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Structure and Dynamics of Combustion Waves in Premixed Gases

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ECM & CNRS (IRPHE)

Theoretical analyses (analytical studies of simplified models)
+ laboratory experiments


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Contents

Combustion is a fascinating phenomenon coupling complex chemistry to transport mechanisms and nonlinear fluid dynamics. This book provides an up-to-date and comprehensive presentation of the nonlinear dynamics of combustion waves and other non-equilibrium energetic systems. The major advances in this field have resulted from analytical studies of simplified models performed in close relation with carefully controlled laboratory experiments. The key to understanding the complex phenomena is a systematic reduction of the complexity of the basic equations.

Focusing on this fundamental approach, the book is split into three parts. Part I provides physical insights for physics-oriented readers, part II presents detailed technical analysis using perturbation methods for theoreticians, and part III recalls the necessary background knowledge in physics, chemistry and fluid dynamics. This structure makes the content accessible to newcomers to the physics of unstable fronts in flows, whilst also offering advanced material for scientists who wish to improve their knowledge.

Paul Clavin is Professor Emeritus at Aix-Marseille Université and is an honorary member of the Institut Universitaire de France (Chair of Mécanique Physique 1993-2004). In 1995 he founded a renowned research institute, the Institut de Recherche sur les Phénomènes Hors Équilibre (IRPHE) and has received major awards from the Société Française de Physique (Plumey 1988), French Academy of Sciences (Grand Prix 1995) and from the Combustion Institute (Zeldovich Gold medal, San Francisco, August 2014).

Geoff Searby is retired Director of Research at the Institut de Recherche sur les Phénomènes Hors Équilibre (IRPHE). He is a renowned specialist of the physics of thermo-acoustic instabilities in combustion chambers and rocket motors, and his experiments have made major contributions to the understanding of the dynamics of flame fronts. In 2004 he obtained a major award from the French Academy of Sciences.

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Clavin and Searby **Combustion Waves and Fronts in Flows**

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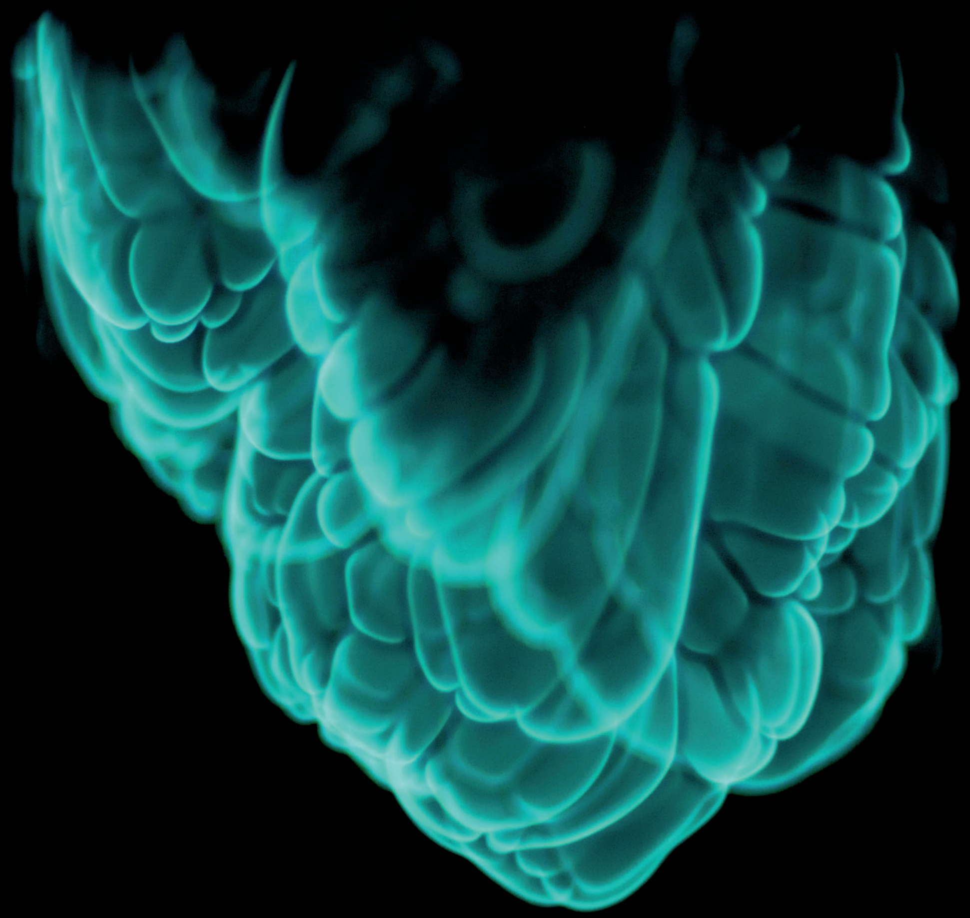
Combustion Waves and Fronts in Flows

