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Structure and Dynamics of Combustion Waves in Premixed Gases

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Lecture XI
Initiation of detonations

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Lecture 11: Initiation of detonation

11-1. Direct initiation

Flow of burnt gas in spherical CJ detonations
Point blast explosions
Zeldovich criterion
Critical energy

11-2. Spontaneous initiation and quenching

Initiation at high temperature
Spontaneous quenching

11-3. Deflagration-to-detonation transition

Basic ingredients
Experiments
Runaway phenomenon
Mechanisms of DDT

Detonability limits

Mixtures in which a planar CJ wave can propagate

Mixtures in which the temperature at the Neumann state (just behind the lead shock) of the CJ wave (controlled by q_m) is larger than the crossover temperature (controlled by the chemical kinetics)

$$\boxed{T_{N_{CJ}} > T^*}$$

composition

chemical kinetics

$$(\gamma - 1)M_{u_{CJ}}^2 > 1 \Rightarrow T_{N_{CJ}} \propto q_m/c_p \qquad 1000\text{ K} < T^* < 1350\text{ K}$$

heat release per unit mass of the deficient species (fuel or oxygen in lean and rich mixtures respectively)

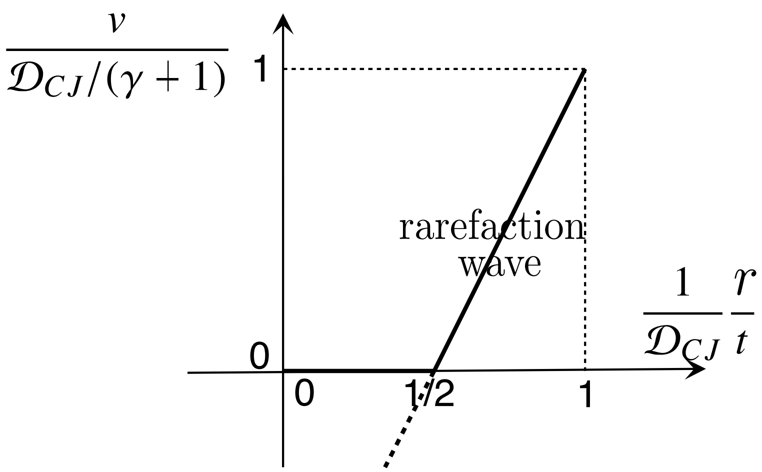
XI-1) Direct initiation of detonation

Flow of burnt gas in a spherical CJ detonation

(CJ detonation viewed as a hydrodynamic discontinuity)

Zeldovich (1942) Taylor (1950)

planar



self-similar form

$$u(r,t) = v(\mathrm{x}) \qquad \boxed{\mathrm{x} \equiv r/t}$$

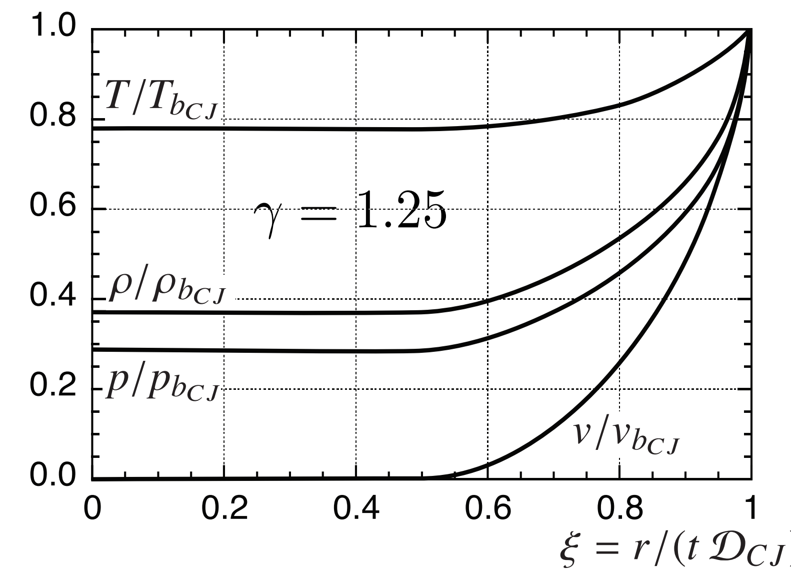
flow velocity in the laboratory frame

$$\frac{\partial}{\partial r} = \frac{1}{t}\frac{\mathrm{d}}{\mathrm{dx}}, \qquad \frac{\partial}{\partial t} = -\frac{r}{t^2}\frac{\mathrm{d}}{\mathrm{dx}} = -\frac{\mathrm{x}}{t}\frac{\mathrm{d}}{\mathrm{dx}}$$

