

Tsinghua-Princeton-CI Summer School
July 19-25, 2016

Lectures on
Dynamics of Combustion Waves
in Premixed Gases

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

Lecture V
Thermo-diffusive phenomena

Copyright 2015 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

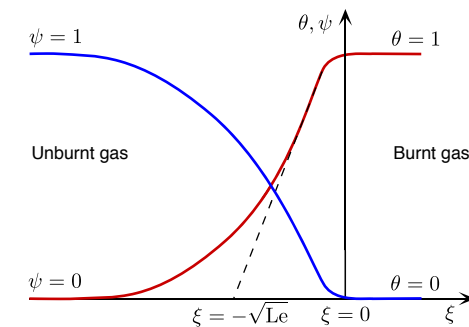
Planar flames for $Le \neq 1$

Jump conditions across the reaction layer

Linear equations and linear analysis

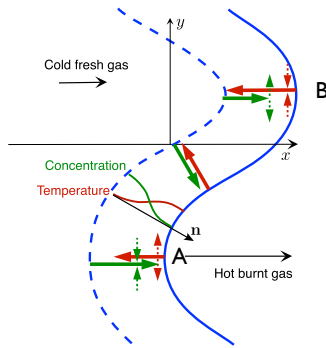
Cellular instability ($Le < 1$)

Oscillatory instability ($Le > 1$)

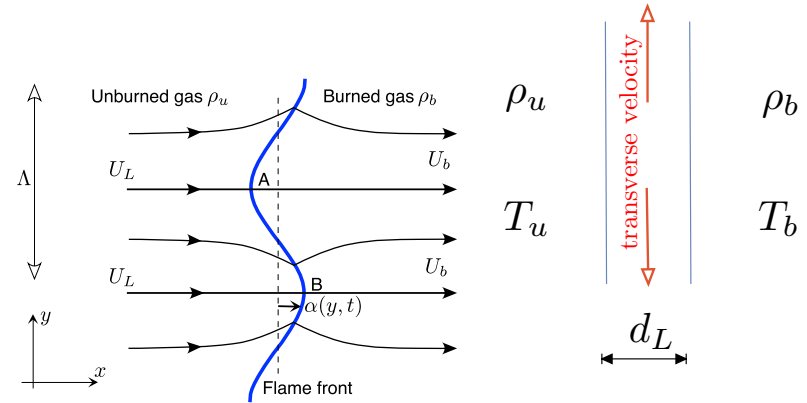
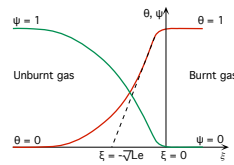


V-I) Flame stretch and Markstein numbers

Two mechanisms modify the inner flame structure



transverse diffusion



transverse convection



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

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

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

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

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

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

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

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

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

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

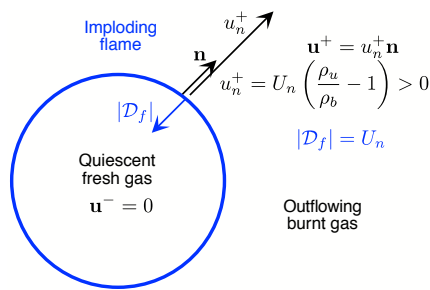
$$1/\tau_s = -U_L \nabla \cdot \mathbf{n}_f + \nabla \cdot \mathbf{u}^-|_f - \mathbf{n}_f \cdot \nabla \mathbf{u}^-|_f \cdot \mathbf{n}_f$$

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

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

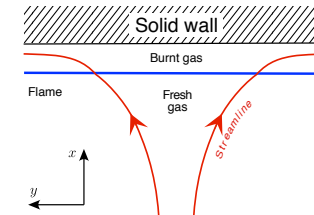
incompressibility

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 $Le = D_T/D$

$v_b \equiv \rho_u/\rho_b > 1$ $\theta \equiv (T - T_u)/(T_b - T_u)$ $l \equiv \beta(Le - 1)$ heat conductivity $\lambda(\theta)$

gas expansion \Rightarrow hydrodynamics 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 $\mathcal{M} \approx 1 - 4$

$$\mathcal{J} = \int_0^1 \frac{(v_b - 1)\lambda(\theta)}{1 + (v_b - 1)\theta} d\theta, \quad \mathcal{D} = - \int_0^1 \frac{(v_b - 1)\lambda(\theta) \ln \theta}{1 + (v_b - 1)\theta} d\theta, \quad \text{Clavin Garcia 1983}$$

