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

Structure and Dynamics of Combustion Waves in Premixed Gases

Paul Clavin

Aix-Marseille Université
ECM & CNRS (IRPHE)

Lecture 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

X-1) Background

shock wave $\approx$ discontinuity in the solution of the Euler equations

Riemann 1860

Model of hyperbolic equations for the formation of discontinuities

$a(u)$ $$\partial u/\partial t + a(u)\partial u/\partial x = 0$$

$t = 0: \quad u = u_o(x)$ $\qquad u = u(x,t)$?

Simple case: linear equation

$a = a_o = \text{cst.}$: $\qquad u = u_o(x - a_o t)$

propagation at constant velocity without deformation

Nonlinear equation $a(u)$ $\quad \mathrm{d}a/\mathrm{d}u \neq 0$

Method of characteristics

The solution is conserved along any trajectory $\mathrm{d}x/\mathrm{d}t = a(u)$ in the phase plan (x,t).

$$u = u(x(t), t) \qquad \mathrm{d}u/\mathrm{d}t = 0$$

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

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

$$\partial u/\partial t + a(u)\partial u/\partial x = 0$$

Riemann 1860

$t = 0: \quad u = u_o(x)$ $\qquad u = u(x,t)$?

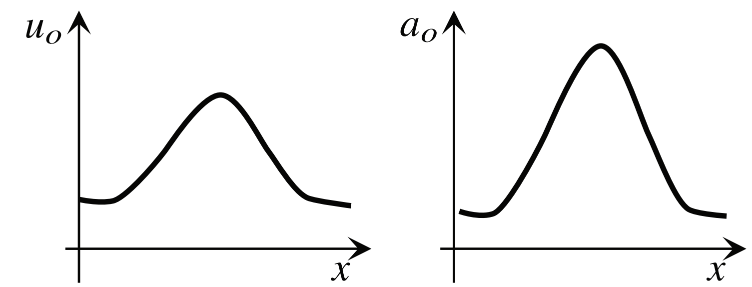
Method of characteristics

The solution is conserved along any trajectory $\mathrm{d}x/\mathrm{d}t = a(u)$ in the phase plan (x, t).

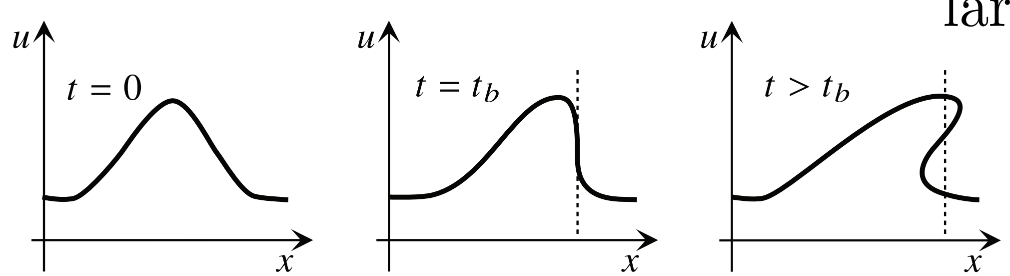
$u(x,t)$ is constant along the straight lines $x = a_o t + x_o$: $\quad u = u_o$

Speed increases with increasing u, $\mathrm{d}a/\mathrm{d}u > 0$

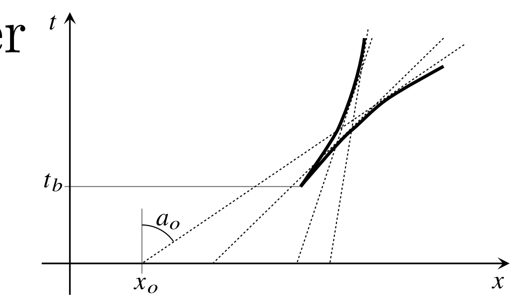
$\Rightarrow$ formation of singularities after a finite time



larger values run faster



$t > t_b$: multivalued solution. Wave breaking



$t > t_b$: characteristics intersect

$u(x,t) = u_o(x_o(x,t))$, $\quad x(x_o,t) = a_o(x_o)t + x_o$, (trajectory) $\quad \partial x/\partial x_o = 1 + t(\mathrm{d}a_o/\mathrm{d}x_o) \quad \partial x_o/\partial x = [1 + t(\mathrm{d}a_o/\mathrm{d}x_o)]^{-1}$

$$\frac{\partial u}{\partial x} = \frac{\partial x_o}{\partial x}\frac{\mathrm{d}u_o}{\mathrm{d}x_o} \qquad \frac{\partial u}{\partial x} = \frac{\mathrm{d}u_o/\mathrm{d}x_o}{[1 + t(\mathrm{d}a_o/\mathrm{d}x_o)]}$$

diverges at time $t = \dfrac{1}{-\mathrm{d}a_o/\mathrm{d}x_o}$ where $da_o/\mathrm{d}x_o < 0$

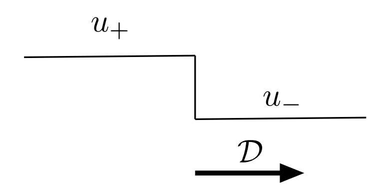
$t_b \equiv$ **time of wave breaking** (shortest time for the divergence of $\partial u/\partial x$)

$$t_b = \frac{1}{\max\,|\mathrm{d}a_0/\mathrm{d}x_0|}$$

Discontinuous solutions

$\partial u/\partial t + a(u)\partial u/\partial x = 0$ conservative form $\partial u/\partial t + \partial j/\partial x = 0$ $j(u)$ $\mathrm{d}j/\mathrm{d}u = a(u)$

Are step functions $u_+ \neq u_-$ propagating at constant velocity $\mathcal{D}$ solutions ?