planar $\neq$ spherical

$$\Delta = \frac{\partial^2}{\partial r^2} \qquad \Delta = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)$$

spherical



constant velocity $\mathcal{D}_{CJ}$ $\Rightarrow$ entropy of burnt gas = cst. $\quad p/\rho^\gamma = \text{cst.} \;\Rightarrow\; a(\rho) = (\rho/\rho_{b_{CJ}})^{\frac{\gamma-1}{2}}\, a_{b_{CJ}}$

CJ condition: $v_{bCJ} = \mathcal{D}_{CJ} - a_{bCJ}$,

$q_m \gg c_p T_u:\; a_{bCJ}/\mathcal{D}_{CJ} = \gamma/(\gamma+1)$

$$q_m \gg c_p T_u \;\Rightarrow\; v_{bCJ} = \mathcal{D}_{CJ}/(\gamma+1)$$

Planar detonation

$$\left.\begin{aligned} \frac{1}{\rho}\frac{\partial\rho}{\partial t} + \frac{u}{\rho}\frac{\partial\rho}{\partial r} &= 0 \\ \frac{\partial u}{\partial t} + u\frac{\partial u}{\partial r} + -\frac{a^2}{\rho}\frac{\partial\rho}{\partial r} &= 0 \end{aligned}\right\} \Rightarrow \left\{\begin{aligned} (v-\mathrm{x})\frac{1}{\rho}\frac{\mathrm{d}\rho}{\mathrm{dx}} + \frac{\mathrm{d}v}{\mathrm{dx}} &= 0 \\ a^2\frac{1}{\rho}\frac{\mathrm{d}\rho}{\mathrm{dx}} + (v-\mathrm{x})\frac{\mathrm{d}v}{\mathrm{dx}} &= 0 \end{aligned}\right. \Rightarrow \left[1 - \left(\frac{v-\mathrm{x}}{a}\right)^2\right]\frac{\mathrm{x}}{v}\frac{\mathrm{d}v}{\mathrm{dx}} = 0$$

Riemann invariant:

$2a/(\gamma-1) - v = 2a_{bCJ}/(\gamma-1) - v_{bCJ}$

$$\Rightarrow \quad \boxed{(\gamma+1)\frac{v - v_{bCJ}}{\mathcal{D}_{CJ}} = 2\left[\frac{\mathrm{x}}{\mathcal{D}_{CJ}} - 1\right]} \quad \Leftarrow \quad v = \mathrm{x} - a$$

Spherical CJ detonation

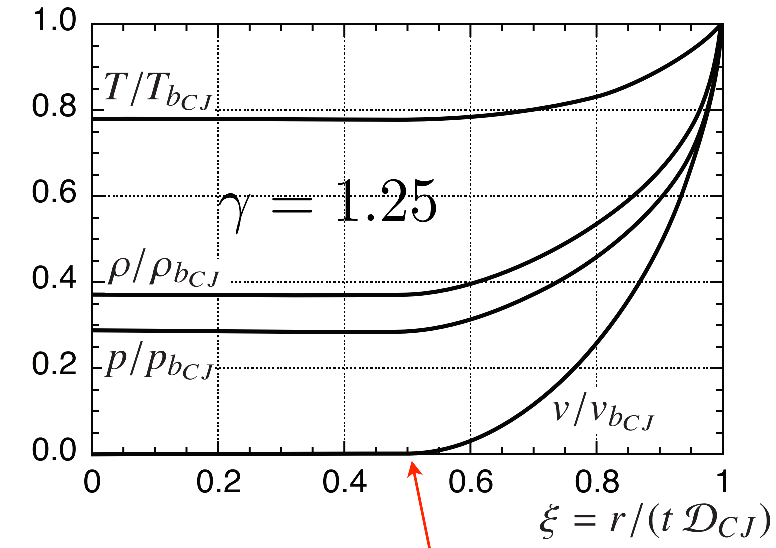
self-similar form

$v(\mathrm{x})$ $\boxed{\mathrm{x} \equiv r/t}$

flow velocity in the laboratory frame

$$\frac{\partial}{\partial r} = \frac{1}{t}\frac{\mathrm{d}}{\mathrm{dx}}, \qquad \frac{\partial}{\partial t} = -\frac{r}{t^2}\frac{\mathrm{d}}{\mathrm{dx}} = -\frac{\mathrm{x}}{t}\frac{\mathrm{d}}{\mathrm{dx}}$$

