Structure and Dynamics of Combustion Waves in Premixed Gases

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Lecture VI
Thermal quenching of flames and flammability limits
Lecture 6: **Thermal quenching and flammability limits**

6-1. Extinction through thermal loss

6-2. Basic concepts in chemical kinetics
   
   *Combustion of hydrogen*
   
   *Two-step model. Crossover temperature*
   
   *One-step model with temperature cutoff*

6-3. Flame speed near flammability limits
VI-1) Extinction through thermal loss

a small heat loss can quench the flame

Formulation (volumetric heat loss in a planar flame)

\[
\frac{\mu}{d} \frac{d\theta}{dx} - \frac{d^2 \theta}{d^2 x} = w - \frac{\tau_L}{\tau_{cool}} \theta, \quad \frac{\mu}{d} \frac{d\psi}{dx} - \frac{1}{Le} \frac{d^2 \psi}{dx^2} = -w
\]

\[
\xi \equiv x/d_L \quad \mu = U_L/U_{Ladia} \quad 1/\tau_{cool} \approx D_T/R^2
\]

\[
\tau_L \approx D_T/U_L^2 \Rightarrow \frac{\tau_L}{\tau_{cool}} \approx \left(\frac{D_T}{RU_L}\right)^2 \quad R = \text{tube radius}
\]

\[
\xi = -\infty : \theta = 0, \, \psi = 1, \quad \xi = +\infty : \theta = 0, \, \psi = 0
\]

Asymptotic analysis for small heat release and a one step reaction

(Joulin Clavin 1976)

\[
\beta \to \infty \quad \frac{\tau_L}{\tau_{cool}} = h/\beta \quad h = O(1) \quad \beta(1 - \theta_f) = O(1) \quad w(\theta, \psi) = (\beta^2/2)\psi \exp[-\beta(1-\theta)]
\]

unknown flame temperature < adiabatic flame temperature : \( \theta_f < 1 \)

jumps across the thin reaction zone:

\[
\frac{d\theta}{d\xi}|_{\xi = 0^-} = e^{-\beta(1-\theta_f)/2} \quad \left[\frac{d\theta}{d\xi} + \frac{1}{Le} \frac{d\psi}{d\xi}\right]_{0^-}^{0^+} = 0
\]

external solutions : \( w = 0 \)

\[
\xi < 0 : \begin{cases} \theta_-(\xi) = \theta_f e^{[\mu + h/(\beta \mu)]\xi}, \\ \psi_-(\xi) = 1 - e^{Le \mu \xi} , \end{cases} \quad \xi > 0 : \begin{cases} \theta_+(\xi) = \theta_f e^{-[h/(\beta \mu)]\xi}, \\ \psi_+(\xi) = 0, \end{cases}
\]

up to first order \( O(1/\beta) \)
\[ \xi < 0 : \begin{cases} \theta_-(\xi) = \theta_f e^{[\mu + h/(\beta \mu)]\xi}, \\ \psi_-(\xi) = 1 - e^{Le \mu \xi}, \end{cases} \quad \xi > 0 : \begin{cases} \theta_+(\xi) = \theta_f e^{-[h/(\beta \mu)]\xi}, \\ \psi_+(\xi) = 0, \end{cases} \]

\[ \left[ \frac{d\theta}{d\xi} + \frac{1}{Le} \frac{d\psi}{d\xi} \right]_{0-}^{0+} = 0 \quad \Rightarrow \quad -(h/\beta \mu)\theta_f - (\mu + h/\beta \mu)\theta_f + \mu = 0 \]

\[ \theta_f - 1 = O(1/\beta) \quad \Rightarrow \quad \beta(1 - \theta_f) = 2h/\mu^2 \]

\[ \mu^2 \ln \mu^2 = -2h \]

C-shaped curve: no solution for \(2h > 1/e\)

quenching at finite flame velocity \(U_L/U_{Ladia} = 1/\sqrt{e}\)
VI-2) Basic concepts in chemical kinetics

Combustion of hydrogen  Sanchez Williams 2014

<table>
<thead>
<tr>
<th>Label</th>
<th>Reaction</th>
<th>( \tilde{k}_j )</th>
<th>( \tilde{B}_j )</th>
<th>( \nu_j )</th>
<th>( T_{aj} )</th>
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Shuffle reactions

- (1f), (2f), (3f)
- (4f) chain breaking

Rate:
- \( \omega_{1f} = c_{\text{HCO}_2}k_{1f} \)
- \( k_{4f} = B_{4f} \)

\( \text{O}_2 + 3\text{H}_2 \rightarrow 2\text{H}_2\text{O} + 2\text{H} \)

\( \text{M} + \text{H} + \text{O}_2 \rightarrow \text{M} + \text{HO}_2 \)

Rate:
- \( \omega_{4f} = c_{\text{HCO}_2}nk_{4f} \)

Simplified two-step model: crossover temperature


\( \omega_B = c_Rc_XB_Be^{-E/k_BT}, \quad E \gg k_BT \)

\( \omega_R = c_XnBR, \quad E_R = 0 \)

\[ c_RB_Be^{-E_1/k_BT^*} = nBR \quad T^* \in [900K - 1400K] \]

Hydrogen combustion:

\( k_{1f}(T^*) \equiv B_{1f}e^{-E_1/k_BT^*} = nB_{4f} \)

Flammability limit

\( T_b = T^* \Rightarrow q_RW^*_u \equiv c_p(T^* - T_u) \)
Two-step model for rich hydrogen flames near the flammability limit
(consumption of hydroperoxide included)

\[ \text{O}_2 + 3\text{H}_2 \rightarrow 2\text{H}_2\text{O} + 2\text{H}, \]
\[ \omega_{1f} = c_{\text{H}}c_{\text{O}_2}k_{1f}(T), \quad k_{1f}(T) = B_{1f}e^{-E_1/k_BT} \]

\[ \text{H} + \text{H} \rightarrow \text{H}_2 + Q, \]
\[ \omega_{4f} + \omega_{5f} = nc_{\text{H}}c_{\text{O}_2}B_{4f} + nc_{\text{H}}^2B_{5f} \]

\[ \frac{dc_H}{dt} = \left[ B_{1f}e^{-E_1/k_BT} - nB_{4f} \right]c_{\text{O}_2}c_H - nB_{5f}c_H^2 \]

\[ (B_{1f}e^{-E_1/k_BT} - nB_{4f})/nB_{4f} \ll 1 \]

tri molecular recombination reaction \((5f) \Rightarrow H\) in quasi-steady state

\[ T > T^* : \quad c_{\text{H}} \approx c_{\text{O}_2} \frac{[B_{1f}e^{-E_1/k_BT} - nB_{4f}]}{nB_{5f}} \]
\[ T < T^* : \quad c_{\text{H}} = 0 \]

One-step model \((\text{near the flammability limit})\)

\[ nB_{4f} = B_{1f}e^{-E_1/k_BT^*} \quad 1/\tau^* = (nB_{4f}^2c_{\text{O}_2}^*)/B_{5f} \]

\[ m\frac{d\theta}{dx} - \rho D_{T}\frac{d^2\theta}{dx^2} \approx \frac{\rho}{\tau^*}\psi^2J(T) \]
\[ m\frac{d\psi}{dx} - \rho D_{O_2}\frac{d^2\psi}{dx^2} \approx -\frac{\rho}{\tau^*}\psi^2e^{-\frac{E}{k_BT^*}}(\frac{1}{T^*} - \frac{1}{T})J(T) \]

\[ x = -\infty : \theta = 0, \quad x = +\infty : \theta = 1 \]

reaction of order 2 with a temperature cutoff

very close to the flammability limit

\[ \frac{T_b - T^*}{T^*} \ll \frac{k_BT^*}{E} \quad \Rightarrow \quad [e^{-\frac{E}{k_BT^*}}(\frac{1}{T^*} - \frac{1}{T}) - 1] \approx \frac{E}{k_BT^*}(\frac{1}{T^*} - \frac{1}{T}) \ll 1 \]

\[ m\frac{d\theta}{dx} - \rho D_{T}\frac{d^2\theta}{dx^2} \approx \frac{\rho}{\tau^*}\psi^2J(T) \]
\[ m\frac{d\psi}{dx} - \rho D_{O_2}\frac{d^2\psi}{dx^2} \approx -\frac{\rho}{\tau^*}\psi^2J(T) \]

\[ \begin{align*}
T > T^* : \quad J(T) & \approx \frac{T_u}{T^*}\frac{E}{k_BT^*} \frac{T - T^*}{T^*} \\
T < T^* : \quad J(T) & = 0
\end{align*} \]
VI-3) Flame speed near flammability limits

\[ \theta \equiv \frac{(T - T_u)}{(T_b - T_u)} \in [\theta^*, 1] \quad \theta^* \equiv \frac{(T^* - T_u)}{(T_b - T_u)} \quad T_b > T^* \Rightarrow \theta^* < 1 \text{ but close to 1} \]

\[ \frac{m}{dx} \frac{d\theta}{dx} - \rho_b D_T \frac{d^2 \theta}{dx^2} \approx \frac{\rho_b}{\tau^*} \psi^2 j(\theta) \]
\[ \frac{m}{dx} \frac{d\psi}{dx} - \rho_b D_{O_2} \frac{d^2 \psi}{dx^2} \approx -\frac{\rho_b}{\tau^*} \psi^2 j(\theta) \]

\[ \left\{ \begin{array}{l} \theta > \theta^* : \quad j(\theta) \approx b^*(\theta - \theta^*) \\ \theta < \theta^* : \quad j(\theta) = 0 \end{array} \right. \]

\[ b^* \equiv \frac{T_u}{T^*} \frac{E}{k_B T^*} \frac{T_b - T_u}{T^*} \]

reaction zone: \( \psi = \text{Le}(1 - \theta) \), \[ D_T \frac{d^2 \theta}{dx^2} = \frac{\text{Le}^2 b^*}{\tau^*} (1 - \theta)^2 [(\theta - 1) - (\theta^* - 1)] \]

\[ \begin{array}{c} \text{Le} \equiv D_T / D_{O_2} \\ \rho_u \frac{U_L}{\rho_b \sqrt{D_T / \tau^*}} \approx \text{Le} \sqrt{\frac{b^*}{6}} (1 - \theta^*)^2 \end{array} \]