Flames, Shocks, Detonations, Ablation Fronts and Explosion of Stars

Paul Clavin and Geoff Searby



Lecture 1: Orders of magnitude

1-1: Overall combustion chemistry

1-2: Combustion waves in gaseous mixtures

1-3: Arrhenius law

1-4: Hydrocarbon/air flames

1-5: Instabilities of flames

$I-1)$ Overall combustion chemistry

$$\text{reactants} \longrightarrow \text{products} + \text{heat release}$$

Lavoisier 1777

binding energy of small molecules $\approx$ a few eV

$1eV/\text{molecule} \approx 23$ kcal/mole $\quad\Rightarrow\quad T_b - T_u \approx 2000$ K

$(C_p \approx 10\,\text{cal/mole/K})$

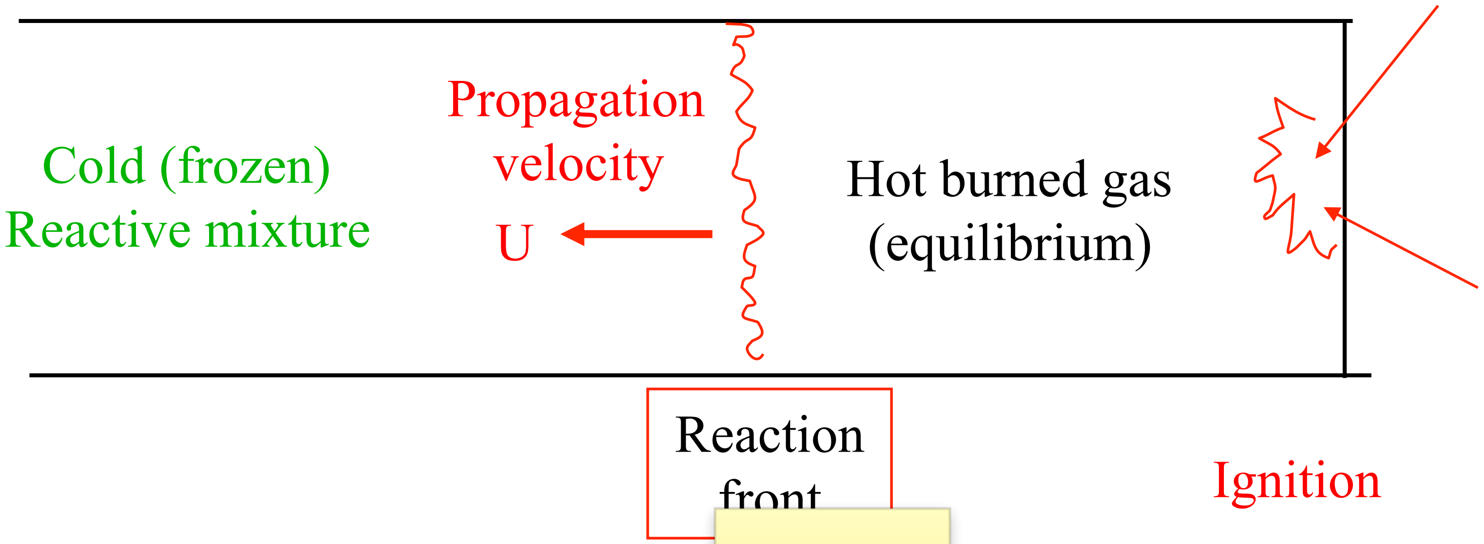
reaction time $\tau_r(T)$ extremely sensitive to temperature:

$T < 500K : \tau_r(T) \approx \infty$ (frozen mixture of reactants)

$T \approx 2500K : \tau_r(T) \approx 10^{-6}s.$

Euler 1738

thermal feedback $\Rightarrow$ combustion waves



Cold (frozen)
Reactive mixture

Propagation
velocity
U

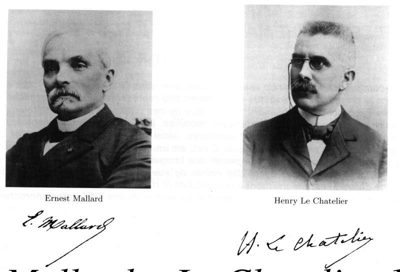
Hot burned gas
(equilibrium)

