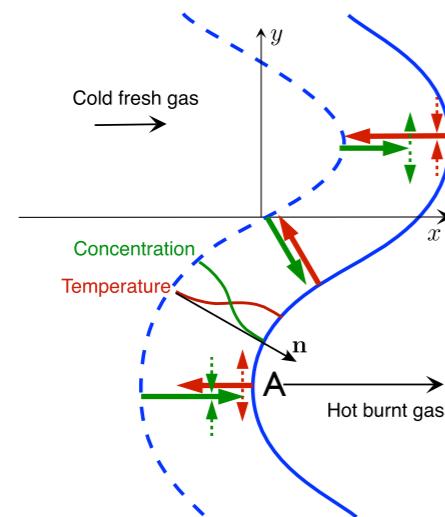
Cellular instability ($\text{Le} < 1$)

Oscillatory instability ($\text{Le} > 1$)

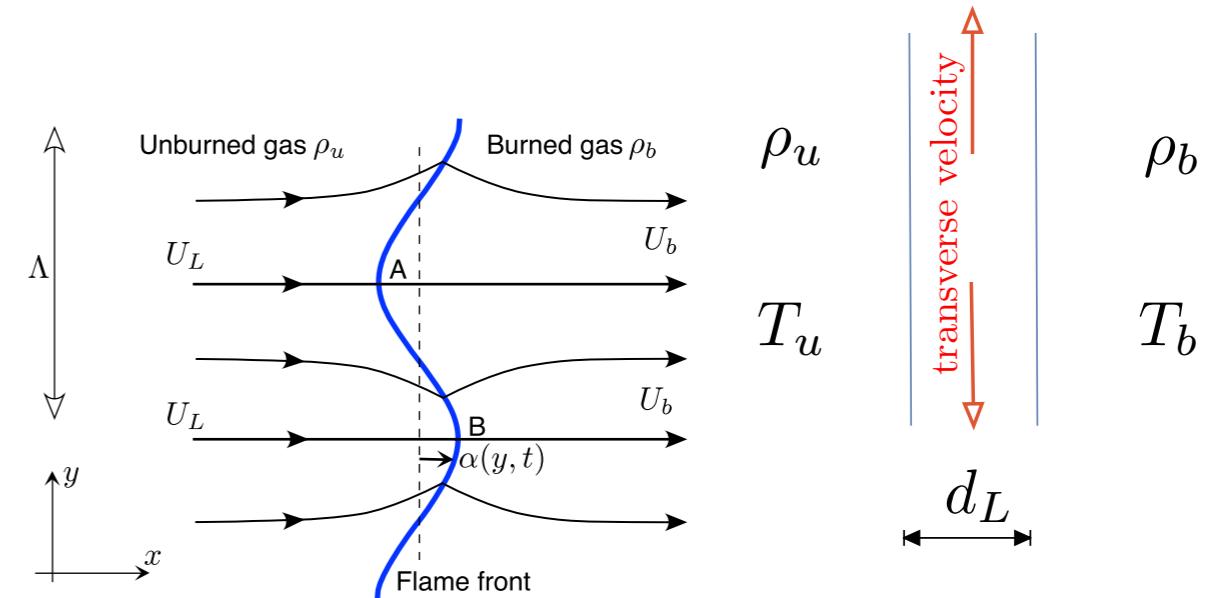
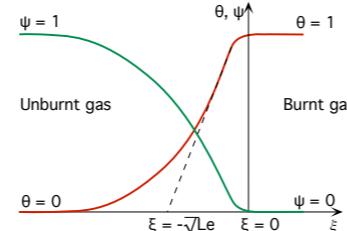


V-I) Flame stretch and Markstein numbers

Two mechanisms modify the inner flame structure



transverse diffusion



transverse convection

One-step model



A single scalar: the Markstein number \mathcal{M}

$$(U_n^- - U_L)/U_L = -\mathcal{M}(\tau_L/\tau_s)$$

U_n^- normal flame velocity in the fresh mixture

$1/\tau_s$ rate of stretch of flame surface

$$U_n^- = u_n^- - \mathcal{D}_f, \quad u_n^- \equiv \mathbf{n}_f \cdot \mathbf{u}_f^-$$

Stretch rate, strain and curvature of a flame Passive interface

$$\text{element of surface area } \delta^2 s \quad \frac{1}{\tau_s} = \frac{1}{\delta^2 s} \frac{d\delta^2 s}{dt} \quad d\mathbf{r}_f/dt = \mathbf{u}^e(\mathbf{r}_f)$$

$$\text{element of volume} \quad \delta^3 r = \delta^2 s \delta \zeta \quad \frac{1}{\delta^3 r} \frac{d}{dt} \delta^3 r = \nabla \cdot \mathbf{u}^e|_f$$

coordinate normal to the front ζ continuity

$$\frac{1}{\delta^3 r} \frac{d}{dt} \delta^3 r = \frac{1}{\delta^2 s} \frac{d}{dt} \delta^2 s + \frac{1}{\delta \zeta} \frac{d}{dt} \delta \zeta$$