Peters 1997

the flame velocity decreases smoothly to zero when approaching the flammability limit \( T_b \rightarrow T^* \)

the flame thickness \( d_L^* \) diverges, \( T_b \rightarrow T^* \):

\[ \frac{d_L^*}{d_L} \propto \frac{1}{\beta^2} \left( \frac{T^* - T_u}{T_b - T^*} \right)^2 \]

Divergence of the thermal sensitivity: Thermal quenching

\[ \frac{T_b}{U_L} \frac{dU_L}{dT_b} = \frac{2T_b}{T_b - T^*} \rightarrow \infty \]

the least heat loss quenches the flame at a non zero velocity
Methane flames

Peters Williams 1987   Peters 1997

$\text{H}_2 - \text{O}_2$ flames

Sanchez Williams 2014
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Lecture VII
Flame kernels and quasi-isobaric ignition
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-1) 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

Turbulence facilitates ignition of hydrocarbon lean mixtures
Turbulence may suppress ignition of hydrocarbon rich mixtures
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

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

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

No flow

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

\[R \leq R_f: \quad \theta = \theta_f, \quad \psi = 0; \quad R \to \infty: \quad \theta = 0, \quad \psi = 1\]

**Flame temperature**

\[L_e \neq 1 \Rightarrow T_f \neq T_b\]

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

(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**

\[\text{Le} < 1 \Rightarrow T_f > T_b\]

\[\text{Le} > 1 \Rightarrow T_f < T_b\]
Unstable steady spherical solution for the one-step model of adiabatic flames

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

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

\[ R \leq R_f : \quad \theta = \theta_f; \quad \psi = 0; \quad R \to \infty : \quad \theta = 0, \quad \psi = 1 \]

**Asymptotic analysis** \( \beta \gg 1 \)

**Thin reaction zone**: \( \beta \to \infty \) 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

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

**External zones**

\[ \frac{d}{dR} \left( R^2 \frac{d\theta}{dR} \right) = 0 \quad R^2 \frac{d\theta}{dR} = \text{cst.} \]

\[ R \geq R_f : \quad \theta = \frac{1}{\text{Le}} \frac{R_f}{R}; \quad R = R_f : \quad D_T \frac{d\theta}{dR} = - \frac{1}{\text{Le}} \frac{D_T}{R_f} \]

\[ R < R_f : \theta = \theta_f \]

**Radius of the kernel**

Matching \( \Rightarrow \)

\[ \frac{1}{\text{Le}} \frac{D_T}{R_f} = e^{\beta \left( \frac{1}{\text{Le}} - 1 \right)} \sqrt{\text{Le} \frac{D_T}{\tau_{rb}}} \iff \frac{R_f}{d_L} = \text{Le}^{-3/2} e^{\beta \left( \frac{1}{\text{Le}} - 1 \right)} \]

\[ \tau_{rb} \equiv \beta^2 \tau_{rb}/2, \quad d_L \equiv \sqrt{D_T \tau_{rb}} \]

\[ \text{Le} < 1 : \quad R_f \ll d_L \quad \text{Le} > 1 : \quad R_f \gg d_L \]
Instability? (adiabatic condition)

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

\[ \frac{d\theta}{dR} \big|_{R=R_f} = -\frac{\theta_f}{R_f} \]

Heat flux towards the preheated zone

Convective flux \( dR_f / dt > 0 \) \( R_f \)

Convective flux \( dR_f / dt < 0 \) \( R_f \)

**Positive feedback: amplification**

\( R_f \uparrow R_f > \overline{R}_f : |\text{diffusion fluxes}| \propto 1/R \)

\( R_f \downarrow R_f < \overline{R}_f : |\text{diffusion fluxes}| \propto 1/R \)

Quasi-isobaric ignition as a nucleation problem

\( \text{Le} < 1 : \overline{R}_f \ll d_L \quad \text{Le} > 1 : \overline{R}_f \gg d_L \)

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, Romney 1990)

Flame balls in micro-gravity experiments (Ronney 1985-2004) (Deshais 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)

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

\[R \leq R_f : \quad \theta = \theta_f, \quad \psi = 0; \quad R \to \infty : \quad \theta = 0, \quad \psi = 1\]

\[T > T^* : \quad \ddot{W} = \frac{\rho_b}{\rho_u} \frac{\psi^2}{\tau_{rb}} [e^{-\beta(1-\theta)} - e^{-\varepsilon}]\]

\[T < T^* : \quad \ddot{W} = 0\]

\[\frac{1}{\tau_{rb}} = \frac{1}{\tau^*} e^{\frac{E}{k_b T_b}} \left( \frac{1}{\tau^*} - \frac{1}{\tau^*} \right) = \frac{B_{if}}{B_{5f}} \frac{B_{1f}}{B_{3f}} e^{-\frac{E}{k_b T_b}} c_{O_2}\]

\[\varepsilon = O(1) : \text{near to flammability limits} \quad (\varepsilon = 0 : \text{quenching } \ddot{W} = 0)\]

\[\varepsilon \gg 1, \ e^{-\varepsilon} \approx 0 : \text{far from flammability limits}\]

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

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

\[\ddot{w} = (\beta^3/4) Le^2 \beta(\theta_f - 1) \left[ \frac{e^{\beta(\theta - \theta_f)} - e^{-\varepsilon - \beta(\theta_f - 1)}}{\varepsilon} \right] \]

\(\theta^* \leq \theta < \theta_f\)

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

\[\beta^3(\theta_f - \theta) \int_{\theta^*}^{\theta_f} \left\{ e^{\beta(\theta - \theta_f)} - e^{-\varepsilon - \beta(\theta_f - 1)} \right\} d\theta\]

\(\varepsilon = 1 - e/\beta\)

\(\ddot{w} = 0\)

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

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

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

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

measure of the distance from the flammability limit: \( \Theta_f \in [0, \infty] \)

\[
(d\theta/d\zeta)^2 = Le^2 e^{\beta(\theta_f-1)} J(\Theta_f)
\]

\[
J(\Theta_f) \equiv \frac{1}{2} \int_0^{\Theta_f} \Theta^2 (e^{-\Theta} - e^{-\Theta_f}) d\Theta \in [0, 1]
\]

\[
J(\Theta_f) = 1 - e^{-\Theta_f} \left( 1 + \Theta_f + \frac{\Theta_f^2}{2!} + \frac{\Theta_f^3}{3!} \right)
\]

\[
\left\{ \begin{array}{c}
\Theta_f \gg 1 : \quad J \approx 1 \\
0 \leq \Theta_f \ll 1 : \quad J \approx \Theta_f^4/(4!)
\end{array} \right.
\]

**Preheated zone and matching**

flame temperature of the spherical flame

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

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

\[
\beta \to \infty : \quad \frac{d_L}{R_f} = Le^2 e^{\frac{\beta}{2} (\frac{1}{Le} - 1)} \sqrt{J(\Theta_f)}
\]

\[
T_f \to T^* \Rightarrow R_f/d_L \to \infty \quad \Theta_f \to 0
\]
$T_b$ is determined by the composition of the mixture $Y_{Ru}$ (mass fraction of the limiting component)

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

$\theta^*$ depends on the composition

\[ \theta^* \equiv \frac{T^* - T_u}{T_b - T_u} \]

temperature of the spherical flame kernel

\[ \theta_f = \frac{T_f - T_u}{T_b - T_u} = \frac{1}{Le} \]

temperature of the planar flame

depends on the composition

\[ T_b = T^* \quad \theta^* = 1 \]

\[ T_f = T^* \quad \theta^* < \frac{1}{Le} < 1 \]

\[ \theta_f = \frac{1}{Le} \]

\[ \theta < \frac{1}{Le} \]

$Le > 1 \Rightarrow T_f < T_b$

$Le < 1 \Rightarrow T_f > T_b$

$T_f = T^*$

Flammable limit

flamible mixtures that cannot be ignited (infinite critical radius)

energetic mixtures

$T_b$ / \[ Y_{Ru}^* \]

Flammable mixtures

non-flammable mixtures that can be ignited (flame balls)

energetic mixtures

$T_b$ / \[ Y_{Ru}^* \]

Flammable mixtures

Le $> 1$ : Heavy hydrocarbon lean mixtures

Hydrogen rich mixtures

Le $< 1$ : Heavy hydrocarbon rich mixtures

Hydrogen lean 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

Turbulence facilitates ignition of hydrocarbon lean mixtures.
Turbulence may suppress ignition of hydrocarbon rich mixtures.

simplest explanation:
Turbulent diffusion coefficients are all equal \( \Leftrightarrow \) \( \begin{cases} 
\text{Le} > 1 \Rightarrow \text{Le} = 1 \\
\text{Le} < 1 \Rightarrow \text{laminar} \quad \text{turbulent}
\end{cases} \)
VII-4) Dynamics of slowly expanding flame kernels

Quasi-steady preheated zone of flame kernel?

preheated zone in the reference frame attached to \( R_f(t) \)
\[
\frac{\partial \theta}{\partial t} - \dot{R}_f \frac{\partial \theta}{\partial R} - D_T \frac{1}{R^2} \frac{\partial}{\partial R} \left( R^2 \frac{\partial \theta}{\partial R} \right) = 0
\]

quasi-steady state? \( t_{\text{relax}} \equiv \frac{R^2}{D_T} \ll t_{\text{evol}} \equiv \frac{R_f}{\dot{R}_f} \) \( R \ll \sqrt{D_T t_{\text{evol}}} \), 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
\[
\frac{\partial T}{\partial t} = D_T \Delta T \quad \text{point source, } R = 0, t > 0 : \dot{Q}(t)\]