$\partial/\partial t = -\mathcal{D}\mathrm{d}/\mathrm{d}\xi$ $\partial/\partial x = \mathrm{d}/\mathrm{d}\xi$

$u(\xi)$ $\xi = x - \mathcal{D}t$

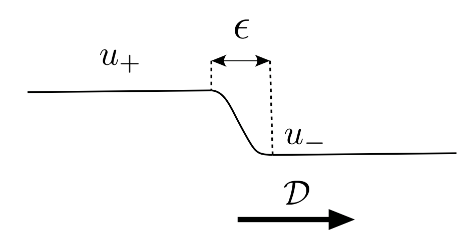
$$-\mathcal{D}\frac{\mathrm{d}u}{\mathrm{d}\xi} + \frac{\mathrm{d}j}{\mathrm{d}\xi} = 0 \qquad j - \mathcal{D}u \quad \text{is a conserved scalar}$$

$$\mathcal{D} = \frac{j(u_+) - j(u_-)}{u_+ - u_-}$$

Infinite numbers of solutions !! *Ill posed problem*

$$f(u) \times \left(-\mathcal{D}\frac{\mathrm{d}u}{\mathrm{d}\xi} + \frac{\mathrm{d}j}{\mathrm{d}\xi}\right) = 0 \qquad G - \mathcal{D}F = \text{ cst.} \qquad \mathcal{D} = \frac{G(u_+) - G(u_-)}{F(u_+) - F(u_-)} \quad \text{where} \quad \frac{\mathrm{d}F}{\mathrm{d}u} \equiv f(u) \quad \frac{\mathrm{d}G}{\mathrm{d}u} \equiv f(u)a(u)$$

Adding a small dissipative term makes the problem well posed



$$\partial u/\partial t + a(u)\partial u/\partial x = \epsilon \partial^2 u/\partial x^2, \quad \epsilon > 0$$

$$\frac{\mathrm{d}}{\mathrm{d}\xi}\left[-u\mathcal{D} + j(u) - \epsilon\frac{\mathrm{d}u}{\mathrm{d}\xi}\right] = 0 \qquad \epsilon\frac{\mathrm{d}u}{\mathrm{d}\xi} = j(u) - u\mathcal{D} + \text{cst} \qquad \frac{\xi}{\epsilon} = \int_0^u \frac{\mathrm{d}u}{j(u) - u\mathcal{D} + \text{cst}}$$

$\xi = \pm\infty$: $\mathrm{d}u/\mathrm{d}\xi = 0$ $\Rightarrow$ 2 expressions of the cst that should be equal $\Rightarrow$ a single value of $\mathcal{D}$

$j(u_+) - u_+\mathcal{D} + \text{cst} = 0$

$j(u_-) - u_-\mathcal{D} + \text{cst} = 0$

$$\mathcal{D} = \frac{j(u_+) - j(u_-)}{u_+ - u_-}$$

independent of ϵ !

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

$a(u) = u$: Burgers equation. Analytical solution to the initial value problem

Riemann invariants (1860)

Euler equation + constant entropy + ideal gas: $a^2 = \frac{\mathrm{d}p}{\mathrm{d}\rho} = \gamma \frac{p}{\rho}$ $\quad \frac{p}{\rho^\gamma} = \mathrm{cst}$ $\quad 2\frac{\mathrm{d}a}{a} = \frac{\mathrm{d}p}{p} - \frac{\mathrm{d}\rho}{\rho} \Rightarrow 2\frac{\mathrm{d}a}{a} = (\gamma - 1)\frac{\mathrm{d}\rho}{\rho}$

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

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

choose λ such that $\quad \lambda u + a^2/\rho = \lambda(\lambda\rho + u), \qquad \lambda = \pm a/\rho \qquad \lambda\rho = \pm a$

$$\lambda\left[\frac{\partial}{\partial t} + (\lambda\rho + u)\frac{\partial}{\partial t}\right]\rho + \left[\frac{\partial}{\partial t} + (\lambda\rho + u)\frac{\partial}{\partial t}\right]u = 0$$