Reaction
front

Ignition

Davy 1830

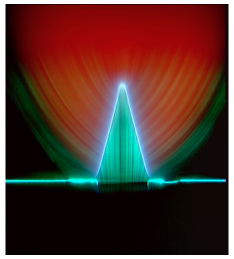
$I-2)$ Combustion waves in gaseous mixtures



Mallard, Le Chatelier 1883

$$\text{Flames :}\quad 10\ \mathrm{cm/s} - \overset{\text{acethylen/oxygen}}{10\ \mathrm{m/s}}, \quad \Delta p/p \approx -10^{-5}$$

Laminar propagation



Laser Tomography
L.Boyer 1980

Bec Bunsen
J. Quinard 2000

$$\text{Fast deflagrations :}\quad \approx 100\ \mathrm{m/s}, \quad \Delta p/p \approx -10^{-1}$$

Turbulent propagation

John H.S. Lee 1990

$$\text{Detonations :}\quad \approx 2000\ \mathrm{m/s}, \quad \Delta p/p \approx +30$$

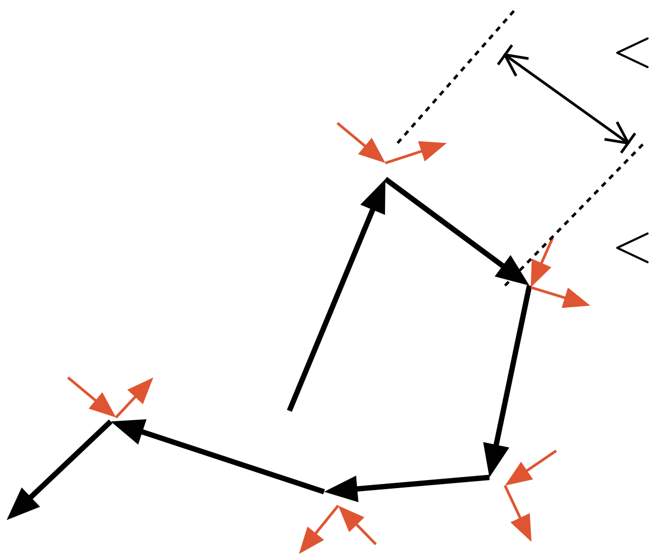
Cellular structure

Berthelot, Vielle 1884

Shchelkin 1960

Back to the kinetic theory of gases

Binary collisions of molecules



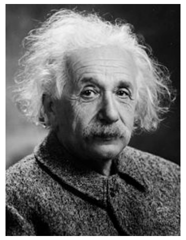
$< \text{distance} >= l$ ← mean free path

$< \text{velocity} >= V \equiv \sqrt{3k_B T/m}$

$< \text{time} >= \tau_{coll} \equiv l/V$

Maxwell 1867

Bolzmann 1877



Einstein 1905

speed of sound: $a \approx V$

τ_{coll} : collision time $\approx$ relaxation time

Equilibrium state. The Maxwell-Boltzmann distribution

m : mass of molecules, n : number density, T : temperature, k_B : Boltzmann cst.

$$f^{(eq)}(\mathbf{v}, n, T)\, \mathrm{d}^3\mathbf{v}\, \mathrm{d}^3\mathbf{r} = n \frac{m^{3/2}}{(2\pi k_B T)^{3/2}} \mathrm{e}^{-m|\mathbf{v}|^2/(2k_B T)} \mathrm{d}^3\mathbf{v}\, \mathrm{d}^3\mathbf{r}$$