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

\( \dot{Q} = \text{cst.} \)

\( X' \equiv R/\sqrt{4D_T \tau} \quad dX' = -2D_T R \frac{d\tau}{(4D_T \tau)^{3/2}} \)

\[
T - T_u = \frac{1}{4\pi D_T \rho c_p R} \frac{1}{\sqrt{\pi}} \int_0^\infty dX' e^{-X'^2}
\]

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

\[
R^2/(4D_T t) \rightarrow 0
\]
For $\text{Le} < 1$ and near to the Zeldovich radius the slow evolution of flame kernels is governed by the diffusion at large distance

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

Joulin’s equation (Joulin 1985)

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

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

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)

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

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 \( (R > R_f) \)

\[ x \equiv (R - R_f) \begin{array}{c} \partial \theta \partial t \end{array} - \left( \dot{R}_f + 2 \frac{D_T}{R} \right) \frac{d \theta}{d x} - D_T \frac{d^2 \theta}{d x^2} = 0 \]

\[ \frac{\dot{R}_f}{R_f} \ll \frac{D_T}{(D_T/\dot{R}_f)^2} \Rightarrow R_f \dot{R}_f \gg D_T \]

Semi-phenomenological model

\[ - \left( \dot{R}_f + 2 \frac{D_T}{R} \right) \frac{d \theta}{d x} - D_T \frac{d^2 \theta}{d x^2} = 0 \]

\[ - \left( \dot{R}_f + 2 \frac{D}{R} \right) \frac{d \psi}{d x} - D \frac{d^2 \psi}{d x^2} = 0 \]

+ asymptotic analysis \( \beta \to \infty \)

thin reaction zone \( \Rightarrow F(\dot{R}_f, R_f) = 0 \)

numerical results for a constant heat source


numerical results of He (2000) extended to \( R_f \dot{R}_f \approx D_T \)!

qualitative agreements with the experiments by Kelley et al. (2009)

**Steady converging flames. Opened-tip Bunsen flames**

Frankel Sivashinsky (1984)

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

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

\[ -(Le^{-1} - 1) \beta \frac{d_L}{R_f} \]

no solution below a minimum radius
Structure and Dynamics of Combustion Waves in Premixed Gases

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Lecture VIII
Thermo-acoustic instabilities. Vibratory flames
Lecture 8: **Thermo-acoustic instabilities**

**Lecture 8-1. Rayleigh criterion**

*Acoustic waves in a reactive medium*

*Sound emission by a localized heat source*

*Linear growth rate*

**Lecture 8-2. Admittance & transfer function**

*Flame propagating in a tube*

*Pressure coupling*

*Velocity and acceleration coupling*

**Lecture 8-3. Vibratory instability of flames**

*Acoustic re-stabilisation and parametric instability (Mathieu’s equation)*

*Flame propagating downward (sensitivity to the Markestein number)*

*Bunsen flame in an acoustic field*
VIII-1) Rayleigh criterion

Acoustic waves in a reactive medium

Ideal gas

\[ p = (c_p - c_v) \rho T \]

\[ \frac{c_p}{c_p - c_v} \frac{Dp}{Dt} = c_p T \frac{D\rho}{Dt} + c_p \rho \frac{DT}{Dt} \quad \text{D}/\text{Dt} \equiv \partial/\partial t + \mathbf{u}.\nabla \]

\[ a^2 = (c_p/c_v)(c_p - c_v)T \]

\[ \rho c_p \frac{DT}{Dt} = \frac{c_p}{c_p - c_v} \frac{Dp}{Dt}p - \frac{c_v}{c_p - c_v}a^2 \frac{D\rho}{Dt}\rho \]

Energy conservation

\[ \rho c_p \frac{D\rho}{Dt} = \frac{Dp}{Dt} + \nabla.(\lambda \nabla T) + \sum_j Q^{(j)} \dot{W}^{(j)} \]

\[ \frac{c_v}{c_p - c_v} \frac{Dp}{Dt} - \frac{c_v}{c_p - c_v}a^2 \frac{D\rho}{Dt} = \nabla.(\lambda \nabla T) + \sum_j Q^{(j)} \dot{W}^{(j)} \]

\[ \text{D}p/\text{Dt} - a^2 \text{D}\rho/\text{Dt} = \dot{q}_\gamma \]

isentropic acoustic

\[ \delta p = a^2 \delta \rho \]

\[ \dot{q}_\gamma \equiv (\gamma - 1) \left[ \nabla.(\lambda \nabla T) + \sum_j Q^{(j)} \dot{W}^{(j)} \right] \quad \gamma \equiv c_p/c_v \]

\[ \dot{q}_\gamma (r, t) = \text{heat transfer} + \text{heat release} \]

(rate of energy transfer per unit volume)
Green's retarded propagator
\[ \psi(r, t) = \left( \frac{1}{\alpha^2} \right) \frac{\partial^2 G}{\partial t^2} - \Delta G = \delta(r) \delta(t), \quad G(r, t) = \bar{a} \delta(r - \bar{a}t)/4\pi r \]

spherical geometry 
\[ p'(r, t) = \frac{1}{4\pi \alpha^2} \int \int \frac{1}{r'} \frac{\partial}{\partial t} \dot{q}'(r', t - r/\bar{a}) d^3r' = \frac{\dot{\Omega}(t - r/\bar{a})}{4\pi \alpha^2 r}, \quad r = |r| \]
Liner growth rate

retro-action loop:

Rocket engines, gas turbines...

Simplest retro-action mechanism: pressure coupling + 1-D geometry

\[ \frac{\partial^2 p'}{\partial t^2} - \bar{a}^2 \Delta p' = \frac{\partial q'_\gamma}{\partial t} \]

\[ \frac{\partial^2 \tilde{p}_k}{\partial t^2} - \frac{b}{\tau_{ins}} \frac{\partial \tilde{p}_k}{\partial t} + \bar{a}^2 k^2 \tilde{p}_k = 0 \]

\[ \tilde{p}_k = e^{\sigma t} \]

\[ 2\sigma \tau_{ins} = b \pm \sqrt{b^2 - 4\bar{a}^2 k^2 \tau_{ins}^2} \]

\[ \frac{1}{\tau_{ins}} \ll \omega_k = \bar{a}k \]

\[ \text{Im}(\sigma) = \omega_k + ..., \quad \text{Re}(\sigma) = \frac{b}{(2\tau_{inst})} + ... \]

\[ \{ \begin{array}{ll}
    b > 0 & \text{fluctuations of heat release and pressure in phase: instability} \\
    b < 0 & \text{fluctuations of heat release and pressure out of phase: stability}
\end{array} \]

More general retro-action mechanism

\[ \delta q'_\gamma(x, t) = \frac{1}{\tau_{ins}} \int_{-\infty}^{t} b(t - t') \delta p'(x, t') \, dt' \]

\[ b(\tau) = \int_{-\infty}^{+\infty} r(\omega) e^{i\omega \tau_d(\omega)} e^{i\omega \tau} \, d\omega + \text{c.c.} \quad r(\omega) > 0 \quad \omega \tau_d(\omega) \text{ is the phase lag} \]

\[ -\pi/2 < \omega_k \tau_d(\omega_k) < +\pi/2 : \text{Instability} \]

Nonlinear study: limit cycles in the unstable case
VIII-2) Admittance & transfer function

Flame propagating in a tube

thicknes of the flame brush $\gg$ acoustic wavelength

gas expansion $\Rightarrow$ jump of the fluctuations of the flow velocity (acoustics)

$$\frac{\delta u_b - \delta u_u}{U_L} = O(1)$$

acoustic pressure

$$\delta p = \rho a \delta u$$

$$\frac{p}{\rho a^2} = O(1)$$

jump of the pressure is negligible

$$\frac{\delta p_b - \delta p_u}{p} = \frac{\delta p_f}{O(U_L/a)}$$

$$\delta p_f$$: fluctuation of the pressure at the flame

averaged energy flux (/period) combustion $\rightarrow$ acoustic

$$\dot{\mathcal{E}}_t = (\delta u_b - \delta u_u) \delta p_f$$

Pressure coupling

Definition of the admittance function $Z(\omega)$

$$\delta u(t) = \text{Re} \left[ \hat{u}(\omega) e^{i\omega t} \right]$$

$$\delta p(t) = \text{Re} \left[ \hat{p}(\omega) e^{i\omega t} \right]$$

$$(\hat{u}_b - \hat{u}_u) = Z(\omega) \hat{p}_f / \rho_b a_b$$

$$\left(\hat{q}_\gamma / (\gamma - 1)\right) = \frac{\dot{\mathcal{E}}_t}{\rho a^2}$$

$$(\delta u_b - \delta u_u) = \int \frac{\delta \hat{q}_\gamma}{\rho a^2} \, dx$$

mass conservation (quasi-isobaric combustion)

$$\nabla \cdot \mathbf{u} = \frac{1}{T} \frac{\partial T}{\partial t} = \frac{\dot{q}_\gamma}{\rho c_p T} = \frac{\dot{q}_\gamma}{\rho a^2}$$

Analytical study of a planar flame submitted to a fluctuation of pressure $(\beta \rightarrow \infty)$

$$\delta T_f / T_f \propto \delta p_f / p_f$$

$$|Z| = O(M_b)$$

gaseous flame

$$\frac{\text{Re}(Z)}{M_b}$$

$$\frac{\tau_a}{\tau_{\text{ins}}} \propto \frac{E}{(\gamma - 1)M_b k_B T_b}$$

coeff depends on the position in the tube as $\delta p_f$ does

$$\rho_f, \hat{u}_b$$

Solid propellant

$$\text{Re}(Z)$$

Unsteady calculation Quasi steady state

Clavin Lazimi 1992

Zeldovich 1942

Clavin et al. 1990

Clavin Searby 2008

Laser tomography (Boyer 1980)
Velocity and acceleration coupling

fluctuating velocity ⇒ modification to flame geometry
⇒ fluctuation of heat release through the flame surface