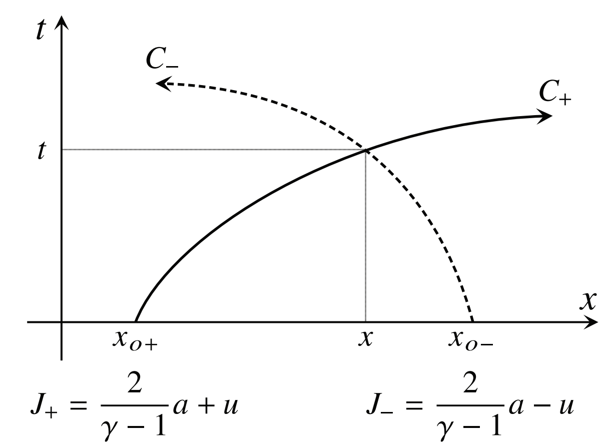
$\lambda\rho + u = u \pm a$

2 characteristics : $\quad C_+ : \frac{\mathrm{d}x}{\mathrm{d}t} = u + a, \qquad C_- : \frac{\mathrm{d}x}{\mathrm{d}t} = u - a$

invariants : $\quad C_+ : \frac{a}{\rho}\mathrm{d}\rho + \mathrm{d}u = 0 \qquad C_- : \frac{a}{\rho}\mathrm{d}\rho - \mathrm{d}u = 0$

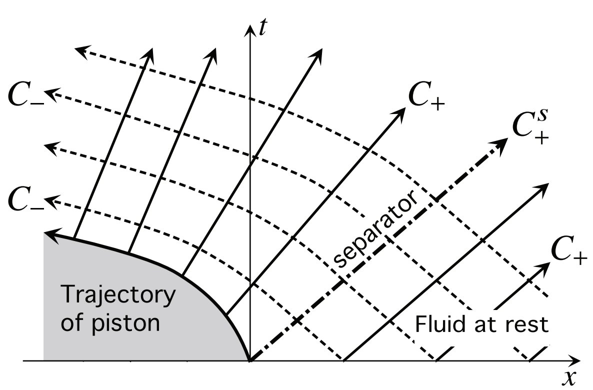
$\lambda\mathrm{d}\rho + \mathrm{d}u = 0 \qquad \pm\frac{a}{\rho}\mathrm{d}\rho + \mathrm{d}u = 0$

$$J_+ \equiv \frac{2}{\gamma - 1}a + u = \ \mathrm{cst\ sur}\ C_+ \qquad J_- \equiv \frac{2}{\gamma - 1}a - u = \ \mathrm{cst\ sur}\ C_-$$