$$d\delta\zeta/dt = \mathbf{n}_f \cdot [\mathbf{u}^e(\mathbf{r}_f + \delta\zeta \mathbf{n}_f) - \mathbf{u}^e(\mathbf{r}_f)]$$

first order correction in $d_L/L \ll 1$ $\mathbf{u}^e(\mathbf{r}_f + \delta\zeta \mathbf{n}_f) \approx \mathbf{u}^e(\mathbf{r}_f) + \delta\zeta \mathbf{n}_f \cdot \nabla \mathbf{u}^e$

$$\frac{1}{\delta \zeta} \frac{d}{dt} \delta \zeta = \mathbf{n}_f \cdot \nabla \mathbf{u}^e \cdot \mathbf{n}_f$$

$$\frac{1}{\tau_s} = \frac{1}{\delta^2 s} \frac{d}{dt} \delta^2 s = \nabla \cdot \mathbf{u}^e|_f - \mathbf{n}_f \cdot \nabla \mathbf{u}^e|_f \cdot \mathbf{n}_f.$$

Flame (first order correction) $d_L/\Lambda \ll 1$

$$\mathbf{n}_f \cdot \mathbf{n}_f = 1$$

$$\mathbf{u}^e(\mathbf{r}_f) = \mathbf{u}_f^- - U_L \mathbf{n}_f$$

$$\mathbf{n}_f \cdot \nabla \mathbf{n} \Big|_f \cdot \mathbf{n}_f = 0$$

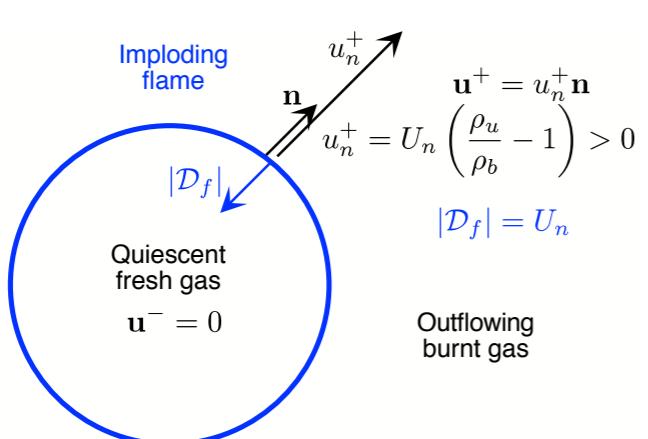
$$1/\tau_s = -U_L \nabla \cdot \mathbf{n}_f + \nabla \cdot \mathbf{u}^-|_f - \mathbf{n}_f \cdot \nabla \mathbf{u}^-|_f \cdot \mathbf{n}_f$$

Flame (first order correction) $d_L/\Lambda \ll 1$

$$1/\tau_s = -U_L \nabla \cdot \mathbf{n}_f + \nabla \cdot \mathbf{u}^-|_f - \mathbf{n}_f \cdot \nabla \mathbf{u}^-|_f \cdot \mathbf{n}_f$$

incompressibility

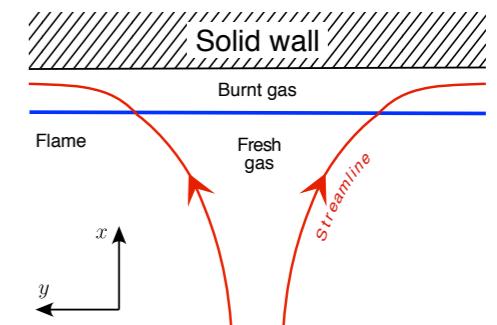
differential geometry $-\nabla \cdot \mathbf{n}_f = 1/R \equiv (1/R_1 + 1/R_2)$



$$1/\tau_s = U_L/R - \mathbf{n}_f \cdot \nabla \mathbf{u}^-|_f \cdot \mathbf{n}_f$$

front curvature

strain rate



study of structure of the one-step flame model $R \rightarrow P + Q$

Clavin, Williams 1982

Clavin, Garcia 1983

$$(U_n^- - U_L)/U_L = -\mathcal{M}(\tau_L/\tau_s)$$

reduced activation energy β Lewis number $\text{Le} = D_T/D$

$$v_b \equiv \rho_u/\rho_b > 1$$

$$\theta \equiv (T - T_u)/(T_b - T_u)$$

$$l \equiv \beta(\text{Le} - 1)$$

gas expansion \Rightarrow hydrodynamicsheat conductivity $\lambda(\theta)$
kinetics + diffusion

$$\mathcal{M} = \frac{v_b}{v_b - 1} \mathcal{J} + \frac{l}{2} \frac{\mathcal{D}}{(v_b - 1)}$$

lean hydrocarbon air mixtures $\mathcal{M} \approx 1 - 4$

$$\mathcal{J} = \int_0^1 \frac{(v_b - 1)\lambda(\theta)}{1 + (v_b - 1)\theta} d\theta, \quad \mathcal{D} = - \int_0^1 \frac{(v_b - 1)\lambda(\theta) \ln \theta}{1 + (v_b - 1)\theta} d\theta,$$