Transfer function for a flame in a tube $T_r(\omega)$

$$\hat{u} \hat{p}_f^* = -\hat{u}^* \hat{p}_f$$

phase quadrature (acoustic mode of a tube)

Weakly cellular flame propagating downward in an acoustic wave

acceleration of a curved flame ⇒ modulation of the flame surface $S = \int dy \sqrt{1 + \alpha'^2_y}$

$$\int \delta \hat{q} \, dx = \rho_u U_L c_p (T_b - T_u) \delta S/S_o$$

fluctuation of heat release rate/ cross-section aera

Consider a curved front slightly perturbed

$$x = \alpha(y, t)$$

$$\alpha(y, t) = \tilde{\alpha}(t) \cos(ky)$$

$$\tilde{\alpha}(t) = \tilde{\alpha}_0 + \tilde{\alpha}_1 e^{i\omega t} + c.c$$

$$k \tilde{\alpha}_0 \ll 1 \quad |\tilde{\alpha}_1| \ll \tilde{\alpha}_0 \quad (\text{linear response ok}) \quad \Rightarrow \quad \delta S/S_o = (T_b/T_u - 1) U_L \delta S/S_o$$

$$\delta u_b - \delta u_u = \int \frac{\delta \hat{q}}{\rho a^2} \, dx \quad \Rightarrow \quad \delta u_b - \delta u_u = (T_b/T_u - 1) U_L \delta S/S_o$$

$$\hat{u} \hat{p}_f^* = -\hat{u}^* \hat{p}_f$$

Real number (sign depends on position)

$$(\delta u_b - \delta u_u) = \frac{1}{4} \left( T_r \hat{u}_u \hat{p}_f^* + T_r^* \hat{u}_u^* \hat{p}_f \right)$$

$$\dot{\epsilon}_t = \frac{1}{2} \left( T_r \hat{u}_u \hat{p}_f^* + T_r^* \hat{u}_u^* \hat{p}_f \right)$$

Analytical expression ($k = k_c$)

(Pelcé Rocheweger 1992)

ok for the primary instability
VIII-3) Vibratory instability of flames

primary instability + re-stabilisation + parametric instability

Acoustic instability in Premixed Flames

Acoustic re-stabilisation and parametric instability

Markstein 1964

\[ \tau' \equiv t / \tau_h, \quad \tau_h \equiv 1 / (U_L k), \quad \varpi \equiv \omega \tau_h, \quad = (\omega \tau_L) / (k d_L) \quad \kappa = k d_L \]

\[ v_b \equiv \rho_u / \rho_b > 1 \]

\[ B \equiv \frac{v_b}{v_b + 1} \]

\[ D \equiv \frac{v_b}{v_b + 1} \left( \frac{v_b - 1}{v_b + 1} \right) \frac{N}{\kappa} \]

\[ C \equiv \left( \frac{v_b - 1}{v_b + 1} \right) \frac{u_a}{\varpi}, \]

\[ g'(t) = \omega u_a U_L \cos(\omega t) \]

Mathieu’s equation. Kapitza pendulum

\[ t \equiv \varpi \tau' \quad Y(t) \equiv e^{B \tau'} \tilde{\alpha} \]

\[ \frac{d^2 Y}{dt^2} + \left\{ \Omega + h \cos(t) \right\} Y = 0 \]

\[ \Omega = - \frac{(D + B^2)}{\varpi^2} \]

\[ h = C \]

Kapitza 1951
Mathieu’s equation. Kapitza pendulum

\[
\frac{d^2 Y}{dt^2} + \{\Omega + h \cos(t)\} Y = 0
\]

\(\Omega > 0\) : Oscillator whose frequency \(\sqrt{\Omega}\) is modulated  

Prametric instability (Faraday 1831)

\(\Omega < 0\) : Re-stabilization of an unstable position of a pendulum by oscillations (Kapitza 1951)

Stability limits of the solutions to Mathieus’s equation

White regions: stable. Grey regions unstable

Flame propagating downward

\[
\frac{d^2 \tilde{\alpha}}{d\tau^2} + 2B \frac{d\tilde{\alpha}}{d\tau} + \left[-D + \omega^2 \cos(\omega \tau') \right] \tilde{\alpha} = 0
\]

Markstein 1960

\[
u_{aI}^* \approx 2v_b \frac{(v_b + 1)}{(v_b - 1)} \left(1 - \frac{U_{Le}}{U_L}\right), \quad \frac{k_I^*}{k_m} \approx \frac{1}{2} \frac{U_{Le}}{U_L}
\]

Bychkov 1999  

Clavin 2015  

ok with experiments Searby Rochewerger 1991
Sensitivity of the acoustic instability to the Markstein number and the acoustic frequency

Flattening of Bunsen flames in an acoustic field (Hahnemann Ehret 1943, Durox et al. 1997, Baillot et al. 1999)

Rich Bunsen methane flame + intense axial acoustic field 140 Hz
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Lecture IX
Turbulent flames
Lecture 9: Turbulent flames

9-1. Introduction

9-2. Turbulent diffusion

\textit{Einstein-Taylor’s diffusion coefficient}
\textit{Rough model of turbulent transport}
\textit{Well-stirred flame regime}

9-3. Strongly corrugated flammmelets regime

\textit{Kolmogorov’s cascade}
\textit{Gibson’s scale}
\textit{Elements of fractal geometry}
\textit{Self similarity of strongly corrugated flames}
\textit{Co-variant laws}

9-4. Turbulent combustion noise

\textit{Monopolar sound emission}
\textit{Sound generated by a turbulent flame}
\textit{Blow torch noise}
IX-1) Introduction

The problem of premixed flames in a turbulent flow is still widely open.

Experiments are difficult. Experimental data are very scattered.

The simplest model has no known solution (Nonlinear stochastic equation)

Reaction-diffusion wave in a turbulent flow (no gas expansion)

\[
\frac{\partial \theta}{\partial t} + \mathbf{v}(\mathbf{r}, t) \cdot \nabla \theta - D_T \Delta \theta = \omega'(\theta)/\tau_{rb}.
\]

prescribed turbulent flow (stochastic field)

Same model in the wrinkled flame regime  
\((l_{tur} \gg d_L, \tau_{tur} \gg \tau_L \Rightarrow U_n = U_L)\)

eq. flame surface  
\[ G(\mathbf{r}, t) = G_0 \quad \partial G/\partial t + (\mathbf{d}/\mathbf{d}t).\nabla G = 0 \quad \mathbf{d}/\mathbf{d}t = \mathbf{v}(\mathbf{r}, t) - U_n \mathbf{n} \quad \mathbf{n} = \nabla G/|\nabla G| \]

\[ \mathbf{v} = (u, w_y, w_z) \quad x = \alpha(y, z, t) \quad G - G_0 = x - \alpha(y, z, t) \quad \partial \alpha/\partial t - u(\mathbf{r}_f, t) + w(\mathbf{r}_f, t) \cdot \nabla yz \alpha = U_{tur} - U_n \sqrt{1 + |\nabla yz \alpha|^2} \]

\[ \langle S \rangle = \int \int \mathbf{d}x \mathbf{d}y \left\{ \sqrt{1 + |\nabla yz \alpha|^2} \right\} \quad U_{tur}/U_L = \left\{ \sqrt{1 + |\nabla yz \alpha|^2} \right\} \]

\[ U_{tur} S_o = U_L \langle S \rangle \]

The very existence of \( \langle S \rangle \) and \( d_{tur} \) is questionable.

\(|\mathbf{v}| \ll U_L : U_{tur}/U_L \approx 1 + (|\mathbf{v}|/U_L)^2 \quad |\mathbf{v}| \gg U_L : U_{tur} \approx |\mathbf{v}| \)

(Bending effect  
modification to the laminar flame structure (Shchelkin 1943, Clavin Williams 1979)  
(Damköler 1940)
IX-2) Turbulent diffusion

**Taylor’s diffusion coefficient** (analogy with Einstein random walk for molecular diffusion)

1-D for simplicity: \(\frac{dx}{dt} = v(t), \quad x(t) = \int_0^t v(t')dt'\)

\[\langle x^2(t) \rangle = \int_0^t dt' \int_0^t dt'' \langle v(t')v(t'') \rangle \]

\[\langle x^2(t) \rangle = 2 \int_0^t dt' \int_0^t d\tau \langle v(t')v(t' - \tau) \rangle\]

turbulence: homogeneous in time \(\langle v(t)v(t - \tau) \rangle = \langle v^2 \rangle g(\tau) \quad g(0) = 1, \quad \lim_{\tau \to \infty} g = 0\)

integration by parts \(\langle x^2(t) \rangle = 2 \langle v^2 \rangle \int_0^t (t - \tau)g(\tau)d\tau\) where \(\int_0^\infty \tau g(\tau)d\tau = O(\tau_I^2) \quad t \gg \tau_I: \quad g = 0\)

t \(\gg \tau_I, 1-D: \langle x^2(t) \rangle = 2D_{tur} t, \quad 3-D: \langle x^2(t) \rangle = 6D_{tur} t, \quad \text{where} \quad D_{tur} \equiv \langle v^2 \rangle \tau_I \quad \langle v^2 \rangle = (\text{turbulence intensity})^2\)

**Rough model for the turbulent transport** (analogy with molecular diffusion)

\(\langle v \theta \rangle \approx -D_{tur} \nabla \langle \theta \rangle, \quad \langle \nabla . (v \theta) \rangle \approx -D_{tur} \Delta \langle \theta \rangle\)

limited to scalar mixing with small displacement / size (blobs, sheets ..) \(l_I \ll L \quad (v_I \approx \langle v^2 \rangle^{1/2} l_I \equiv v_I \tau_I)\)

\[D_{tur} \equiv l_I v_I\]