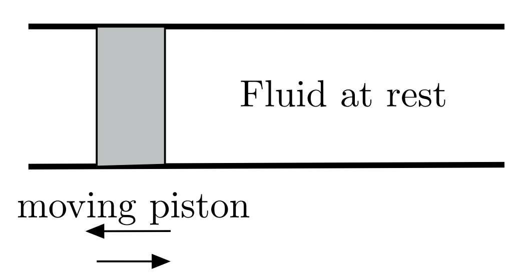


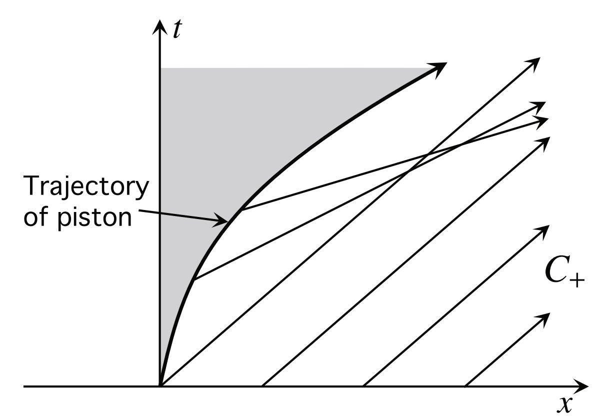
Simple waves

C_+ are straight lines



Rarefaction wave

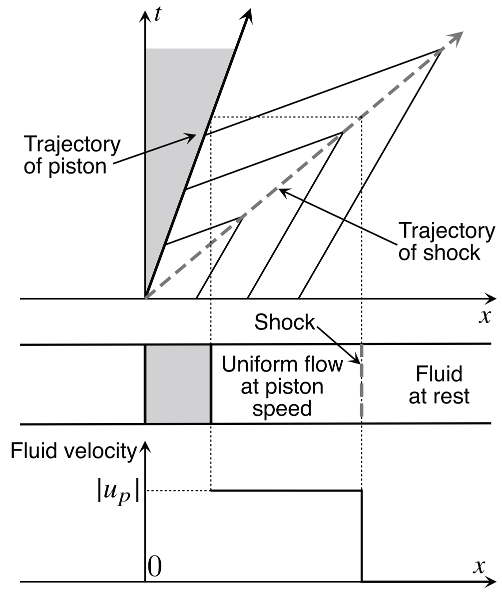




Compression wave

formation of a singularity: shock wave

compression



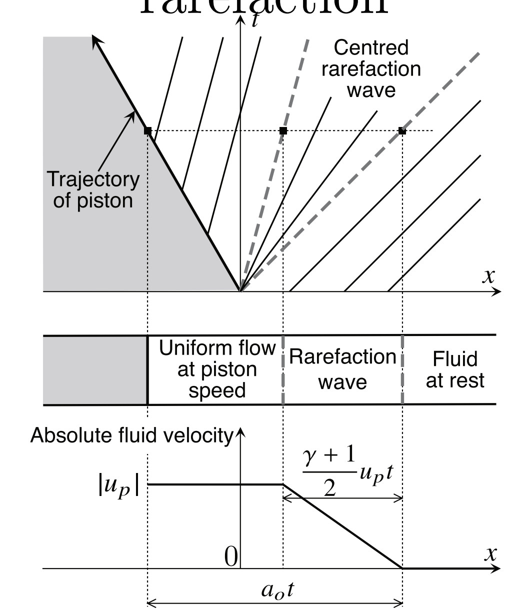
Centred waves

$t < 0:$ piston velocity $= 0$

$t > 0:$ piston velocity $=$ cst $\neq 0$

Sel-similar solutions x/t

rarefaction



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 $\nearrow$ $u_p\, t$

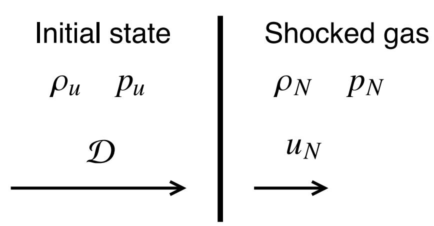
Rankine 1870

Hugoniot 1880

Rankine-Hugoniot conditions for shock waves

(1870 – 1880)

Eqs for the conservation of mass, momentum and energy



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

$$\boxed{m \equiv \rho_u \mathcal{D}} = \rho_N u_N \qquad p_u + \frac{m^2}{\rho_u} = p_N + \frac{m^2}{\rho_N} \qquad h_N - h_u + (u_N^2 - \mathcal{D}^2)/2 = 0$$

written in the moving frame of the shock at velocity $\mathcal{D}$

steady problem

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

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

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 $\gamma \equiv c_p/c_v$

$$p = (c_p - c_v)\rho T, \qquad h = c_p T = \frac{\gamma}{\gamma - 1}\frac{p}{\rho}$$

$$h(p,\rho) - h(p_u,\rho_u) - \frac{1}{2}\left(\frac{1}{\rho_u} + \frac{1}{\rho}\right)(p - p_u) = 0 \qquad p - p_u = -m^2\left(\frac{1}{\rho} - \frac{1}{\rho_u}\right)$$

$$\mathcal{P} \equiv \frac{(\gamma+1)}{2\gamma}\left(\frac{p}{p_u} - 1\right), \quad \mathcal{V} \equiv \frac{(\gamma+1)}{2}\left(\frac{\rho_u}{\rho} - 1\right)$$

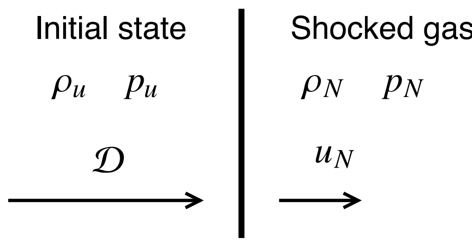
$(\mathcal{P}+1)(\mathcal{V}+1) = 1$ Hugoniot curve $\qquad \mathcal{P} = -M_u^2\mathcal{V}$ Michelson-Rayleigh line

quadratic equation for $\mathcal{V}$, 2 solutions: $\mathcal{V} = 0$, $\mathcal{V} = \mathcal{V}_N$

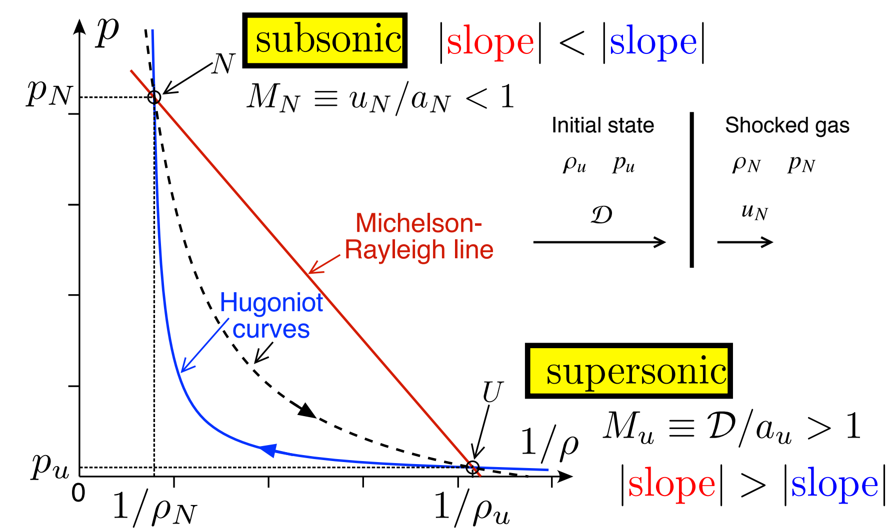
Shocked gas (Neumann state) vs M_u

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

$$M_N^2 = \frac{(\gamma-1)M_u^2 + 2}{2\gamma M_u^2 - (\gamma-1)} \quad \Leftrightarrow \quad 2\gamma M_u^2 M_N^2 - (\gamma-1)(M_u^2 + M_N^2) - 2 = 0$$



General comments



The Hugoniot curve is tangent to the isentropic

the entropy change along the Hugoniot curve is of third order $\Rightarrow$ $M_u \equiv \mathcal{D}/a_u > 1$

$$\delta s = s - s_u \qquad \delta p = p - p_u$$

$$\delta s \nearrow \delta p \nearrow$$

$$\delta s = \frac{1}{12}\frac{1}{T_u}\left(\frac{\partial^2(1/\rho)}{\partial p^2}\right)_s (\delta p)^3$$