velocity of molecules

element of volume

Molecular diffusion $\equiv$ Random Walk

spreading : $\dfrac{1}{(4\pi D t)^{3/2}} \mathrm{e}^{-r^2/4Dt}$

$D = lV = l^2/\tau_{coll} \approx a^2 \tau_{coll}$

Diffusion coefficient

Dimensional parameters

chemical energy/unit mass $q_m \quad \Rightarrow \quad T_b/T_u = 5 - 10$

sound speed, $\quad a_b/a_u = \sqrt{T_b/T_u}$

reaction rate $1/\tau_r(T_b)$

molecular and thermal diffusion coefficients $D \approx D_T$

Dimensional analysis

$[q_m] = (\text{velocity})^2$

$[D] = (\text{velocity})^2 \times \text{time}$

$D \approx 10^{-3} \text{m}^2/\text{s}$

propagation velocity

detonation: $\quad \mathcal{D} \approx \sqrt{q_m} \approx a_b$

$\approx 1000 \text{ m/s}$

supersonic $\quad \mathcal{D}/a_u > 1$

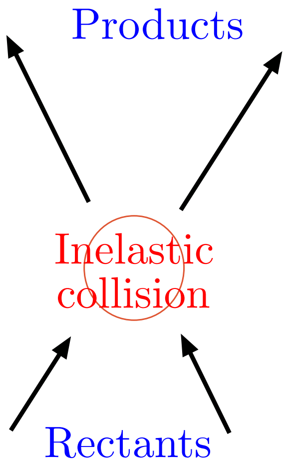
laminar flames: $\quad U_L \approx \sqrt{D/\tau_r(T_b)}$

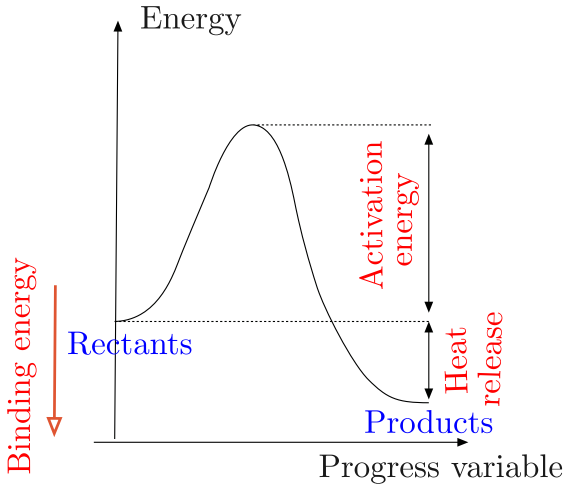
$\approx 1 \text{ m/s}$

subsonic $\quad U_L/a_u < 1$

$I-3)$ Overall reaction rate. Arrhenius factor

Collision in gases





$$\boxed{\frac{E}{k_BT_b}\approx 8}$$

$$\mathrm{e}^{-E/k_BT_b}\approx 3\times 10^{-4}$$

$$T_b/T_u=8\ \Rightarrow\ \mathrm{e}^{-E/k_BT_u}\approx 1.6\times 10^{-28}$$

Kinetic theory of gases $\Rightarrow$ Arrehnius law

MB distribution $\propto \mathrm{e}^{-\frac{1}{2}\frac{mv^2}{k_BT}}$ $\Rightarrow$ $\boxed{\dfrac{1}{\tau_r(T)}=\dfrac{1}{\tau_{coll}}\mathrm{e}^{-E/k_BT}}$

Arrhenius factor

elastic collision rate $1/\tau_{coll}\approx 10^9\mathrm{s}^{-1}$

$\Rightarrow$ $1/\tau_r(T_b)\approx 3\times 10^5\mathrm{s}^{-1}$

$T_b/T_u=8\Rightarrow$ $\tau_r(T_u)\approx 10^{10}$ years !!

Kinetic theory of gases $\Rightarrow$ Flame properties

sound speed $\searrow$ $\swarrow$ men free path

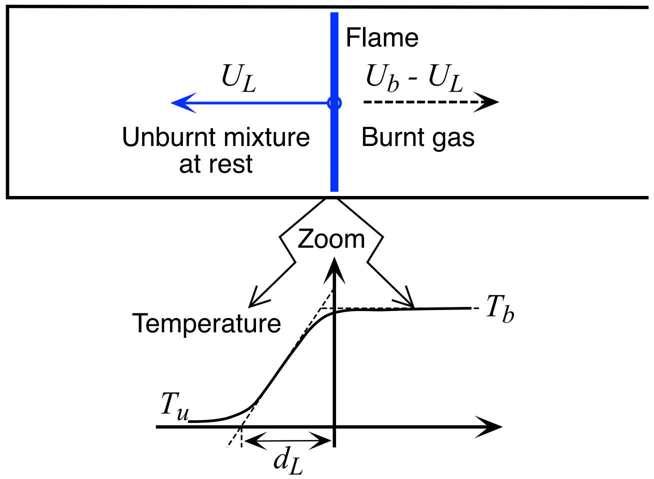
$D\approx a^2\,\tau_{coll}\approx l^2/\tau_{coll}$ $\qquad a\approx l/\tau_{coll}$