Clavin Garcia 1983

The second Markstein number

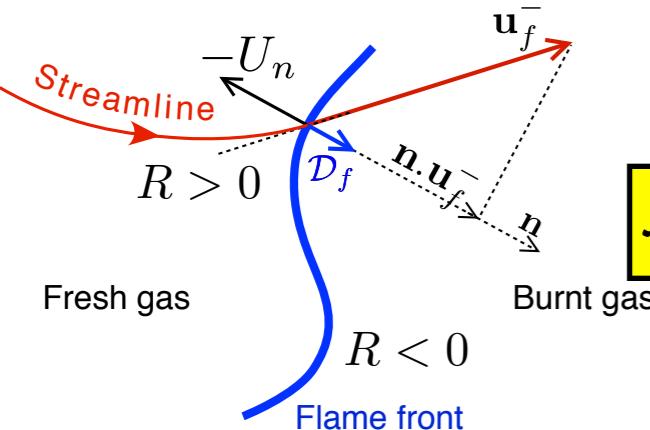
multiple-step flame model

$$\mathcal{M}_{fc} \neq \mathcal{M}_{sr}$$

Clavin Grana-Otero 2011

$$(U_n^- - U_L)/U_L = -\mathcal{M}_{fc}(d_L/R) + \mathcal{M}_{sr}(\tau_L \mathbf{n}_f \cdot \nabla \mathbf{u}^-|_f \cdot \mathbf{n}_f)$$

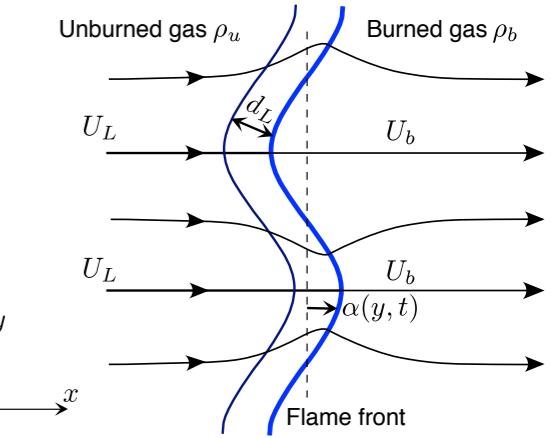
front curvature flow strain rate



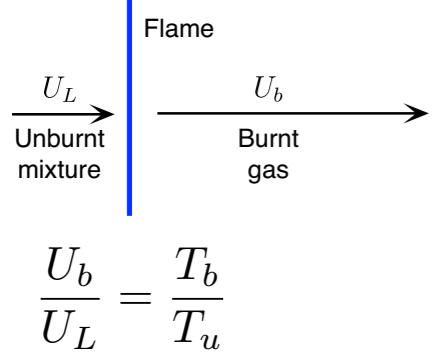
difficulty with the finite thickness:

$$\mathcal{M}_{sr} \text{ varies with the position inside the flame structure}$$

$$\mathcal{M}_{sr}(\tau_L \mathbf{n}_f \cdot \nabla \mathbf{u}^-|_f \cdot \mathbf{n}_f) = \text{cst.}$$



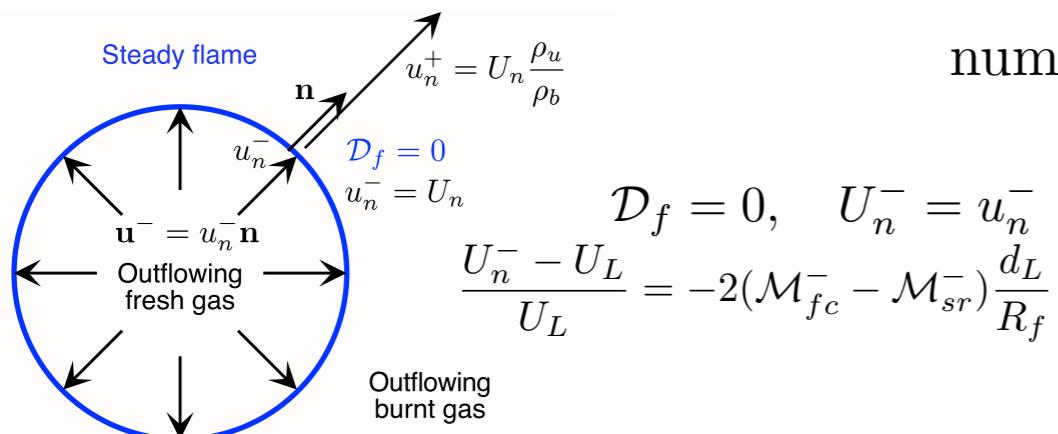
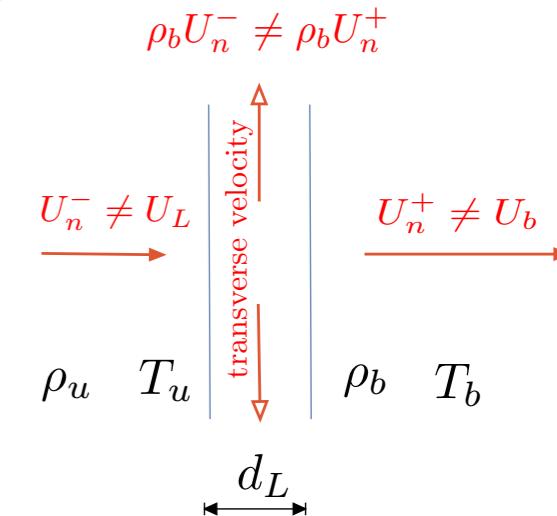
Markstein numbers in the burned gas