The Hugoniot relation is not an iso-function of state

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

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

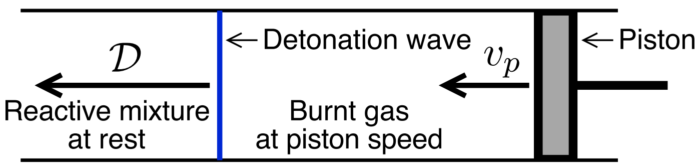
Rarefaction shock does not exist. The entropy of the fluid increases through the shock (Irreversibility)

can be proved for weak shock by the entropy balance $\quad \rho u \frac{\mathrm{d}s}{\mathrm{d}x} = \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\lambda}{T}\frac{\mathrm{d}T}{\mathrm{d}x}\right) + \dot{\omega}_s \qquad \dot{\omega}_s > 0$

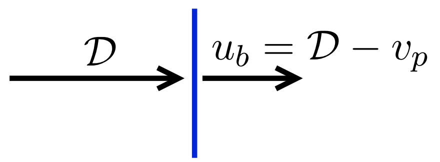
or by the H-theorem using the Boltzmann equation

Mikhelson condition for the CJ detonation (1893)

REFERENCE FRAME OF LABORATORY



$\rho_u \mathcal{D} = \rho_u \rho_b \quad u_b \leqslant a_b$



REFERENCE FRAME OF SHOCK WAVE

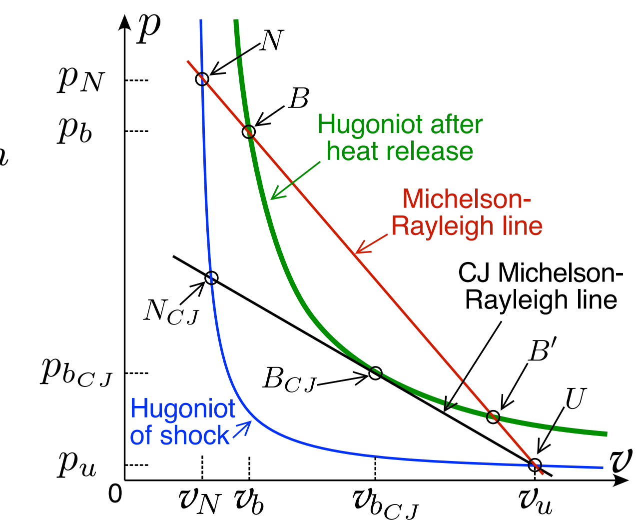
$$\frac{\partial \rho}{\partial t} = -\frac{\partial(\rho u)}{\partial x}, \qquad \frac{\partial(\rho u)}{\partial t} = -\frac{\partial}{\partial x}\left(p + \rho u^2 - \mu\frac{\partial u}{\partial x}\right), \qquad \frac{\partial(\rho e_{tot})}{\partial t} = -\frac{\partial}{\partial x}\left[\rho u\left(c_p T + \frac{u^2}{2} - q_m\psi\right) - \lambda\frac{\partial T}{\partial x} - \mu u\frac{\partial u}{\partial x}\right]$$

$$c_p(T_b - T_u) + (u_b^2 - \mathcal{D}^2)/2 = q_m$$

$$\frac{\gamma}{\gamma - 1}\left(\frac{p_b}{\rho_b} - \frac{p_u}{\rho_u}\right) - \frac{1}{2}(p_b - p_u)\left(\frac{1}{\rho_u} + \frac{1}{\rho_b}\right) = q_m$$

$$\mathcal{P} \equiv \frac{(\gamma+1)}{2\gamma}\left(\frac{p}{p_u} - 1\right), \quad \mathcal{V} \equiv \frac{(\gamma+1)}{2}\left(\frac{\rho_u}{\rho} - 1\right) \qquad \mathcal{Q} \equiv \frac{\gamma+1}{2}\frac{q_m}{c_p T_u}$$

$$(\mathcal{P}+1)(\mathcal{V}+1) = 1 + \mathcal{Q}$$
$$\mathcal{P} = -M_u^2 \mathcal{V}$$



quadratic equation for $\mathcal{V}$ $\qquad M_u^2\mathcal{V}^2 + (M_u^2 - 1)\mathcal{V} + \mathcal{Q} = 0$

supersonic combustion wave $\qquad M_u \equiv \mathcal{D}/a_u > 1$

Lower bound of propagation velocity $\mathcal{D} = \mathcal{D}_{CJ}$
(called Chapmann-Jouguet 1899 – 1904)

$$(M_u^2 - 1)^2 \geqslant 4\mathcal{Q}M_u^2 \qquad M_u \geqslant M_{u_{CJ}} \equiv \sqrt{\mathcal{Q}} + \sqrt{\mathcal{Q}+1},$$ 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 $\mathcal{D} > \mathcal{D}_{CJ}$ 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
$U \rightarrow N \rightarrow B$
(large Arrhenius factor)