laminar flame velocity $\searrow$ $\swarrow$ sound speed

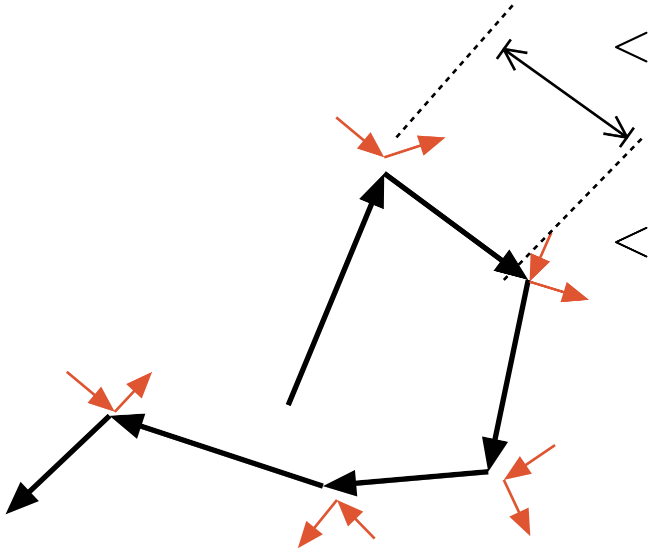
$U_L\approx\sqrt{D_T/\tau_r}$ $\qquad$ $\boxed{\text{subsonic}}$ $\quad U_L/a\approx\sqrt{\mathrm{e}^{-E/k_BT_b}}\ll 1$

$d_L\approx D_T/U_L$ $\qquad$ $\boxed{\text{macroscopic structure}}$ $\quad d_L\approx l\sqrt{\mathrm{e}^{E/k_BT_b}}\gg l$

flame thickness $\nearrow$ $\nwarrow$ mean free path $\nearrow$



Molecular diffusion $\equiv$ Random Walk



$< \text{distance} >= l$

mean free path

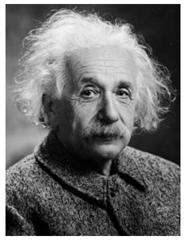
$< \text{velocity} >= V \equiv \sqrt{3k_B T/m}$

$a \approx V$

$< \text{time} >= \tau_{coll} \equiv l/V$

Maxwell 1867

Bolzmann 1877

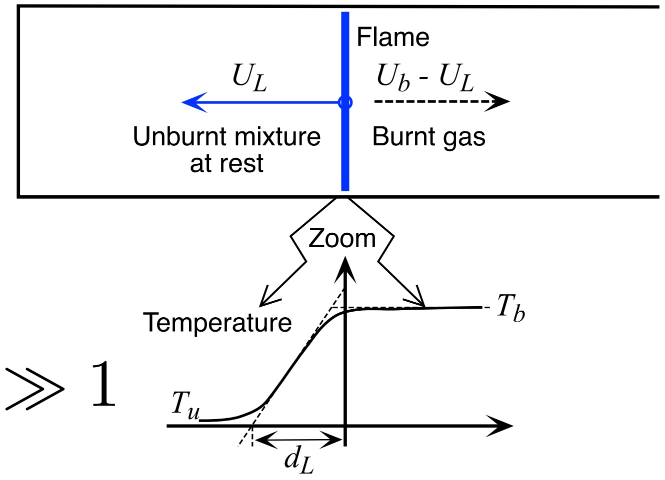


Einstein 1905

spreading : $\dfrac{1}{(4\pi Dt)^{3/2}} \mathrm{e}^{-r^2/4Dt}$

$$D = lV = l^2/\tau_{coll} \approx a^2 \tau_{coll}$$

Flame structure



$$U_L \approx \sqrt{D/\tau_r(T_b)}$$

$$\frac{1}{\tau_r(T_b)} = \frac{1}{\tau_{coll}} \mathrm{e}^{-E/k_B T_b}$$

$$U_L/a \approx \sqrt{\mathrm{e}^{-E/k_B T_b}} \ll 1$$

$$d_L/l \approx U_L \tau_r/l \approx \sqrt{D\tau_r}/l \approx \sqrt{\mathrm{e}^{E/k_B T_b}} \gg 1$$