$$U_n^+ \equiv u_n^+ - \mathcal{D}_f \quad u_n^+ \equiv \mathbf{n}_f \cdot \mathbf{u}^+(\mathbf{r}_f)$$

$$\frac{(U_n^+ - U_b)}{U_b} = -\mathcal{M}_{fc}^+ \frac{d_L}{R} + \mathcal{M}_{sr}^+ \tau_L \mathbf{n}_f \cdot \nabla \mathbf{u}^+|_f \cdot \mathbf{n}_f$$

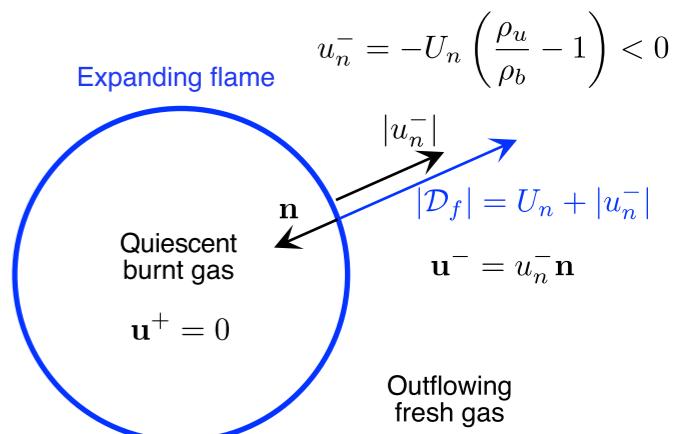
$$\mathcal{M}_{fc}^+ \neq \mathcal{M}_{fc}^- \quad \mathcal{M}_{sr}^+ \neq \mathcal{M}_{sr}^-$$



numerical and experimental data

$$u_n^+ = 0 \quad U_n^+ = -\mathcal{D}_f$$

$$\frac{U_n^+ - U_b}{U_b} = -2\mathcal{M}_{fc}^+ \frac{d_L}{R_f}$$



V-2) Thermo-diffusive instabilities of planar flames

Sivashinsky 1977 Joulin Clavin 1979

instability mechanism \neq hydrodynamic instability

~~$\rho T \neq \rho_o T_o$~~ $\rho c_p D\bar{T}/Dt = \nabla \cdot (\lambda \nabla T) + \sum_j Q^{(j)} \dot{W}^{(j)}(T, \dots Y_k \dots)$ ~~+ fluid mechanics~~

equations $\rho D\bar{Y}_i/Dt = \nabla \cdot (\rho D_i \nabla Y_i) + \sum_j \vartheta_i^{(j)} m_i \dot{W}^{(j)}(T, \dots Y_k \dots),$

Thermo-diffusive flame model for a one-step kinetics ($\beta \gg 1$)

$$\theta \equiv \frac{T - T_u}{T_b - T_u} \in [0, 1] \quad \psi \equiv Y/Y_u \quad \beta \equiv \frac{E}{k_B T_b} \left(1 - \frac{T_u}{T_b}\right) \quad \frac{1}{\tau_{rb}} \equiv \frac{e^{-E/k_B T_b}}{\tau_{coll}}$$

$\rho = \text{cst.}$

$\frac{\partial \theta}{\partial t} - D_T \Delta \theta = \frac{\psi}{\tau_{rb}} e^{-\beta(1-\theta)}$	$\frac{\partial \psi}{\partial t} - D \Delta \psi = -\frac{\psi}{\tau_{rb}} e^{-\beta(1-\theta)}$
$x = -\infty : \theta = 0, \psi = 1$	$x = +\infty : \theta = 1, \psi = 0$

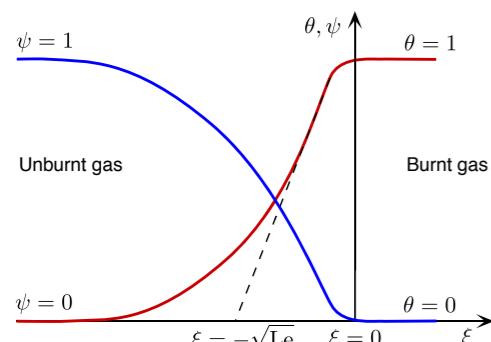
Planar flame for $\text{Le} \equiv D_T/D \neq 1$

$$\xi \equiv \frac{x}{d_L(\text{Le} = 1)} \quad \mu \equiv \frac{U_L}{U_L(\text{Le} = 1)}$$