**Well-stirred flame regime of Damköhler** (1940) \(l_I \ll d_L \quad \text{and} \quad D_{tur} \gg D_T\)

little practical importance

\[U_{tur} \approx \sqrt{D_{tur}/\tau_b} \quad \frac{U_{tur}}{U_L} \approx \sqrt{\left(\frac{l_I}{d_L}\right) \left(\frac{v_I}{U_L}\right)} \gg 1, \quad d_{tur} \approx D_{tur}/U_{tur} \gg d_L\]
IX-3) Strongly corrugated flammelets regime

Kolmogorov’s cascade (homogeneous, isotropic and fully-developed turbulence)

Decomposition into a sum of vorties of different length and time scales

\[ l_i, \tau_i, v_i \equiv l_i/\tau_i \]

turn-over velocity \( \text{Re}_i \equiv l_i v_i/\nu \)

local Reynolds nb \( \nu \equiv \mu/\rho \)

Kolmogorov scale \( l_K, \tau_K, v_K \) \( \text{Re}_K = 1 \)

\( l_i > l_K \) \( v_i > v_K \) \( \forall i \)

Integral scale \( l_I, \tau_I, v_I \) \( \text{Re}_I \gg 1 \)

\( l_I > l_i \) \( v_I > v_i \) \( \forall i \)

Scaling laws (dimensional analysis) \( l_K \ll l_i \ll l_I \)

energy transfer in NS eqs : \( \rho (v \cdot \nabla) v^2/2 \) \( v_i^3/l_i \equiv \epsilon \approx \text{cst} \Rightarrow \epsilon \approx \epsilon^{1/3} l_i^{1/3}, \quad v_i^2 \approx \epsilon^{2/3} l_i^{2/3}, \quad \tau_i \approx \epsilon^{-1/3} l_i^{2/3} \)

dissipation rate of energy : \( \nu \nabla \Delta v \Rightarrow \epsilon = \nu v_K^2/l_K^2 \quad \epsilon = v_i^3/l_I \)

\[ \text{Re}_K \equiv v_K l_K/\nu = 1 \Rightarrow l_I/l_K \approx \text{Re}_I^{3/4}, \quad v_I/v_K \approx \text{Re}_I^{1/4}, \quad \tau_I/\tau_K \approx \text{Re}_I^{1/2} \]

Re\(_I \gg 1 \)

energy spectrum : \( \langle v^2 \rangle /2 = \int_0^\infty dk E(k) \) \( E(k) \approx \epsilon^{2/3} k^{-5/3} \)

definition of strongly corrugated flames

\[ v_K \ll U_L \ll v_I \Rightarrow d_L \ll l_K, \quad \tau_L \ll \tau_K \]

no modification to the laminar flame structure

definition of the Gibson scale: smallest size of the wrinkles on the flame front

\[ l_L^3 \]

turn-over time = transit time across the vortex \( \tau_i \approx l_i/U_L \Rightarrow v_i \approx U_L \)

\[ l_G \equiv U_L^3/\epsilon \Rightarrow l_K \ll l_G \ll l_I \]

many scales of wrinkles \( l_G \ll l_I \Rightarrow \) fractal geometry of the flame front
Elements of fractal geometry

Total surface area in a cube of size $l_i$, $l_G < l_i < l_I$ \[ S_i \approx N_{i,G} l_G^2. \]

nb of cubes of size $l_G$ that intersect the surface within the volume $l_i^3$

Weaker resolution $l_j$, $l_G < l_j < l_i$ \[ S_{i,j} \approx N_{i,j} l_j^2 \]

nb of cubes of size $l_j$ that intersect the surface within the volume $l_i^3$

Details of small scales are lost as the size of the box $l_j$ increases \[ S_{i,j+k} < S_{i,j} < S_i \quad N_{i,j+k} < N_{i,j} < N_i \]

Fractal dimension $D_f > 2$ : $N_{i,j} \approx (l_i/l_j)^{D_f}$, $S_{i,j}/l_i^2 \approx (l_i/l_j)^{D_f-2}$

Regular surface: $D_f = 2 \Rightarrow$ total area $S_i$ in a box of size $l_i$ \[ S_i/l_i^2 = \lim_{l_j \to 0} S_{i,j}/l_i^2 = \text{finite cst.} \]

For a flame of thickness $d_L$ its area is well defined for wrinkles whose scale is larger than $d_L$, $l_j > d_L$

The fractal dimension $D_f > 2$ can concern only scales greater than the smallest wrinkles

Fractal dimension of a turbulent flame can be meaningful only for $d_L < l_G < l_j < l_i < l_I$
Self similarity of strongly corrugated flames

\[ v_K \ll U_L \ll v_I \quad d_L \ll l_K \ll l_G \ll l_I \]

Assumption: the Kolmogorov cascade is not modified by gas expansion \( \text{ok for } l_i \gg l_G \)

Contamination time vs combustion time

Kolmogorov cascade

\[ \tau_i \approx \epsilon^{-1/3} l_i^{2/3} \quad l_i \quad v_i \approx \epsilon^{1/3} l_i^{1/3} \quad l_i \]

Fastest contamination: integral scale \( v_I \gg v_i \). \( U_{\text{tur}} = v_I \)?

\( \text{ok if the combustion time of the vortex is not longer than the turnover time} \)

Self similar law

An effective front of thickness \( l_i \) is defined at each scale

A flame velocity \( U_i \) can be defined at each scale if

\[ U_i = (S_{i,j}/l_i^2)U_j \quad U_i/U_j = \langle S_{i,j} \rangle /l_i^2 \]

At the Gibson scale the combustion time of the vortex = turnover time \( U_L = v_G \)

Self similarity: same law at all scales \( \Rightarrow \) combustion time of the vortex = the turnover time \( \forall l_i \)

\[ l_i/U_i = \tau_i \quad \Rightarrow \quad U_i = v_i \]

Kolmogorov cascade \( \Rightarrow \) small vortices burn faster than larger ones

\[ U_{\text{tur}} = v_I, \quad l_{\text{tur}} = l_I \]

Fractal dimension of the flame surface:

\[ U_i/U_j = \langle S_{i,j} \rangle /l_i^2 \quad \Rightarrow \quad u_i/u_j = \langle S_{i,j} \rangle /l_i^2 \quad \Rightarrow \quad \langle S_{i,j} \rangle /l_i^2 = (l_i/l_j)^{1/3} \quad \Rightarrow \quad D_f = 7/3 \]

\[ \langle S_{i,j} \rangle /l_i^2 = (l_i/l_j)^{D_f-2} \]

The result is the same for all mixtures...??
Co-variant laws

P. Clavin IX

More general law independent of the turbulent scaling and satisfying additivity

Turbulent energy contained in the range \([l_i, l_j]\) : 
\[v_{i,j}^2 \equiv \sum_{k=i}^{j-1} v_k^2\]

Co-variant law = same for each couple of length scales \(l_i, l_j\) \(l_i \geq l_j\)

The only co-variant law for the flame velocity \(U_i\) at scale \(l_i\) satisfying additivity is 
\[U_i^2 = U_j^2 + c v_{i,j}^2\]

Co-variance ? \(l_i > l_k > l_j\), 
\[v_{i,j}^2 = v_{i,k}^2 + v_{k,j}^2\]
\[U_i^2 = U_j^2 + c v_{i,k}^2 + c v_{k,j}^2 = U_k^2 + c v_{i,k}^2\]

co-variance ok 
\[U_i^2 = U_k^2 + c v_{i,k}^2\]

\[\frac{\nu^2}{U_{L}^2} = O(1), \frac{l_I}{l_K} \approx 180\]

Pocheau 1994

Pocheau 1996
IX-4) Turbulent combustion noise

wavelength \( a/\omega \gg L \) size of the flame

**Monopolar sound emission**

Deformable (small) body with fluctuating volume \( V(t) \)

\[
u = \nabla \phi(r, t) \quad \text{acoustic potential} \quad \phi(r, t) = -\frac{\dot{V}(t - a r)}{4\pi r} \quad r \equiv |r|, \quad \dot{V}(t) \equiv \frac{dV}{dt}\]

\( r \gg L : \quad v = (4\pi ar)^{-1}\ddot{V}(t - r/a), \quad \ddot{V}(t) \equiv \frac{d^2V(t)}{dt^2} \)

Radiated flux of energy (intensity of sound) \( I \equiv \rho a \langle v^2 \rangle \)

\[
I = (\rho/4\pi a) \left\langle \left(\frac{dV}{dt}\right)^2 \right\rangle
\]

**Sound generated by a turbulent flame**

\[
\dot{M}_b = \rho_b \int_S (D_f + U_b) d^2\sigma
\]

\[
\dot{M}_u = \rho_u \int_S (D_f + U_L) d^2\sigma
\]

\( \rho_u U_L = \rho_b U_b \)

\[
dV/dt = \dot{M}_b/\rho_b
\]

\[
\dot{M}_u/\rho_u + (U_b - U_L)S
\]

\[
dV/dt = (U_b - U_L)S(t)
\]

\[
I = (\rho/4\pi a)(U_b - U_L)^2 \left\langle \left(\frac{dS}{dt}\right)^2 \right\rangle
\]

Intensity of sound

Strahle 1985

\[
d\tilde{I}(\omega)/d\omega = \frac{\rho}{4\pi a} (U_b - U_L)^2 \int_0^\infty dt e^{i\omega t} \left\langle \dot{S}(t)\dot{S}(0) \right\rangle
\]

Power spectrum of sound
\[ I = \left(\frac{\rho}{4\pi a}\right) \left(U_b - U_L\right)^2 \langle (dS/dt)^2 \rangle \]

Stongly corrugated regime with a Kolmogorov cascade:

\[ D_f = 4/3 \Rightarrow I \approx \frac{1}{4\pi} \left(\frac{T_b}{T_u} - 1\right)^2 \rho \Delta V \frac{v_I^4}{a l_I} \]

\[ \text{total volume of the flame brush} \]

\[ d\tilde{I}(\omega)/d\omega = \frac{\rho}{4\pi a} \left(U_b - U_L\right)^2 \int_{0}^{\infty} dt e^{i\omega t} \langle \dot{S}(t)\dot{S}(0) \rangle \]

\[ d\tilde{I}(\omega) \propto \omega^{-5/2} d\omega \]