Limitations of the dimensional analysis

$$\left. \begin{array}{l} \mathrm{e}^{-E/k_B T_b} \approx 3 \times 10^{-4} \\ a \approx 500 \mathrm{m/s} \\ l \approx 10^{-7} \mathrm{\ m} \end{array} \right\} \Rightarrow$$

$U_L \approx 8.6\,\mathrm{m/s}$ too large

$d_L \approx 0.6 \times 10^{-5}$ m too small

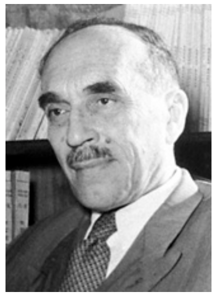
||

10 – 50 cm/s

hydrocarbon/air

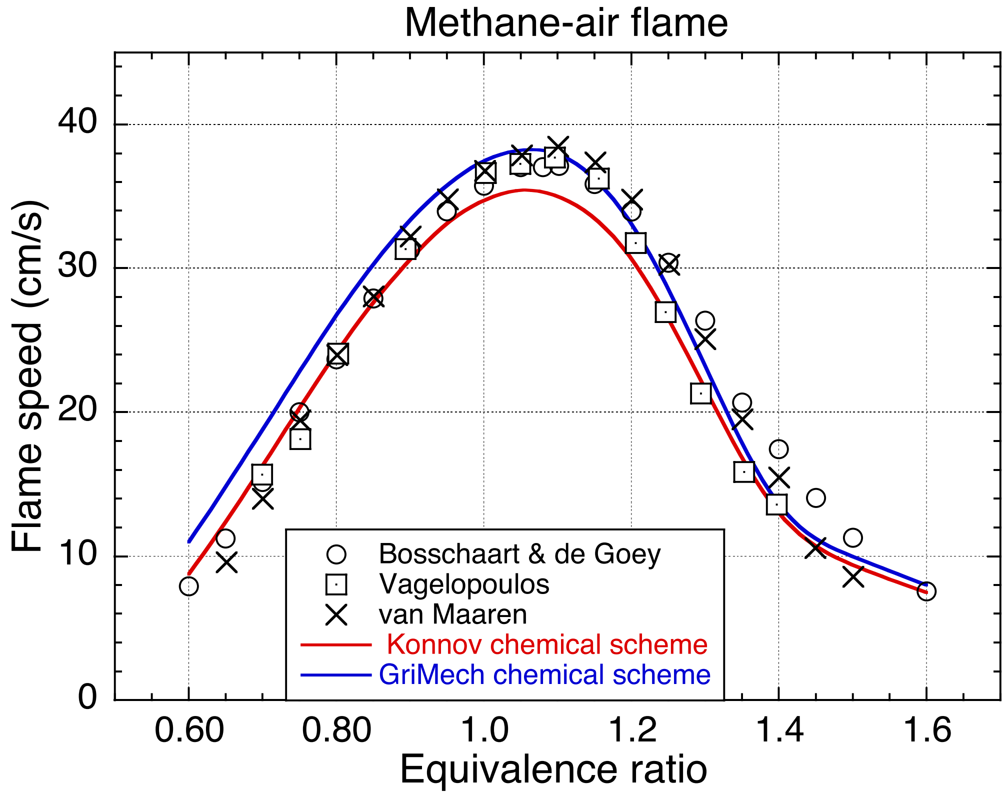
1 – 10^{-1} mm

$I-4)$ Hydrocarbon/air flames



Semenov 1934

Methane-air flame



$$\vartheta_F^+ F + \vartheta_o^+ O_2 \rightleftharpoons P$$

Equivalence ratio

$$\phi = \frac{N_F/N_{O_2}}{\vartheta_F^+/\vartheta_{O_2}^+}$$

$\phi = 1$: stoichiometry