?

$$\mu \frac{d\theta}{d\xi} - \frac{d^2\theta}{d\xi^2} = \frac{\beta^2}{2} \psi e^{-\beta(1-\theta)} \quad \mu \frac{d\psi}{d\xi} - \frac{1}{\text{Le}} \frac{d^2\psi}{d\xi^2} = -\frac{\beta^2}{2} \psi e^{-\beta(1-\theta)}$$

reaction layer



$$-\frac{d^2\theta}{d\xi^2} \approx \frac{\beta^2}{2} \psi e^{-\beta(1-\theta)}$$

matching

$$\frac{d^2\theta}{d\xi^2} + \frac{1}{\text{Le}} \frac{d^2\psi}{d\xi^2} = 0$$

$\mu = \sqrt{\text{Le}}$

(first order reaction rate)

Flame temperature of curved flame for $\text{Le} \neq 1$

$$\begin{aligned} \text{Le} \neq 1 &\Rightarrow \theta_f \neq 1 \\ \beta \gg 1 \quad \text{Le} - 1 = O(1/\beta) &\Rightarrow (\theta_f - 1) = O(1/\beta) \end{aligned}$$

the thin reaction layer of curved flame is quasi-planar

$$-\frac{d^2\theta}{d\xi^2} \approx \frac{\beta^2}{2} \psi e^{-\beta(1-\theta)}$$

$$\theta = \theta_f - \Theta_1/\beta + ..$$

$$\beta(\theta_f - 1) = O(1)$$

$$\frac{d^2\theta}{d\xi^2} + \frac{1}{\text{Le}} \frac{d^2\psi}{d\xi^2} = 0$$

$$\psi = -\Psi_1/\beta + ..$$

$$d\theta/d\xi|_{0+} = O(1/\beta)$$

$$\xi = \text{non-dimensional normal coordinate} \quad \xi \equiv \frac{x}{d_L(\text{Le} = 1)}$$

$$\Theta_1 = \Psi_1/\text{Le} \quad \frac{1}{\beta^2} \frac{d^2\Theta_1}{d\xi^2} = \frac{1}{2} e^{-\beta(1-\theta_f)} \Psi_1 e^{-\Theta_1}$$

integration and matching

$$d\theta/d\xi|_{\xi=0-} \approx \text{Le}^{1/2} e^{-\beta(1-\theta_f)/2}$$

jump conditions across the reaction layer

$$d\theta/d\xi|_{\xi=0-} = e^{-\beta(1-\theta_f)/2}$$

valid at the leading order

$$\left[\frac{d\theta}{d\xi} + \frac{1}{\text{Le}} \frac{d\psi}{d\xi} \right]_{0-}^{0+} = 0$$

valid up to 1st order

θ_f ?

Joulin Clavin 1979

Preheated zone

non-dimensional equations in the reference frame attached to the unperturbed flame

$$\xi \equiv x/d_L, \quad \eta = y/d_L, \quad \tau \equiv t/\tau_L$$

$$\frac{\partial\theta}{\partial\tau} + \frac{\partial\theta}{\partial\xi} - \Delta\theta = 0, \quad \frac{\partial\psi}{\partial\tau} + \frac{\partial\psi}{\partial\xi} - \frac{1}{\text{Le}} \Delta\psi = 0$$

boundary conditions: jump conditions and

$$\xi \rightarrow \infty : \theta = 0, \psi = 1, \quad \xi = \infty : \theta = 1, \psi = 0.$$

Linear equations

frame of reference attached to the reaction sheet (ζ, η, τ)

$$\zeta \equiv \xi - a(\eta, \tau) \quad \boxed{\zeta = 0 : \text{reaction sheet}}$$

$$\frac{\partial}{\partial \xi} = \frac{\partial}{\partial \zeta}, \quad \frac{\partial}{\partial \eta} \rightarrow \frac{\partial}{\partial \eta} - \frac{\partial a}{\partial \eta} \frac{\partial}{\partial \zeta}, \quad \frac{\partial}{\partial \tau} \rightarrow \frac{\partial}{\partial \tau} - \frac{\partial a}{\partial \tau} \frac{\partial}{\partial \zeta}$$

linearization

$$\theta = \bar{\theta}(\zeta) + \delta\theta, \quad \theta_f = 1 + \delta\theta_f, \quad \psi = \bar{\psi}(\zeta) + \delta\psi$$