spherical



$$\left.\begin{aligned} \frac{1}{\rho}\frac{\partial\rho}{\partial t} + \frac{u}{\rho}\frac{\partial\rho}{\partial r} + \frac{1}{r^2}\frac{\partial}{\partial r}(r^2 u) = 0 \\ \frac{\partial u}{\partial t} + u\frac{\partial u}{\partial r} = -\frac{a^2}{\rho}\frac{\partial\rho}{\partial r} \end{aligned}\right\} \Rightarrow \left\{\begin{aligned} (v-\mathrm{x})\frac{1}{\rho}\frac{\mathrm{d}\rho}{\mathrm{dx}} + \frac{\mathrm{d}v}{\mathrm{dx}} + \boxed{\frac{2v}{\mathrm{x}}} = 0 \\ a^2\frac{1}{\rho}\frac{\mathrm{d}\rho}{\mathrm{dx}} + (v-\mathrm{x})\frac{\mathrm{d}v}{\mathrm{dx}} = 0 \end{aligned}\right. \Rightarrow \frac{\mathrm{x}}{v}\frac{\mathrm{d}v}{\mathrm{dx}} = \frac{2}{\left[1 - \left(\frac{v-\mathrm{x}}{a}\right)^2\right]}$$

weak discontinuity

$\boxed{r = a_o t}$

self-similar solution of the first kind (Zeldovich-Barenblatt 1958)

$$\xi \equiv r/(\mathcal{D}_{CJ} t), \quad v = v_{b_{CJ}}\mathcal{U}(\xi), \quad \rho = \rho_{b_{CJ}}\mathcal{R}(\xi)$$

$$v_{b_{CJ}} = \mathcal{D}_{CJ} - a_{b_{CJ}}$$

$M^2_{u_{CJ}} \gg 1$ strong shock approximation: $\mathcal{D}_{b_{CJ}}/v_{b_{CJ}} = \gamma + 1, \quad a/v_{b_{CJ}} = \gamma\mathcal{R}^{(\gamma-1)/2}$

$$\boxed{\begin{gathered}[\mathcal{U} - (\gamma+1)\xi]\,\frac{1}{\mathcal{R}}\frac{\mathrm{d}\mathcal{R}}{\mathrm{d}\xi} + \frac{\mathrm{d}\mathcal{U}}{\mathrm{d}\xi} + \frac{2\mathcal{U}}{\xi} = 0 \qquad \gamma^2\mathcal{R}^{\gamma-1}\frac{1}{\mathcal{R}}\frac{\mathrm{d}R}{\mathrm{d}\xi} + [\mathcal{U} - (\gamma+1)\xi]\,\frac{\mathrm{d}\mathcal{U}}{\mathrm{d}\xi} = 0 \\ \xi = 1:\ \mathcal{U} = 1,\ \mathcal{R} = 1.\end{gathered}}$$

CJ condition

$\mathrm{d}\mathcal{U}/\mathrm{d}\xi$ diverges at $\xi = 1$

$$\lim_{\xi\to 1}(1-\mathcal{U})^2 = \frac{2\gamma}{\gamma+2}(1-\xi)$$

start the numerical integration at $\xi = 1$

$\xi = 0:\ \mathcal{U} = 0,\ \mathrm{d}\mathcal{U}/\mathrm{d}\xi = 0 \Rightarrow$ stop the calculation at ξ_o at which $\mathcal{U} = 0$; uniform solution in $0 \leqslant \xi \leqslant \xi_o$

spherical kernel of burnt gas at rest whose radius increasing linearly with time

Direct initiation of detonation ?

Initiation by releasing an amount of energy E at a concentrated location in a short time (e.g. explosive charge)

Critical condition $\boxed{E > E_c}$ $\quad E_c$?