Clavin Siggia 1991

in agreement with experiments on very large burners

(Abugov Obrezkov 1978)

**Blowtorch noise**

Combustion noise is two orders of magnitude higher
the noise is not resulting from the direct interaction of upstream turbulence on the flame front
amplification by the intrinsic flame instability is essential

(Searby 2001)
Structure and Dynamics of Combustion Waves in Premixed Gases

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Lecture X
Supersonic waves
Lecture 10: **Supersonic waves**

10-1. Background

*Model of hyperbolic equations for the formation of discontinuity*

*Riemann invariants*

*Rankine-Hugoniot conditions for shock waves*

*Mikhelson (Chapman-Jouguet) conditions for detonations*

10-2. Inner structure of a weak shock wave

*Formulation*

*Dimensional analysis*

*Analysis*

10-3. ZND structure of detonations

10-4. Selection mechanism of the CJ wave
PLANAR SHOCK WAVE
INERT GAS

$D > a_u$

$U_N = D - v_p$

Supersonic

Subsonic

thickness: few mean free paths

Poisson 1808, Stokes 1848, Riemann 1860, Rankine 1869, Hugoniot 1889, Rayleigh 1910
SHOCK WAVE AS A SINGULARITY OF THE EULER EQUATIONS
shock wave \approx \text{discontinuity in the solution of the Euler equations}

**Model of hyperbolic equations for the formation of discontinuities**

\[ a(u) \frac{\partial u}{\partial t} + a(u)\frac{\partial u}{\partial x} = 0 \]

\[ t = 0 : \quad u = u_o(x) \quad \text{and} \quad u = u(x,t) ? \]

Simple case: linear equation

\[ a = a_o = \text{cst.} : \quad u = u_o(x - a_o t) \]

propagation at constant velocity without deformation

Nonlinear equation \( a(u) \neq 0 \)

**Method of characteristics**

The solution is conserved along any trajectory \( \frac{dx}{dt} = a(u) \) in the phase plan \((x,t)\).

\[ u = u(x(t), t) \quad \text{and} \quad \frac{du}{dt} = 0 \]

\( u(x,t) \) is constant along the straight lines \( x = a_o t + x_o \):

\[ u = a_o \equiv u(a_o) \]

Finite-time singularity
Nonlinear equation \[
\frac{\partial u}{\partial t} + a(u) \frac{\partial u}{\partial x} = 0
\]
\[
t = 0 : \quad u = u_o(x)
\]
\[
u = u(x, t) ?
\]

**Method of characteristics**

Trajectories \(x(t)\) : \[
dx/dt = a(u) \quad u = u(x(t), t) \quad du/dt = 0
\]

\[
u(x, t) = \text{cst.} \Rightarrow a(x, t) = \text{cst.}
\]

\(u(x, t)\) is constant along the straight lines; \[
t = 0 : \quad x = a_o t + x_o, \quad u = u_o
\]

\[
x = a_o t + x_o \quad \quad u_o \equiv u(a_o)
\]

Speed increases with increasing \(u\), \(da/du > 0\)

\(\Rightarrow\) formation of singularities after a finite time

larger values run faster

\[
u_o(x) \equiv u(x, t = 0)
\]

\(t > t_b : \) multivalued solution. Wave breaking

\(t > t_b : \) characteristics intersect
\[ \partial u / \partial t + a(u) \partial u / \partial x = 0 \]

Speed increases with increasing \( u \), \( da/du > 0 \)

\[ \Rightarrow \text{formation of singularities after a finite time} \]

\[ u_o(x) \equiv u(x, t = 0) \]

\[ u(x, t) = u_o(x_o(x, t)) \]

\[ x(x_o, t) = a_o(x_o)t + x_o \text{, trajectory} \]

\[ \frac{\partial u}{\partial x} = \frac{\partial x_o}{\partial x} \frac{du_o}{dx_o} \quad \text{diverges at time} \quad t = \frac{1}{-da_o/dx_o} \text{ where } da_o/dx_o < 0 \]

\[ t_b \equiv \text{time of wave breaking} \text{ (shortest time for the divergence of } \partial u / \partial x \text{)} \]

\[ t_b = \frac{1}{\max |da_o/dx_o|} \]
Discontinuous solutions

\[ \frac{\partial u}{\partial t} + a(u) \frac{\partial u}{\partial x} = 0 \quad \text{conservative form} \quad \frac{\partial u}{\partial t} + \frac{\partial j}{\partial x} = 0 \]

\[ j(u) \quad \frac{dj}{du} = a(u) \quad j(u) \equiv \int_{u_-}^{u} a(u') du' \]

Are step functions \( u_+ \neq u_- \) propagating at constant velocity \( D \) solutions?

\[ u(\xi) \quad \xi = x - Dt \]

\[ \frac{\partial}{\partial t} = -D \frac{d}{d\xi} \quad \frac{\partial}{\partial x} = \frac{d}{d\xi} \]

\[ -D \frac{du}{d\xi} + \frac{dj}{d\xi} = 0 \quad j - Du \quad \text{is a conserved scalar} \]

\[ j(u_+) - Du_+ = j(u_-) - Du_- \quad D = \frac{j(u_+) - j(u_-)}{u_+ - u_-} \]

Infinite numbers of solutions !! **Ill posed problem**

\[ f(u) \times \left( -D \frac{du}{d\xi} + \frac{dj}{d\xi} \right) = 0 \]

\[ G - DF = \text{cst.} \quad D = \frac{G(u_+) - G(u_-)}{F(u_+) - F(u_-)} \quad \text{where} \quad \frac{dF}{du} \equiv f(u) \quad \frac{dG}{du} \equiv f(u)a(u) \]
**Discontinuous solutions**

\[ \frac{\partial u}{\partial t} + a(u) \frac{\partial u}{\partial x} = 0 \]

Are step functions \( u_+ \neq u_- \) propagating at constant velocity \( D \) solutions?

\[ u(\xi) \quad \xi = x - Dt \]

Infinite numbers of solutions!! \textcolor{red}{Ill posed problem}

---

**adding a dissipative term makes the problem well posed**

\[ \frac{\partial}{\partial t} = -D \frac{d}{d\xi} \quad \frac{\partial}{\partial x} = \frac{d}{d\xi} \]

\[ \frac{d}{d\xi} \left[ -uD + j(u) - \epsilon \frac{du}{d\xi} \right] = 0 \quad \epsilon \frac{du}{d\xi} = j(u) - uD + \text{cst} \quad \xi = \int_0^u \frac{du}{j(u) - uD + \text{cst}} \quad j(u) \equiv \int_{u_-}^u a(u') du' \]

\[ \xi = \pm\infty : \frac{du}{d\xi} = 0 \Rightarrow 2 \text{ expressions of the cst that should be equal} \Rightarrow \text{a single value of } D \]

\[ D = \frac{j(u_+) - j(u_-)}{u_+ - u_-} \quad \text{independent of } \epsilon! \]

\[ u(\xi) \text{ continuous function} \quad \lim_{\epsilon \to 0} u = \text{step function} \]

\[ a(u) = u : \text{Burgers equation. Analytical solution to the initial value problem} \]
Riemann invariants (1860)

Euler equation + constant entropy + ideal gas: \[ a^2 = \frac{dp}{d\rho} = \gamma \frac{p}{\rho} \quad \frac{p}{\rho^\gamma} = \text{cst} \quad 2 \frac{da}{a} = \frac{dp}{p} - \frac{d\rho}{\rho} \Rightarrow 2 \frac{da}{a} = (\gamma - 1) \frac{d\rho}{\rho} \]

\[ \lambda \times \frac{\partial}{\partial t} \rho + u \frac{\partial}{\partial x} \rho + \rho \frac{\partial}{\partial x} u = 0 \quad \frac{a^2}{\rho} \frac{\partial}{\partial x} \rho + \frac{\partial}{\partial t} u + u \frac{\partial}{\partial x} u = 0 \]

\[ \lambda \frac{\partial}{\partial t} \rho + \left( \lambda u + \frac{a^2}{\rho} \right) \frac{\partial}{\partial x} \rho + \frac{\partial}{\partial t} u + (\lambda \rho + u) \frac{\partial}{\partial x} u = 0 \]

choose \( \lambda \) such that \( \lambda u + a^2/\rho = \lambda (\lambda \rho + u) \), \( \Rightarrow \lambda = \pm a/\rho \)

\[ \lambda \rho + u = u \pm a \]

2 characteristics:

invariants:
\[ \lambda d\rho + du = 0 \quad \pm \frac{a}{\rho} d\rho + du = 0 \]

\[ J_+ \equiv \frac{2}{\gamma - 1} a + u = \text{cst sur } C_+ \quad J_- \equiv \frac{2}{\gamma - 1} a - u = \text{cst sur } C_- \]

Simple waves

\( C_+ \) are straight lines

Rarefaction wave

Compression wave

formation of a singularity: shock wave

Riemann 1860
**Centred waves**

\[ t < 0 : \text{piston velocity} = 0 \]
\[ t > 0 : \text{piston velocity} = \text{cst} \neq 0 \]

Sel-similar solutions \(x/t\)

Shock wave at constant velocity > piston velocity

no discontinuity of \(u\)

Discontinuity of \(du/dx\) propagating at the local sound speed

Fully unsteady process: thickness \(u_p t\)
JUMP CONDITIONS ACROSS A SHOCK WAVE
Shock waves

Rankine-Hugoniot conditions for shock waves
(1870 – 1880)