external equations

$$\left[\frac{\partial}{\partial \tau} + \frac{\partial}{\partial \zeta} - \left(\frac{\partial^2}{\partial \zeta^2} + \frac{\partial^2}{\partial \eta^2} \right) \right] \delta\theta = \left(\frac{\partial a}{\partial \tau} - \frac{\partial^2 a}{\partial \eta^2} \right) \frac{d\bar{\theta}}{d\zeta}$$

$$\left[\frac{\partial}{\partial \tau} + \frac{\partial}{\partial \zeta} - \frac{1}{Le} \left(\frac{\partial^2}{\partial \zeta^2} + \frac{\partial^2}{\partial \eta^2} \right) \right] \delta\psi = \left(\frac{\partial a}{\partial \tau} - \frac{1}{Le} \frac{\partial^2 a}{\partial \eta^2} \right) \frac{d\bar{\psi}}{d\zeta}$$

harmonic analysis
(normal modes)

$$\zeta \equiv \sigma\tau_L, \quad \kappa \equiv kd_L$$

$$a(\eta, \tau) = \hat{a}e^{(i\kappa\eta + \zeta\tau)}, \quad \delta\theta_f(\eta, \tau) = \tilde{\theta}_f \hat{a}e^{(i\kappa\eta + \zeta\tau)}$$

$$\delta\psi = \tilde{\psi}(\zeta) \hat{a}e^{(i\kappa\eta + \zeta\tau)} \quad \delta\theta = \tilde{\theta}(\zeta) \hat{a}e^{(i\kappa\eta + \zeta\tau)}$$

$\zeta ?$

reduced linear growth rate

$$\left[\frac{d}{d\zeta} - \frac{d^2}{d\zeta^2} \right] \tilde{\theta}(\zeta) + (\zeta + \kappa^2) \tilde{\theta}(\zeta) = (\zeta + \kappa^2) \frac{d\bar{\theta}}{d\zeta}$$

$$\left[\frac{d}{d\zeta} - \frac{1}{Le} \frac{d^2}{d\zeta^2} \right] \tilde{\psi}(\zeta) + \left(\zeta + \frac{\kappa^2}{Le} \right) \tilde{\psi}(\zeta) = \left(\zeta + \frac{\kappa^2}{Le} \right) \frac{d\bar{\psi}}{d\zeta}$$

boundary conditions: jump conditions and $\zeta = -\infty : \tilde{\theta} = 0, \tilde{\psi} = 0, \quad \zeta = +\infty : \tilde{\theta} = 0, \tilde{\psi} = 0$

Analysis

external equations

$$\left[\frac{d}{d\zeta} - \frac{d^2}{d\zeta^2} \right] \tilde{\theta}(\zeta) + (\varsigma + \kappa^2) \tilde{\theta}(\zeta) = (\varsigma + \kappa^2) \frac{d\bar{\theta}}{d\zeta}$$

$$\left[\frac{d}{d\zeta} - \frac{1}{Le} \frac{d^2}{d\zeta^2} \right] \tilde{\psi}(\zeta) + \left(\varsigma + \frac{\kappa^2}{Le} \right) \tilde{\psi}(\zeta) = \left(\varsigma + \frac{\kappa^2}{Le} \right) \frac{d\bar{\psi}}{d\zeta}$$

κ given
 ς and θ_f ?

temperature in the external zones

particular solutions

$$\begin{aligned} \tilde{\theta} &= d\bar{\theta}/d\zeta & \tilde{\psi} &= d\bar{\psi}/d\zeta \\ \bar{\theta}^- &= e^\zeta & \bar{\theta}^+ &= 1 & \bar{\psi}^- &= 1 - e^{Le\zeta} & \bar{\psi}^+ &= 0 \end{aligned}$$

boundary conditions

$$\begin{aligned} \zeta \rightarrow \pm\infty : \quad \tilde{\theta} &= 0 \\ \theta(\zeta = 0) = \theta_f & \quad \tilde{\theta}^\pm = d\bar{\theta}^\pm/d\zeta + \left(\tilde{\theta}_f - \left. d\bar{\theta}^\pm/d\zeta \right|_{\zeta=0} \right) e^{r^\pm \zeta} \\ r^2 - r - (\varsigma + \kappa^2) &= 0 \quad r^\pm = \frac{1}{2} \left[1 \mp \sqrt{1 + 4(\varsigma + \kappa^2)} \right] \end{aligned}$$

general solution to
the homogeneous equation

$$\begin{aligned} \zeta \rightarrow -\infty : \quad \tilde{\psi} &= 0 \\ \psi(\zeta = 0) &= 0 \end{aligned}$$

mass fraction in the preheated zone zone

$$\tilde{\psi}^- = d\bar{\psi}^-/d\zeta - \left(\left. d\bar{\psi}^-/d\zeta \right|_{\zeta=0} \right) e^{s^- \zeta}$$

$$\frac{1}{Le} s^2 - s - \left(\zeta + \frac{\kappa^2}{Le} \right) = 0 \quad s^- = \frac{Le}{2} \left[1 + \sqrt{1 + \frac{4}{Le} \left(\zeta + \frac{\kappa^2}{Le} \right)} \right]$$