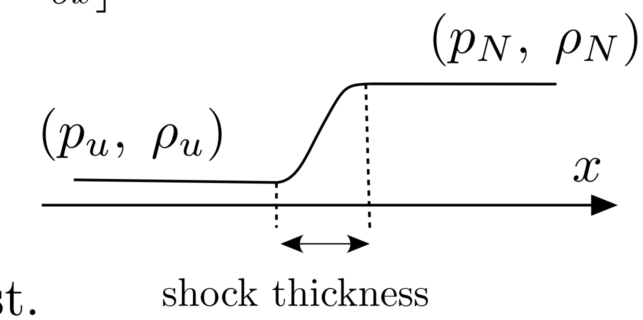
Paul Vieille (1900)

X-2) Inner structure of a weak shock

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

Formulation

(reference frame attached to the shock wave)



$$\rho u = m, \qquad p+\rho u^2-\mu\frac{\mathrm{d}u}{\mathrm{d}x}=\text{cst.} \qquad m\left(h+\frac{u^2}{2}\right)-\lambda\frac{\mathrm{d}T}{\mathrm{d}x}-\mu u\frac{\mathrm{d}u}{\mathrm{d}x}=\text{cst.}$$

$$x\rightarrow-\infty: \quad p=p_u,\ \ \rho=\rho_u,\ \ u=\mathcal{D} \qquad x\rightarrow\infty: \quad \mathrm{d}p/dx=0,\ \ \mathrm{d}p/dx=0,,\ \ \mathrm{d}u/\mathrm{d}x=0$$

$$\frac{p}{\rho}=(\gamma-1)c_vT \qquad h=\frac{\gamma}{\gamma-1}\frac{p}{\rho}$$

Two coupled equations for p *and* $\upsilon\equiv 1/\rho, m$ *given* $\quad (u=m\upsilon, \quad c_vT=p\upsilon/(\gamma-1))$

$$(p-p_u)+m^2(\upsilon-\upsilon_u)=\mu m\frac{\mathrm{d}\upsilon}{\mathrm{d}x},$$

$$\frac{\gamma}{\gamma-1}(p\upsilon-p_u\upsilon_u)-\frac{1}{2}(p-p_u)(\upsilon+\upsilon_u)=\frac{\gamma}{\gamma-1}\frac{\lambda}{mc_p}\frac{\mathrm{d}(p\upsilon)}{\mathrm{d}x}+\frac{\mu m}{2}(\upsilon-\upsilon_u)\frac{\mathrm{d}\upsilon}{\mathrm{d}x}$$

$$\frac{1}{2}(u^2-u_u^2)=\frac{m^2}{2}(\upsilon+\upsilon_u)(\upsilon-\upsilon_u)$$
$$=\frac{1}{2}(\upsilon+\upsilon_u)\left[-(p-p_u)+\mu m\frac{\mathrm{d}\upsilon}{\mathrm{d}x}\right]$$

$$x\rightarrow\infty: \quad \mathrm{d}p/\mathrm{d}x=0,\ \ \mathrm{d}\upsilon/\mathrm{d}x=0$$

Dimensional analysis

$$\rho u^2 \quad \times \quad \mu\frac{\mathrm{d}u}{\mathrm{d}x}$$

$u/a=O(1),$ (speed of sound)

$\mu/\rho=$ viscous diffusion coefficient $\approx \ell/a$ (mean free path; kinetic theory of gases) $\Rightarrow$ thickness of shock waves $\approx$ mean free path

macroscopic equations not valid ?

ok for weak shock !

$M_u \equiv \mathcal{D}/a_u > 1$ **Analysis for** $\epsilon \equiv M_u - 1 \ll 1$ (weak shock)

$$\upsilon \equiv 1/\rho \qquad \nu \equiv (\upsilon - \upsilon_u)/\upsilon_u = O(\epsilon) \qquad \pi \equiv (p - p_u)/p_u = O(\epsilon)$$

mean free path

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

Non dimensional equations

$$a_u = \sqrt{\gamma p_u/\rho_u} \qquad \mathrm{Pr} \equiv \mu/(\rho_u D_{Tu}) \qquad M_u^2 = 1 + 2\epsilon + ..$$

$$(p - p_u) + m^2(\upsilon - \upsilon_u) = \mu m \frac{\mathrm{d}\upsilon}{\mathrm{d}x},$$

$$\frac{\gamma}{\gamma-1}(p\upsilon - p_u\upsilon_u) - \frac{1}{2}(p - p_u)(\upsilon + \upsilon_u) = \frac{\gamma}{\gamma-1}\frac{\lambda}{mc_p}\frac{\mathrm{d}(p\upsilon)}{\mathrm{d}x} + \frac{\mu m}{2}(\upsilon - \upsilon_u)\frac{\mathrm{d}\upsilon}{\mathrm{d}x}$$

O(ϵ^3)

$$\frac{m^2\upsilon_u}{\gamma p_u} = M_u^2 \approx 1 + 2\epsilon$$

anticipating $\left\{ \begin{array}{l} \mathrm{d}\nu/\mathrm{d}\xi = O(\epsilon^2) \\ \mathrm{d}\pi/\mathrm{d}\xi = O(\epsilon^2) \end{array} \right\}$