Eqs for the conservation of mass, momentum and energy

\[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} = 0 \quad \frac{\partial (\rho u)}{\partial t} = -\frac{\partial}{\partial x} \left( p + \rho u^2 - \mu \frac{\partial u}{\partial x} \right) \quad \frac{\partial (\rho e_{tot})}{\partial t} = -\frac{\partial}{\partial x} \left[ \rho u (h + u^2/2) - \lambda \frac{\partial T}{\partial x} - \mu u \frac{\partial u}{\partial x} \right]
\]

\[
m \equiv \rho u D = \rho_N u_N \quad p_u + \frac{m^2}{\rho_u} = p_N + \frac{m^2}{\rho_N} \quad h_N - h_u + (u_N^2 - D^2)/2 = 0
\]

written in the moving frame of the shock at velocity \( D \)

steady problem

\[
p_u - p_N = m^2 \left[ \frac{1}{\rho_N} - \frac{1}{\rho_u} \right] \quad h_u - h_N = \frac{m^2}{2} \left[ \frac{1}{\rho_N^2} - \frac{1}{\rho_u^2} \right]
\]

\[
h(\rho_u, p_u) - h(\rho_N, p_N) + \frac{1}{2} \left( \frac{1}{\rho_u} + \frac{1}{\rho_N} \right) (p_N - p_u) = 0
\]

Hugoniot curve \( (p - 1/\rho) \)

\[
h(p, \rho) - h(p_u, \rho_u) - \frac{1}{2} \left( \frac{1}{\rho_u} + \frac{1}{\rho} \right) (p - p_u) = 0
\]

Michelson-Rayleigh line

\[
p - p_u = -m^2 \left( \frac{1}{\rho} - \frac{1}{\rho_u} \right)
\]
Ideal (polytropic) gas \( \gamma \equiv c_p/c_v \)

\[
p = (c_p - c_v)\rho T, \quad h = c_p T = \frac{\gamma}{\gamma - 1} p
\]

Hugoniot curve \( \mathcal{P} = -M_u^2 \mathcal{V} \)

\[
\mathcal{P} = \frac{(\gamma + 1)}{2}\left(\frac{P}{P_u} - 1\right), \quad \mathcal{V} = \frac{(\gamma + 1)}{2}\left(\frac{\rho_u}{\rho} - 1\right)
\]

Shocked gas (Neumann state) vs \( M_u \)

\[
\frac{u_N}{D} = \frac{\rho_u}{\rho_N} = \frac{(\gamma - 1)M_u^2 + 2}{(\gamma + 1)M_u^2}, \quad \frac{p_N}{p_u} = \frac{2\gamma M_u^2 - (\gamma - 1)}{(\gamma + 1)} \quad \frac{T_N}{T_u} = \frac{[2\gamma M_u^2 - (\gamma - 1)](\gamma - 1)M_u^2 + 2}{(\gamma + 1)^2 M_u^2}
\]

\[M_N^2 = \frac{(\gamma - 1)M_u^2 + 2}{2\gamma M_u^2 - (\gamma - 1)} \implies 2\gamma M_u^2 M_N^2 - (\gamma - 1)(M_u^2 + M_N^2) - 2 = 0\]

General comments

The Hugoniot curve is tangent to the isentropic

the entropy change along the Hugoniot curve is of third order \( \Rightarrow M_u \equiv D/a_u > 1 \)

\[
\delta s = s - s_u, \quad \delta p = p - p_u, \quad \delta s \neq \delta p
\]

The Hugoniot relation is not an iso-function of state

\[
h(p, \rho) - h(p_u, \rho_u) - \frac{1}{2}\left(\frac{1}{\rho_u} + \frac{1}{\rho}\right)(p - p_u) = 0 \quad \text{cannot be written in the form} \quad \mathcal{H}(1/\rho, p) = \mathcal{H}(1/\rho_u, p_u)
\]

\[
h(p, \rho) - h(p_N, \rho_N) - \frac{1}{2}\left(\frac{1}{\rho_N} + \frac{1}{\rho}\right)(p - p_N) = 0 \neq h(p, \rho) - h(p_u, \rho_u) - \frac{1}{2}\left(\frac{1}{\rho_u} + \frac{1}{\rho}\right)(p - p_u) = 0
\]

Rarefaction shock does not exist. The entropy of the fluid increases through the shock \( \text{(Irreversibility)} \)

can be proved for weak shock by the entropy balance or by the H-theorem using the Boltzmann equation

\[
\rho_u \frac{ds}{dx} = \frac{d}{dx} \left(\frac{\lambda}{T} \frac{dT}{dx}\right) + \dot{\omega}_s, \quad \dot{\omega}_s > 0
\]
INNER STRUCTURE OF A SHOCK
Inner structure of a weak shock

\[ \frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} = 0 \]

\[ \frac{\partial (\rho u)}{\partial t} = -\frac{\partial}{\partial x} \left( p + \rho u^2 - \mu \frac{du}{dx} \right) \]

\[ \frac{\partial (\rho e_{\text{tot}})}{\partial t} = -\frac{\partial}{\partial x} \left[ \rho u (h + u^2/2) - \lambda \frac{dT}{dx} - \mu u \frac{du}{dx} \right] \]

Formulation

( reference frame attached to the shock wave )

\[ \rho u = m, \quad p + \rho u^2 - \mu \frac{du}{dx} = \text{cst.} \]

\[ m \left( h + \frac{u^2}{2} \right) - \lambda \frac{dT}{dx} - \mu u \frac{du}{dx} = \text{cst.} \]

\[ x \to -\infty: \quad p = p_u, \quad \rho = \rho_u, \quad u = \mathcal{D} \]

\[ x \to \infty: \quad \frac{dp}{dx} = 0, \quad \frac{dp}{dx} = 0, \quad \frac{du}{dx} = 0 \]

\[ m = \rho_u \mathcal{D} \quad \frac{p}{\rho} = (\gamma - 1) c_v T \quad h = \frac{\gamma p}{\gamma - 1 \rho} \]

Two coupled equations for \( p \) and \( v \equiv 1/\rho, m \) given \((u = mv, \ c_v T = pv/(\gamma - 1))\)

\[ \frac{\gamma}{\gamma - 1} (pv - p_u v_u) - \frac{1}{2} (p - p_u)(v + v_u) = \frac{\gamma}{\gamma - 1} mc_p \frac{d (pv)}{dx} + \frac{\mu m}{2} (v - v_u) \frac{dv}{dx} \]

\[ x \to \infty: \quad \frac{dp}{dx} = 0, \quad \frac{dv}{dx} = 0 \]

Dimensional analysis

\[ \frac{\rho u^2}{\mu \frac{du}{dx}} \]

\[ \frac{\text{speed of sound}}{\text{mean free path}} = O(1), \quad \frac{\mu/\rho}{\ell/a} \approx \text{viscous diffusion coefficient} \approx \text{kinetic theory of gases} \]

\[ \Rightarrow \] thickness of shock waves \( \approx \) mean free path

macroscopic equations not valid ?

ok for weak shock !
\( M_u \equiv D/a_u > 1 \)  

**Analysis for** \( \epsilon \equiv M_u - 1 \ll 1 \)  
(weak shock) \( D/a_u = 1 + \epsilon \)

\[
(p - p_u) + m^2(v - v_u) = \mu m \frac{dv}{dx},
\]

\[
\frac{\gamma}{\gamma - 1} (p v - p_u v_u) - \frac{1}{2} (p - p_u)(v + v_u) = \frac{\gamma}{\gamma - 1} \lambda m c_p \frac{d(p v)}{dx} + \frac{\mu m}{2} (v - v_u) \frac{dv}{dx}
\]

\( x \to -\infty : p = p_u, \ v = v_u \)

\( x \to \infty : dp/dx = 0, \ dv/dx = 0 \)

**Non-dimensional equations**

\[
\nu \equiv 1/\rho \quad \nu \equiv (v - v_u)/v_u = O(\epsilon) \quad \pi \equiv (p - p_u)/p_u = O(\epsilon)
\]

\[
\lambda / m c_p = D_{Tu}/(\rho u D) \approx D_{Tu}/(\rho u a_u) \quad \text{Pr} \equiv \mu / (\rho u D_{Tu}) \]

\[
\xi \equiv x/\ell \quad \ell \equiv D_{Tu}/a_u
\]

mean free path

\[
a_u = \sqrt{\gamma p_u/\rho_u} \quad M_u^2 = 1 + 2 \epsilon + ...
\]

\[
\frac{1}{\gamma} \pi + (1 + 2 \epsilon) \nu = \text{Pr} \frac{d\nu}{d\xi} + O(\epsilon^3), \quad \text{valid up to order } \epsilon^2
\]

\[
\left( \frac{\gamma + 1}{2 \gamma} \right) \pi \nu + \frac{1}{\gamma} \pi + \nu = \frac{d\pi}{d\xi} + \frac{d\nu}{d\xi} + O(\epsilon^3),
\]

\[
\frac{1}{\gamma} \pi + \nu = \text{Pr} \frac{d\nu}{d\xi} - 2 \epsilon \nu + O(\epsilon^3), \quad \Rightarrow \left( \frac{\gamma + 1}{2 \gamma} \right) \pi \nu + \text{Pr} \frac{d\nu}{d\xi} - 2 \epsilon \nu = \frac{d\pi}{d\xi} + \frac{d\nu}{d\xi} + O(\epsilon^3),
\]

\[
\pi = -\gamma \nu + O(\epsilon^2), \quad \Rightarrow \left[ (\gamma - 1) + \text{Pr} \right] \frac{d\nu}{d\xi} = \left( \frac{\gamma + 1}{2} \nu + 2 \epsilon \right) \nu
\]