jump conditions

$d\theta/d\xi _{\xi=0-} = e^{-\beta(1-\theta_f)/2}$	$\left[\frac{d\theta}{d\xi} + \frac{1}{Le} \frac{d\psi}{d\xi} \right]_{0-}^{0+} = 0$	ζ and θ_f ?
valid at the leading order	valid up to 1 st order	

asymptotic analysis $\beta \gg 1$: $Le = 1 + l/\beta$, $l \equiv \beta(Le - 1) = O(1)$

$$\beta(1 - \theta_f) = O(1) \quad \beta\tilde{\theta}_f = O(1)$$

2nd condition $\tilde{\theta}_f(r^+ - r^-) = (s^- - r^-) + (1 - Le)$ $(r^+ - r^-) = -\sqrt{1 + 4(\zeta + \kappa^2)}$
 $Le \rightarrow 1$: $s^- - r^- \rightarrow 0$

to leading order in small values of $(Le-1) = O(1/\beta)$

$$\tilde{\theta}_f \approx \frac{(Le - 1)}{2} \left[\frac{1}{\sqrt{1 + 4(\zeta + \kappa^2)}} - 1 + \frac{2\zeta + 4\kappa^2}{1 + 4(\zeta + \kappa^2)} \right]$$

linearized 1st condition $d\tilde{\theta}^-/d\zeta|_{\zeta=0} = \beta\tilde{\theta}_f/2$ $1 - r^- = r^+ = \beta\tilde{\theta}_f/2$
valid to leading order using $\tilde{\theta}_f = O(1/\beta)$

$$\beta\tilde{\theta}_f = 1 + \sqrt{1 + 4(\zeta + \kappa^2)}$$

dispersion relation (ζ, κ)

$$-\frac{l}{2} \left[1 - \sqrt{1 + 4(\zeta + \kappa^2)} + 2\zeta \right] = \left[1 - \sqrt{1 + 4(\zeta + \kappa^2)} \right] [1 + 4(\zeta + \kappa^2)]$$

$$-\frac{l}{2} \left[1 - \sqrt{1 + 4(\varsigma + \kappa^2)} + 2\varsigma \right] = \left[1 - \sqrt{1 + 4(\varsigma + \kappa^2)} \right] [1 + 4(\varsigma + \kappa^2)]$$

Cellular instability for $\text{Le} \equiv D_T/D < 1$

$$\kappa = 0 : \varsigma(\kappa) = 0$$

Weakly curved limit. Small wavenumber expansion $\kappa \equiv kd_L \ll 1$ $|\varsigma| \equiv |\sigma|\tau_L \ll 1$

$$\tilde{\theta}_f = (\text{Le} - 1)\kappa^2$$

$$\varsigma = -(l + 2)\kappa^2/2$$

$l \equiv \beta(\text{Le} - 1) > -2$: $\sigma < 0$ stable

$l \equiv \beta(\text{Le} - 1) < -2$: $\sigma > 0$

unstable

$$\mathcal{M} < 0$$

$$\frac{\partial \alpha}{\partial t} \propto -D_T \frac{\partial^2 \alpha}{\partial y^2}$$

$$\frac{\partial \alpha}{\partial t} = \left[\frac{\beta(\text{Le} - 1) + 2}{2} \right] D_T \left(\frac{\partial^2 \alpha}{\partial y^2} + \frac{\partial^2 \alpha}{\partial z^2} \right) = [\beta(\text{Le} - 1) + 2] \frac{D_T}{R},$$

$$2/R = 1/R_1 + 1/R_2$$

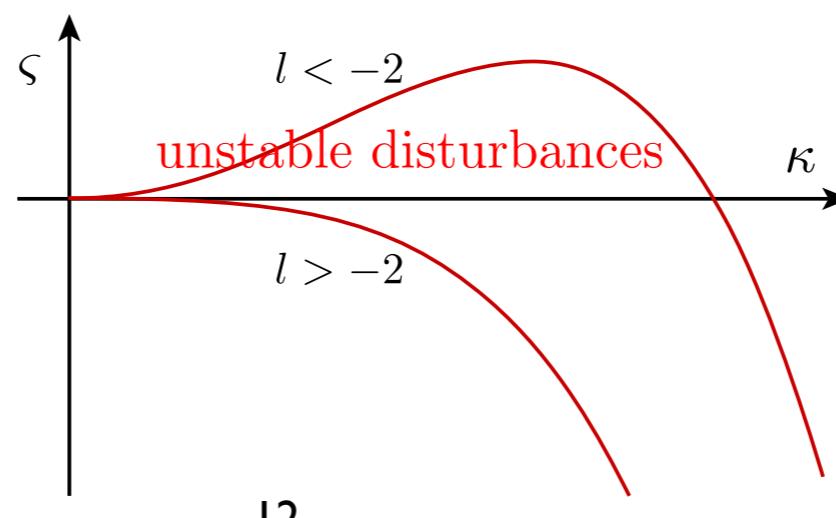
$$\mathcal{M} = \beta(\text{Le} - 1) + 2 \quad \times$$