The second Markstein number

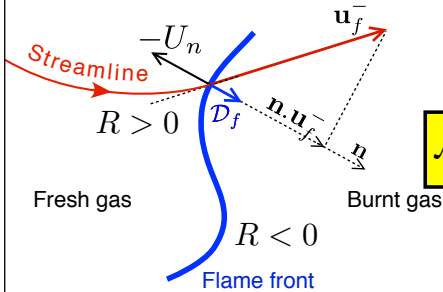
multiple-step flame model

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

Clavin Grana-Otero 2011

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

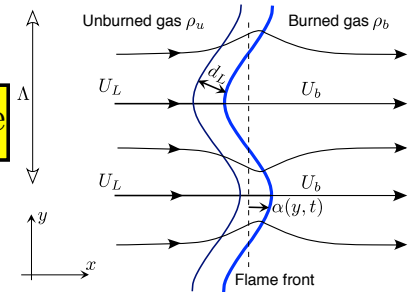
front curvature flow strain rate



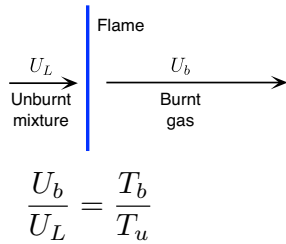
difficulty with the finite thickness:

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

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



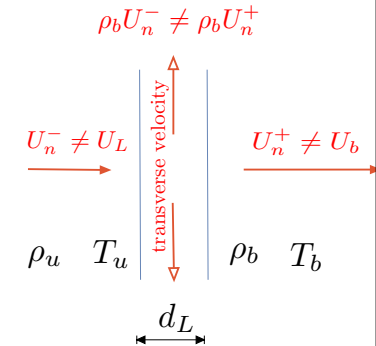
Markstein numbers in the burned gas



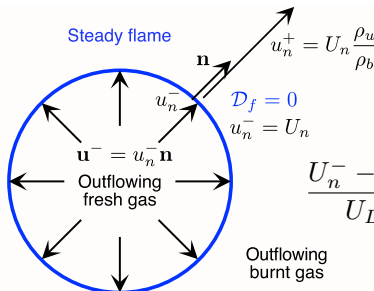
$$U_n^+ \equiv u_n^+ - \mathcal{D}_f \quad u_n^+ \equiv \mathbf{n}_f \cdot \mathbf{u}^+(\mathbf{r}_f)$$

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

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



numerical and experimental data

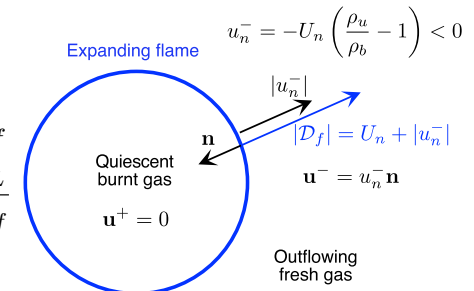


$$\mathcal{D}_f = 0, \quad U_n^- = u_n^-$$

$$\frac{U_n^- - U_L}{U_L} = -2(\mathcal{M}_{fc}^- - \mathcal{M}_{sr}^-) \frac{d_L}{R_f}$$

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

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



V-2) Thermo-diffusive instabilities of planar flames

Sivashinsky 1977 Joulin Clavin 1979

instability mechanism \neq hydrodynamic instability

equations

$$\rho T \neq \rho_o T_o \quad \rho c_p DT/Dt = \nabla \cdot (\lambda \nabla T) + \sum_j Q^{(j)} \dot{W}^{(j)}(T, ..Y_k..)$$

$$\rho DY_i/Dt = \nabla \cdot (\rho D_i \nabla Y_i) + \sum_j \nu_i^{(j)} m_i \dot{W}^{(j)}(T, ..Y_k..),$$