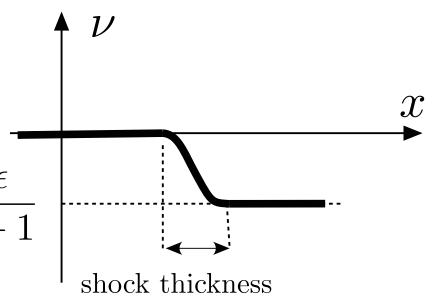
$$\left\{ \begin{array}{l} \frac{1}{\gamma}\pi + (1+2\epsilon)\nu = \mathrm{Pr}\frac{\mathrm{d}\nu}{\mathrm{d}\xi} + O(\epsilon^3), \\ \left(\frac{\gamma+1}{2\gamma}\right)\pi\nu + \frac{1}{\gamma}\pi + \nu = \frac{\mathrm{d}\pi}{\mathrm{d}\xi} + \frac{\mathrm{d}\nu}{\mathrm{d}\xi} + O(\epsilon^3), \end{array} \right.$$

valid up to order ϵ^2

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

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

the Rankine-Hugoniot jumps at order ϵ are recovered when dissipative terms are neglected $\nu_N = -4\epsilon\frac{1}{\gamma+1}$ $\quad \pi_N = -4\epsilon\frac{\gamma}{\gamma+1}$



$$\frac{2}{\gamma+1}[(\gamma-1) + \mathrm{Pr}]\frac{\mathrm{d}\nu}{\mathrm{d}\xi} = \nu(\nu - \nu_N) \leqslant 0$$

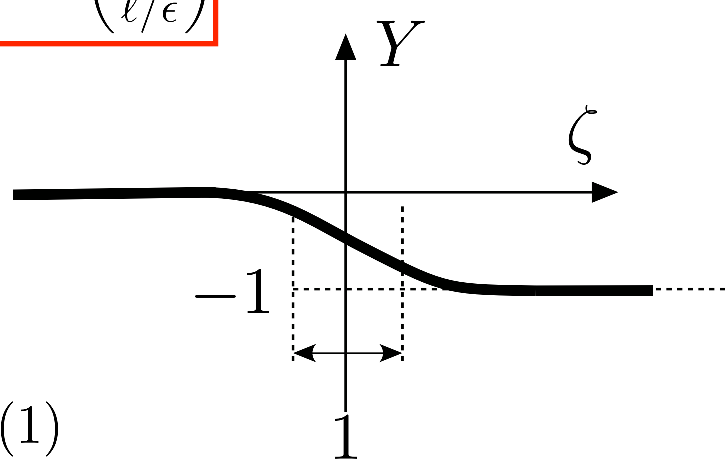
$\xi = -\infty$: initial state, $\nu = 0$, $\qquad \xi = +\infty$: shocked gas, $\nu = \nu_N = -4\epsilon/(\gamma+1)$

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

$$\zeta = O\left(\frac{x}{\ell/\epsilon}\right)$$

$$\frac{\mathrm{d}Y}{\mathrm{d}\zeta} = Y(Y+1) < 0$$

$\zeta = -\infty$: $Y = 0$, $\qquad \zeta = +\infty$: $Y = -1$



$$\zeta = \int \frac{\mathrm{d}Y}{Y(Y+1)} \qquad Y(\zeta) = -\frac{e^\zeta}{e^\zeta + 1}$$

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

microscopic length if $M_u - 1 = O(1)$

macroscopic length if $(M_u - 1) \ll 1$

$$x = O(l/\epsilon)$$

X-3) ZND structure of detonations

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

Orders of magnitude

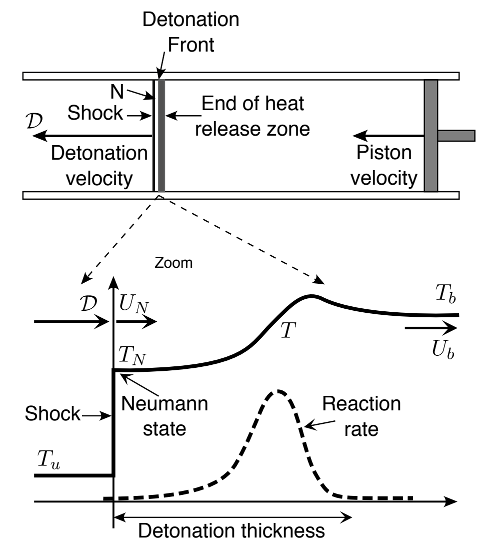
$$\frac{E}{k_B T_N} \gg 1 \;\Rightarrow\; \frac{1}{\tau_r(T_N)} \approx \frac{e^{-E/k_B T_N}}{\tau_{coll}} \ll \frac{1}{\tau_{coll}} \qquad \frac{u_N}{a_N} = O(1), \quad d_N \equiv u_N \tau_r(N) \gg a_N \tau_{coll} \approx \ell$$

thickness of the reaction zone $\gg$ thickness of the lead (inert) shock

structure of the detonation: **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 $\Rightarrow$ **diffusion terms are negligible**