$$\mathcal{M} = \frac{v_b}{v_b - 1} \mathcal{J} + \frac{l}{2} \frac{\mathcal{D}}{(v_b - 1)}$$

$$\mathcal{J} = \int_0^1 \frac{(v_b - 1)\lambda(\theta)}{1 + (v_b - 1)\theta} d\theta, \quad \mathcal{D} = - \int_0^1 \frac{(v_b - 1)\lambda(\theta) \ln \theta}{1 + (v_b - 1)\theta} d\theta,$$

$$\varsigma = -(l + 2)\kappa^2/2 - 8\kappa^4$$

Turing type of instability



Zeldovich



Turing

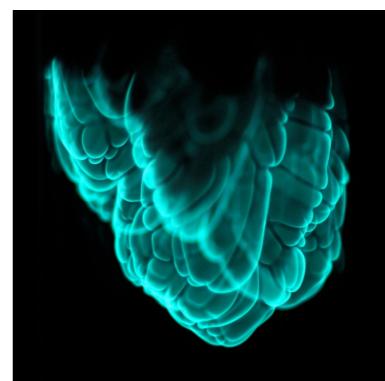
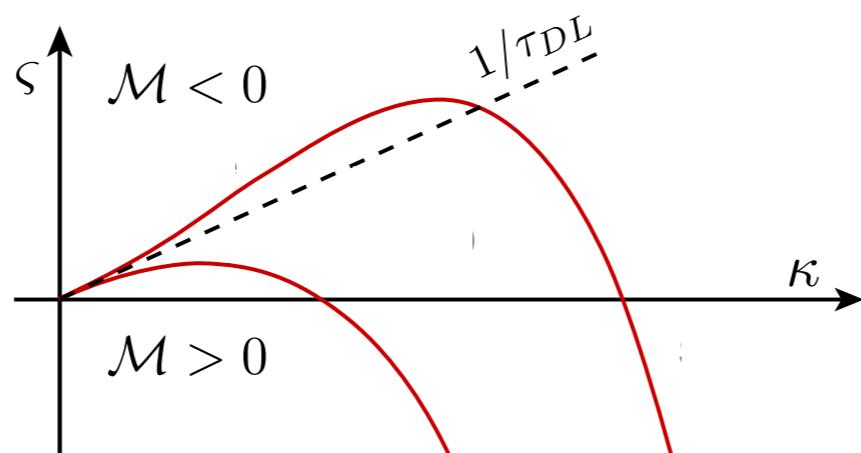
Hydrodynamics + diffusion



Propane lean flame
 $\mathcal{M} > 0$

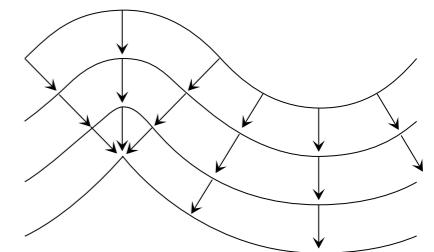
hydrodynamic instability only

Sivashinsky eq. 1977 $\frac{\partial \phi}{\partial \tau} - \mathcal{H}(\phi) - \Delta \phi + \frac{1}{2} |\nabla \phi|^2 = 0$
nonlinear equation



Propane rich flame
 $\mathcal{M} < 0$

hydrodynamic + cellular instabilities
shorter wavelengths are unstable

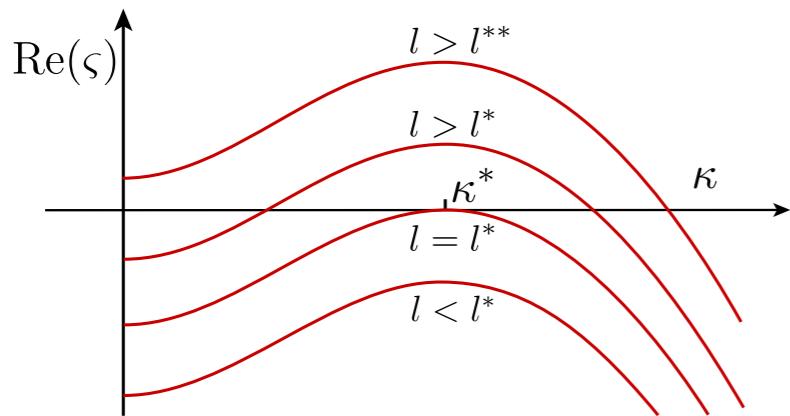


Oscillatory instability $\text{Le} \equiv D_T/D > 1$

$$\text{Im}(\zeta) \neq 0$$

$$l \equiv \beta(\text{Le} - 1) = l^* : \text{Re}(\zeta) = 0, \kappa^* \neq 0$$

Poincaré-Andronov bifurcation $l^* \approx 10$



$l^{**} \approx 11$: planar pulsation. OK for solid combustion