+ fluid mechanics

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

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

$\rho = \text{cst.}$

$$\frac{\partial \theta}{\partial t} - D_T \Delta \theta = \frac{\psi}{\tau_{rb}} e^{-\beta(1-\theta)} \quad \frac{\partial \psi}{\partial t} - D \Delta \psi = -\frac{\psi}{\tau_{rb}} e^{-\beta(1-\theta)}$$

$$x = -\infty : \theta = 0, \psi = 1 \quad x = +\infty : \theta = 1, \psi = 0$$

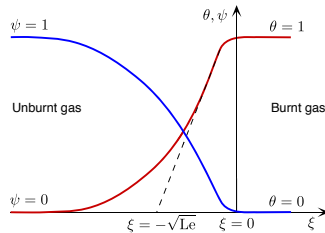
Planar flame for $Le \equiv D_T/D \neq 1$

$$\xi \equiv \frac{x}{d_L(Le = 1)}$$

$$\mu \equiv \frac{U_L}{U_L(Le = 1)} \quad ?$$

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

reaction layer



$$-\frac{d^2\theta}{d\xi^2} \approx \frac{\beta^2}{2} \psi e^{-\beta(1-\theta)} \quad \frac{d^2\theta}{d\xi^2} + \frac{1}{Le} \frac{d^2\psi}{d\xi^2} = 0$$

matching

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

(first order reaction rate)

Flame temperature of curved flame for $Le \neq 1$

$$\beta \gg 1 \quad Le \neq 1 \Rightarrow \theta_f \neq 1$$

$$Le - 1 = O(1/\beta) \Rightarrow (\theta_f - 1) = O(1/\beta)$$

the thin reaction layer of curved flame is quasi-planar

$$-\frac{d^2\theta}{d\xi^2} \approx \frac{\beta^2}{2} \psi e^{-\beta(1-\theta)} \quad \frac{d^2\theta}{d\xi^2} + \frac{1}{Le} \frac{d^2\psi}{d\xi^2} = 0 \quad \xi = \text{non-dimensional normal coordinate}$$

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

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

jump conditions across the reaction layer

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

Joulin Clavin 1979

Preheated zone

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

$$\xi \equiv x/d_L, \quad \eta = y/d_L, \quad \tau \equiv t/\tau_L \quad \frac{\partial\theta}{\partial\tau} + \frac{\partial\theta}{\partial\xi} - \Delta\theta = 0, \quad \frac{\partial\psi}{\partial\tau} + \frac{\partial\psi}{\partial\xi} - \frac{1}{Le} \Delta\psi = 0$$

boundary conditions: jump conditions and $\xi \rightarrow -\infty : \theta = 0, \psi = 1, \quad \xi \rightarrow \infty : \theta = 1, \psi = 0.$

Linear equations

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

$$\zeta \equiv \xi - a(\eta, \tau)$$

$\zeta = 0$: 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

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

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

external equations

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

harmonic analysis
(normal modes)

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

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

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

ς ?

reduced linear growth rate

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

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

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

$$\tilde{\theta} = d\bar{\theta}/d\zeta \quad \tilde{\psi} = d\bar{\psi}/d\zeta$$

$$\bar{\theta}^- = e^\zeta \quad \bar{\theta}^+ = 1 \quad \bar{\psi}^- = 1 - e^{Le\zeta} \quad \bar{\psi}^+ = 0$$

boundary conditions

$$\zeta \rightarrow \pm\infty : \quad \tilde{\theta} = 0$$

$$\theta(\zeta = 0) = \theta_f \quad \tilde{\theta}^\pm = d\bar{\theta}^\pm/d\zeta + \left(\tilde{\theta}_f - d\bar{\theta}^\pm/d\zeta \Big|_{\zeta=0} \right) e^{r^\pm \zeta}$$