Formulation

Reference frame of the lead shock $(x=0)$

$$\frac{\mathrm{d}(\rho u)}{\mathrm{d}x} = 0 \qquad \frac{\mathrm{d}p}{\mathrm{d}x} + \rho u \frac{\mathrm{d}u}{\mathrm{d}x} = 0$$

$$\frac{\gamma}{\gamma-1}\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{p}{\rho}\right) + u\frac{\mathrm{d}u}{\mathrm{d}x} - q_m \frac{\mathrm{d}\psi}{\mathrm{d}x} = 0 \qquad \rho u \frac{\mathrm{d}\psi}{\mathrm{d}x} = \rho \frac{\dot{w}(T,\psi)}{\tau_r(T_N)}$$

$$\psi \in [0,1] \qquad \dot{w}(T,\psi=1) = 1 \qquad \dot{w}(T,\psi=0) = 0.$$

$$x = 0: \quad u = u_N, \quad \rho = \rho_N, \quad p = p_N, \quad \psi = 1, \quad \dot{w} = 1$$

$$x \to \infty: \quad u = u_b, \quad \rho = \rho_b, \quad p = p_b, \quad \psi = 0, \quad \dot{w} = 0$$

detonation thickness $d_N = u_N \tau_r(T_N)$

$a^2 = \gamma \dfrac{p}{\rho}$ *Elimination of* p *and* ρ

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{p}{\rho}\right) = p\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{1}{\rho}\right) + \frac{1}{\rho}\frac{\mathrm{d}p}{\mathrm{d}x} = \frac{p}{\rho u}\frac{\mathrm{d}u}{\mathrm{d}x} + \frac{1}{\rho}\frac{\mathrm{d}p}{\mathrm{d}x} = \frac{a^2}{\gamma u}\frac{\mathrm{d}u}{\mathrm{d}x} - u\frac{\mathrm{d}u}{\mathrm{d}x} \quad \Rightarrow \quad \frac{\gamma}{\gamma-1}\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{p}{\rho}\right) + u\frac{\mathrm{d}u}{\mathrm{d}x} = \frac{1}{(\gamma-1)u}(a^2-u^2)\frac{\mathrm{d}u}{\mathrm{d}x}$$

$$(a^2-u^2)\frac{\mathrm{d}u}{\mathrm{d}x} = (\gamma-1)q_m u \frac{\mathrm{d}\psi}{\mathrm{d}x}, \quad \Rightarrow \quad \boxed{\frac{\mathrm{d}u^2}{\mathrm{d}\psi} = 2(\gamma-1)q_m \frac{u^2}{(a^2-u^2)}}$$

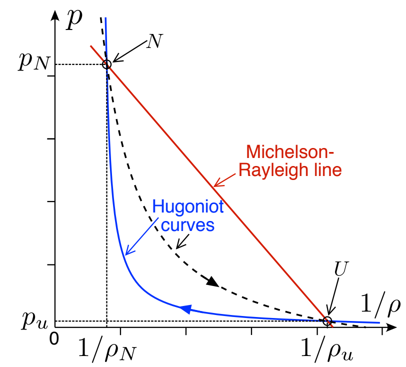
Phase portrait in the plan ψ - u^2

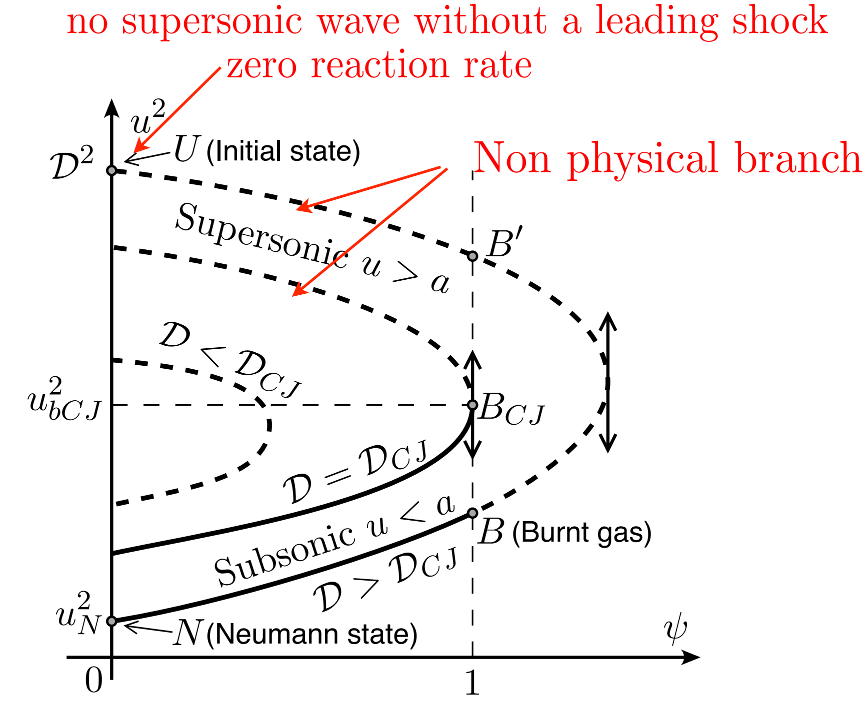
$$\frac{du^2}{d\psi} = 2(\gamma-1)q_m \frac{u^2}{(a^2-u^2)}$$

$$\frac{1}{\gamma-1}a^2 + \frac{1}{2}u^2 - q_m\psi = \frac{1}{\gamma-1}a_u^2 + \frac{1}{2}\mathcal{D}^2$$

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

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





X-4) Selection mechanism of the CJ wave

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