Rankine-Hugoniot

\[
\nu_N = -4 \epsilon \frac{1}{\gamma + 1} \quad \pi_N = -4 \epsilon \frac{\gamma}{\gamma + 1}
\]

\[
\nu_N = - \frac{4 \epsilon}{\gamma + 1}
\]

shock thickness
\[ M_u \equiv \frac{D}{a_u} > 1 \quad \text{Analysis for} \quad \epsilon \equiv M_u - 1 \ll 1 \quad \text{(weak shock)} \]

\[ \left[ (\gamma - 1) + Pr \right] \frac{d\nu}{d\xi} = \left( \frac{\gamma + 1}{2} \nu + 2\epsilon \right) \nu \]

\[ \frac{2}{\gamma + 1} \left[ (\gamma - 1) + Pr \right] \frac{d\nu}{d\xi} = \nu (\nu - \nu_N) \leq 0 \]

\[ \xi = -\infty : \text{initial state, } \nu = 0, \quad \xi = +\infty : \text{shocked gas, } \nu = \nu_N = -4\epsilon/(\gamma + 1) \]

\[ \nu_N = -\frac{4\epsilon}{\gamma + 1} \]

\[ Y \equiv \frac{(\gamma + 1)\nu}{4\epsilon} \in [0, -1] \quad \zeta \equiv \frac{2}{\left[ (\gamma + 1) + Pr \right]} \epsilon \xi = \frac{2}{\left[ (\gamma + 1) + Pr \right]} \frac{x}{(\ell/\epsilon)} \quad \zeta = O\left(\frac{x}{\ell/\epsilon}\right) \]

\[ \frac{dY}{d\zeta} = Y(Y + 1) < 0 \]

\[ \zeta = -\infty : Y = 0, \quad \zeta = +\infty : Y = -1 \]

\[ \zeta = \int \frac{dY}{Y(Y + 1)} \quad Y(\zeta) = -\frac{\epsilon^\zeta}{e^\zeta + 1} \]

shock thickness = mean free path/(\(M_u - 1\))

macroscopic length if \(M_u - 1 = O(1)\)

microscopic length if \((M_u - 1) \ll 1\)

\[ x = O(\ell/\epsilon) \]
OVERDRIVEN DETONATION
REACTING GAS

PISTON SUPPORTED SUPERSONIC WAVE

\[ D > a_u \]

FRESH MIXTURE
AT REST

SUPersonic
Front

\[ U_b < a_b \]

UNIFORM FLOW
OF BURNED GAS

C-J REGIME

\[ U_{bCJ} = a_{bCJ} \]

MOVING
PISTON

\[ U_b = D - v_p \]

FIRE

lead shock

reaction zone

Abel 1870, Berthelot et Vielle 1881, Mallard et Le Chatelier 1881, Mikhail'son 1893, Chapman 1899, Jouguet 1904,
Vielle 1900, Zel'dovich 1940, von Neumann 1942, Döring 1943,
JUMP ACROSS A DETONATION
Mikhelson condition for the CJ detonation (1893)

\[
\begin{align*}
\frac{\partial\rho}{\partial t} &= -\frac{\partial(pu)}{\partial x}, \quad \frac{\partial(pu)}{\partial t} = -\frac{\partial}{\partial x} \left( p + \rho u^2 - \mu \frac{\partial u}{\partial x} \right), \quad \frac{\partial(pu)}{\partial t} = -\frac{\partial}{\partial x} \left[ \rho u \frac{c_p T + \frac{u^2}{2} - q_m}{\mu} - \lambda \frac{\partial T}{\partial x} - \mu \frac{\partial u}{\partial x} \right] \\
c_p(T_b - T_u) + \left( u_p^2 - D^2 \right)/2 &= q_m \\
-\frac{\gamma}{\gamma - 1} \left( \frac{p_b}{\rho_b} - \frac{p_u}{\rho_u} \right) - \frac{1}{2} (p_b - p_u) \left( \frac{1}{\rho_u} + \frac{1}{\rho_b} \right) &= q_m \\
(P + 1)(\mathcal{V} + 1) = 1 + Q \\
\mathcal{P} &= -M_u^2 \mathcal{V}
\end{align*}
\]

quadratic equation for \( \mathcal{V} \)

\[
M_u^2 \mathcal{V}^2 + (M_u^2 - 1)\mathcal{V} + Q = 0
\]

supersonic combustion wave \( M_u \equiv D/a_u > 1 \)

**Lower bound of propagation velocity** \( D = D_{CJ} \)

(called Chapmann-Jouguet 1899 – 1904)

\[
(M_u^2 - 1)^2 \geq 4QM_u^2 \quad M_u \geq M_{uCJ} \equiv \sqrt{Q} + \sqrt{Q + 1},
\]

Mikhelson (1893)

In the CJ wave the velocity of the burned gas is sonic in the frame of the wave \( u_{bCJ} = a_{bCJ} \) (self-sustained wave)

(Rayleigh line is tangent)

In the overdriven detonations \( D > D_{CJ} \) the velocity of the burned gas is subsonic in the frame of the wave \( u_b < a_b \) (piston-supported detonation)

**Vieille conjecture** (1900)

detonation = inert shock wave followed by a exothermal reaction zone

\[
U \to N \to B
\]

(large Arrhenius factor)
Planar detonation

Overdriven regime / Self sustained wave

Marginal solution

the so called Chapman-Jouguet wave

Mikhel’son (1893)

**Arrhenius law**

\[ e^{-E/k_BT} \]

**reaction rate**

\[ \frac{e^{-E/k_BT}}{\tau_{coll}} \]

**elastic collisions**

\[ \frac{E}{k_BT} \approx 10 \]

**Sonic condition**

C-J detonation

**thickn...
ZND structure of detonations

Zeldovich (1940) Neumann (1942) Döring (1944)

Combustion = large activation energy

Orders of magnitude

\[
\frac{E}{k_B T_N} \gg 1 \Rightarrow \frac{1}{\tau_r(T_N)} \approx \frac{e^{-E/k_B T_N}}{\tau_{coll}} \ll \frac{1}{\tau_{coll}} \quad \frac{u_N}{a_N} = O(1), \quad d_N \equiv u_N \tau_r(N) \gg a_N \tau_{coll} \approx \ell
\]

thick\sspace of\sspace the\sspace reaction\sspace zone \gg thick\sspace of\sspace the\sspace lead\sspace (inert)\sspace shock

structure of the detonation: \textbf{inert shock followed by a much larger reaction zone}

conjectured by Vieille (1900)

\[
\frac{D_T}{d_N^2} \approx \frac{a_N^2 \tau_{coll}}{d_N^2} \approx \frac{\tau_{coll}}{(\tau_r(T_N))^2} \approx \frac{e^{-E/k_B T_N}}{\tau_r(T_N)} \ll \frac{1}{\tau_r(T_N)}
\]

diffusion rate \ll reaction rate \Rightarrow \textbf{diffusion terms are negligible}
structure of the detonation: inert shock followed by a much larger reaction zone

\[
\frac{D_T}{d_N^2} \approx a_N^2 \frac{\tau_{\text{coll}}}{(\tau_r(T_N))^2} \approx \frac{\tau_{\text{coll}}}{(\tau_r(T_N))^2} \approx \frac{e^{-E/k_BT_N}}{\tau_r(T_N)} \ll \frac{1}{\tau_r(T_N)}
\]

diffusion rate \ll reaction rate \Rightarrow diffusion terms are negligible

\section*{Formulation}

\textit{Reference frame of the lead shock (}x = 0\textit{)}

\[
\frac{\gamma}{\gamma - 1} \frac{d}{dx} \left( \frac{p}{\rho} \right) + u \frac{du}{dx} - q_m \frac{d\psi}{dx} = 0
\]

\[
\rho u \frac{d\psi}{dx} = \rho \frac{\dot{\psi}(T, \psi)}{\tau_r(T_N)}
\]

\[\psi \in [0, 1]\]

\[\dot{\psi}(T, \psi = 1) = 1\]

\[\dot{\psi}(T, \psi = 0) = 0.\]

\[x = 0: \ u = u_N, \ \rho = \rho_N, \ p = p_N, \ \psi = 1, \ \dot{\psi} = 1\]

\[x \to \infty: \ u = u_b, \ \rho = \rho_b, \ p = p_b, \ \psi = 0, \ \dot{\psi} = 0\]

detonation thickness \[d_N = u_N \tau_r(T_N)\]

\[
a^2 = \gamma \frac{p}{\rho}
\]

\[
\frac{d}{dx} \left( \frac{p}{\rho} \right) = p \frac{d}{dx} \left( \frac{1}{\rho} \right) + \frac{1}{\rho} \frac{dp}{dx} = \frac{p}{\rho u} \frac{du}{dx} + \frac{1}{\rho} \frac{dp}{dx} = a^2 \frac{du}{\gamma u dx} - u \frac{du}{dx} \Rightarrow \frac{\gamma}{\gamma - 1} \frac{d}{dx} \left( \frac{p}{\rho} \right) + u \frac{du}{dx} = \frac{1}{(\gamma - 1)u} \frac{a^2 - u^2}{dx}
\]

\[
(a^2 - u^2) \frac{du}{dx} = (\gamma - 1)q_m u \frac{d\psi}{dx}, \quad \Rightarrow \quad \frac{du^2}{d\psi} = 2(\gamma - 1)q_m \frac{u^2}{(a^2 - u^2)}
\]
Phase portrait in the plan $\psi - u^2$

$$\frac{d u^2}{d \psi} = 2(\gamma - 1)q_m \frac{u^2}{(a^2 - u^2)}$$

Initial state $\psi = 0$ : $u^2 = D^2$, $a^2 = a_u^2$

Neumann state $\psi = 0$ : $u^2 = u_N^2$, $a^2 = a_N^2$

zero reaction rate

no supersonic wave without a leading shock

OK with the Vieille's conjecture
C-J Detonation = self-propagating wave

\[ U_b \leq a_b \]

\[ U_{bCJ} = a_{bCJ} \]

\[ u_{bCJ} = D_{CJ} - a_{bCJ} \]

Selection mechanism

Rarefaction wave in the burnt gas when the piston is suddenly stopped

Speed of discontinuities in lab. frame

leading edge of the rarefaction wave = speed of sound /gas flow
\begin{align*}
\sqrt{\frac{dx_f}{dt} - D_{CJ}} &\sim \frac{x_f}{t} \\
\frac{D_{CJ}}{x_f(t) - D_{CJ}t} &\sim \frac{1}{t} + \text{constant} \\
\lim_{t \to \infty} x_f(t) &= D_{CJ}t + \text{constant}
\end{align*}