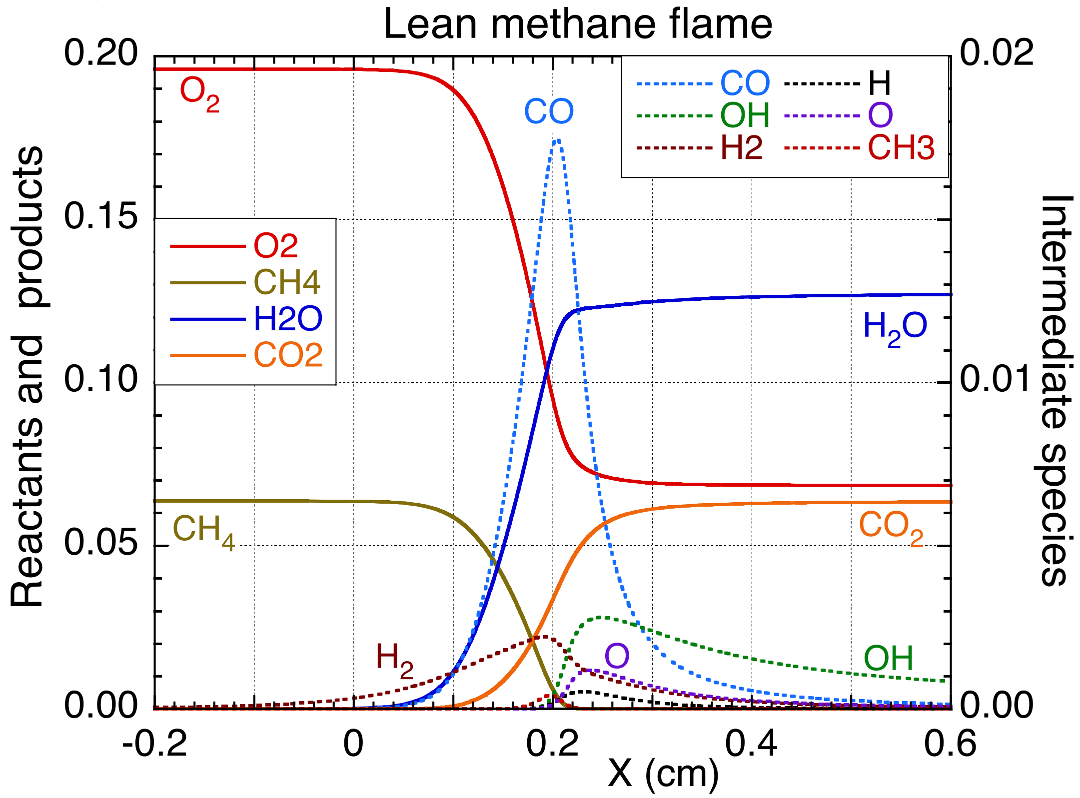
$\phi > 1$: fuel rich

$\phi < 1$: fuel lean

near to the flammability limit

$$\phi = 0.65$$

"thicker flame"

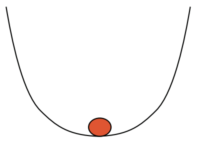


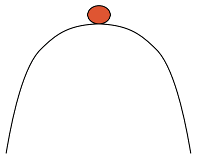
$$d_L \approx U_L \tau_r(T_b)$$
$$\approx \sqrt{D_T \tau_r(T_b)}$$
$$\approx D_T \sqrt{\tau_r(T_b)/D_T}$$
$$\approx D_T/U_L$$

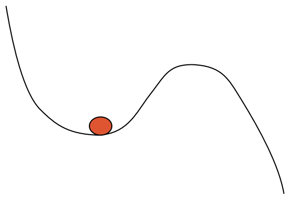
$$U_L \searrow \qquad d_L \nearrow$$

$I-5)$ Instabilities of flames

Intrinsic instabilities

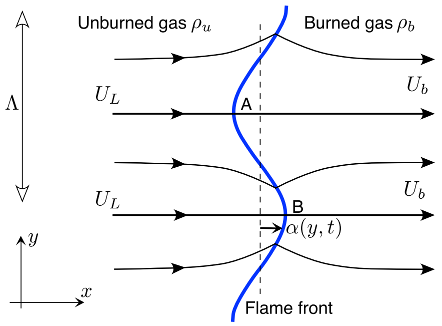

Stable


Linearly unstable


Linearly stable
Nonlinearly unstable

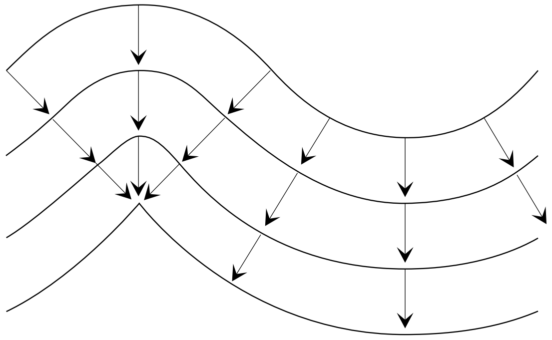
Planar flames are linearly unstable:

- hydrodynamic instability of the flame front $\boxed{\rho_u > \rho_b}$

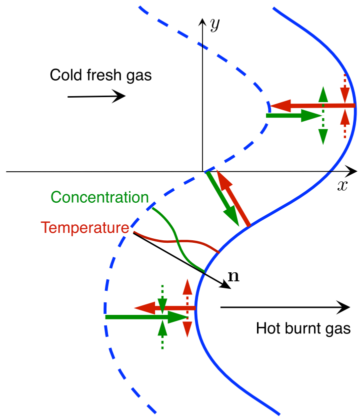


induced flow

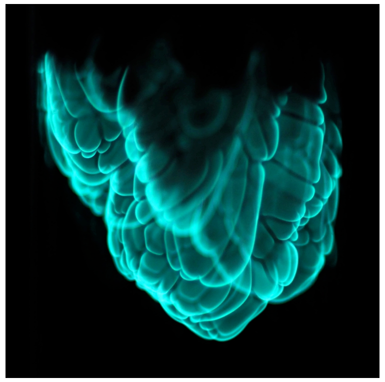

Propane lean flame


Cusp formation
Huygens construction

- diffusional-thermal instability of the inner flame stucture $\boxed{D_T < D}$



Unstable inner structure


Propane rich flame

System instability (combustion in a cavity)

The coupling of flames with acoustics can be unstable

Thermo-acoustic instabilities (Rayleigh criterion)

Lord Rayleigh 1878

Combustion chambers

Rocket engine

Gas turbines

Vibratory instability of flames in tubes

Lean methane-air flame

$\phi = 0.73 \qquad U_L = 23\ \mathrm{cm/s}$

$\phi = 0.8 \qquad U_L = 30\ \mathrm{cm/s}$

Acoustic instability
in
Premixed Flames

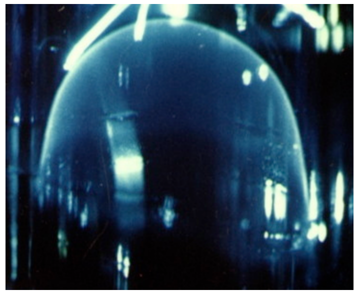
© IRPHE
G. Searby

G. Searby IRPHE 2006

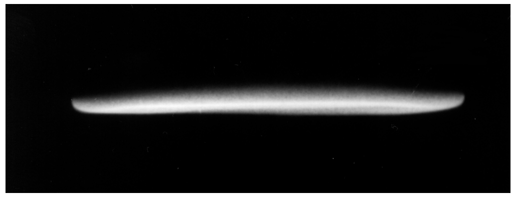
Tomography cut: L. Boyer 1980

Effect of acceleration

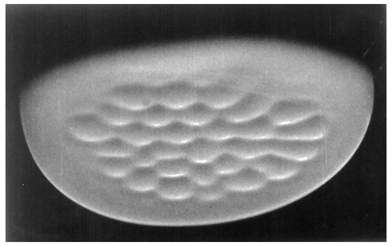
Gravity



Propane flame propagating upwards

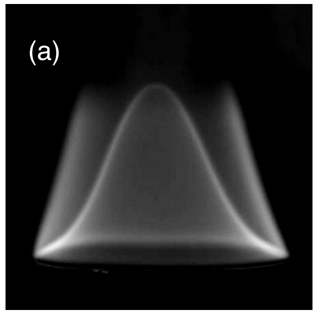


Slow downwards propagating flame

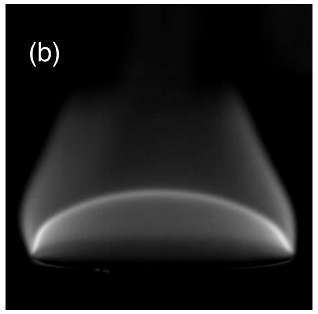


slightly faster

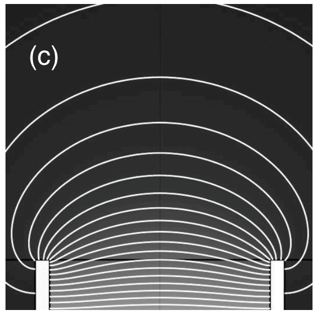
Effect of an acoustic field on a Bunsen flame



Methane rich Bunsen flame
$\phi = 1.5$



in the presence of
an axial acoustic field



equipotential surface
in the absence of flame