$$r^2 - r - (\varsigma + \kappa^2) = 0 \quad r^\pm = \frac{1}{2} \left[1 \mp \sqrt{1 + 4(\varsigma + \kappa^2)} \right]$$

general solution to the homogeneous equation

$$\zeta \rightarrow -\infty : \quad \tilde{\psi} = 0$$

$$\psi(\zeta = 0) = 0$$

mass fraction in the preheated zone zone

$$\zeta > 0 : \quad \tilde{\psi} = \bar{\psi} = 0$$

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

$$\frac{1}{Le} s^2 - s - \left(\varsigma + \frac{\kappa^2}{Le} \right) = 0$$

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

jump conditions

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

ς and θ_f ?

asymptotic analysis

$\beta \gg 1 :$ $Le = 1 + l/\beta, \quad l \equiv \beta(Le - 1) = O(1)$
 $\beta(1 - \theta_f) = O(1) \qquad \beta\tilde{\theta}_f = O(1)$

2nd condition

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

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

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

linearized 1st condition

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

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

dispersion relation (ς, κ)

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

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

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

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

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

$$\tilde{\theta}_f = (Le - 1)\kappa^2 \quad \zeta = -(l + 2)\kappa^2/2$$

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

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

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

$$\mathcal{M} < 0$$

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

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

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

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

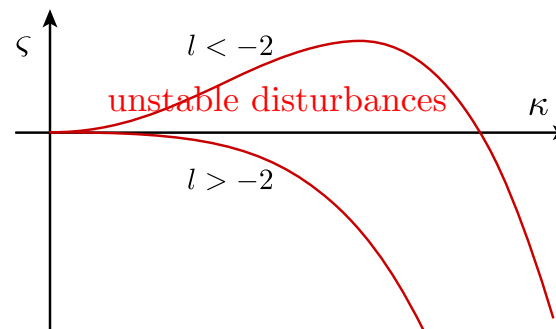


$$\mathcal{M} = \frac{v_b}{v_b - 1} \mathcal{J} + \frac{l}{2} \frac{\mathcal{D}}{(v_b - 1)}$$

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

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

Turing type of instability



Zeldovich



Turing

Hydrodynamics + diffusion



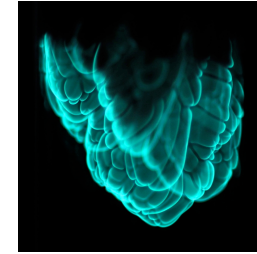
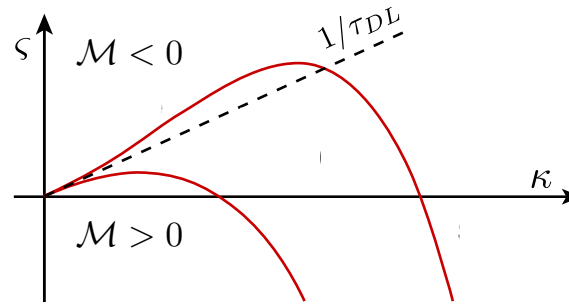
Propane lean flame
 $\mathcal{M} > 0$

hydrodynamic instability only

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

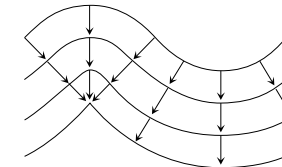
nonlinear equation

geometrical term: Huygens construction



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

hydrodynamic + cellular instabilities
shorter wavelengths are unstable



Oscillatory instability $Le \equiv D_T/D > 1$

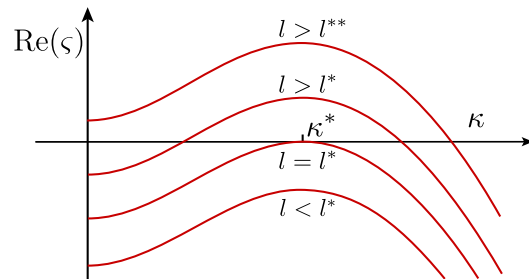
$\text{Im}(\varsigma) \neq 0$

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

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

effect of heat losses

Joulin Clavin 1979



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