At early times the energy liberated by the exothermal reaction is negligible in front of E

$\Rightarrow$ initial condition for direct initiation of detonation: self-similar solution of point blast explosion in an inert gas

Blast wave (Point explosion in an inert gas)

(Taylor 1941 Sedov 1946)

Varying velocity $\mathcal{D}$ $\Rightarrow$ entropy of shocked gas $\neq$ cst. Dissiption neglected $\Rightarrow$ 2 Euler eqs. + $\left(\frac{\partial}{\partial t} + v\frac{\partial}{\partial r}\right)\left(\frac{p}{\rho^\gamma}\right) = 0$

Strong shock $M_u \equiv \mathcal{D}/a_u \gg 1$ $\Rightarrow$ $v_N = \frac{2}{\gamma+1}\mathcal{D}(t)$, $\rho_N = \frac{\gamma+1}{\gamma-1}\rho_u$, $p_N = \frac{2}{\gamma+1}\rho_u\mathcal{D}^2(t)$ where $\mathcal{D}(t) \equiv \frac{\mathrm{d}r_f}{\mathrm{d}t}$

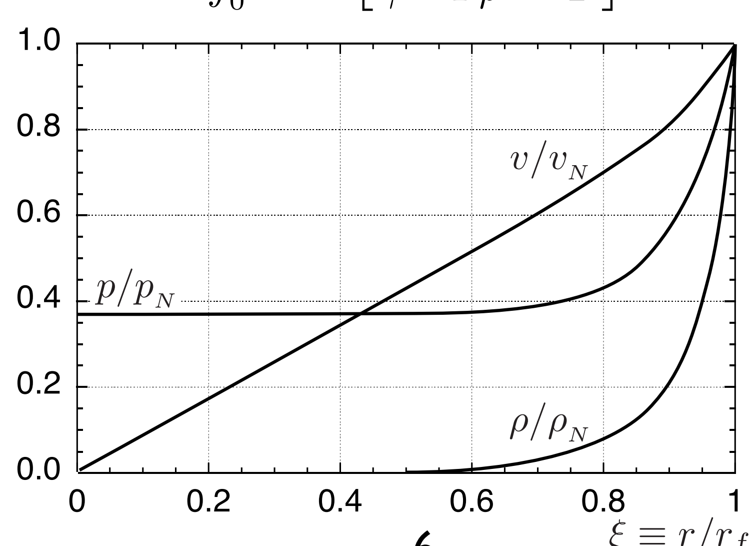
look for a self similar solution in the form $\xi \equiv \frac{r}{r_f(t)}$, $v = \mathcal{D}(t)\mathcal{V}(\xi)$, $\rho = \rho_u\mathcal{R}(\xi)$, $p = \rho_u\mathcal{D}(t)^2\mathcal{P}(\xi)$

$\Rightarrow$ 3 o.d.e. for $\mathcal{V}(\xi)$, $\mathcal{R}(\xi)$, $\mathcal{P}(\xi)$ with $\xi = 1:$ $\mathcal{V} = 2/(\gamma+1)$, $\mathcal{R} = (\gamma+1)/(\gamma-1)$, $\mathcal{P} = 2/\gamma+1$,

$r_f(t)$? 2 dimensional parameters E and ρ_u $\Rightarrow$ a single non-dimensional parameter can be built with r and t $: r(\rho_u/Et^2)^{1/5}$

$$\boxed{r_f(t) = b(\gamma)\left(\frac{E}{\rho_u}\right)^{1/5} t^{2/5}} \Rightarrow \boxed{\mathcal{D}(t) \equiv \dot{r}_f(t) = \frac{2\,b(\gamma)}{5}\left(\frac{E}{\rho_u}\right)^{1/5} t^{-3/5}} \qquad \boxed{\rho_u\mathcal{D}^2r^3 \approx (2/5)^2E}$$

$b(\gamma)$? conservation of energy : $4\pi\int_0^{r_f(t)} \rho\left[\frac{1}{\gamma-1}\frac{p}{\rho} + \frac{v^2}{2}\right] r^2\mathrm{d}r = E$ $\Rightarrow$ $b = 1.0033..$ for $\gamma = 1.4$



Successful direct initiation: Transition between 2 self-similar solutions

$E > E_c$: { point blast explosion (Sedov-Taylor) $\searrow$ spherical CJ wave (Zeldovich-Taylor) $\qquad$ { $D_f(t) \searrow \mathcal{D}_{CJ}$

$E < E_c$: { point blast explosion $\searrow$ fluid at rest $v = 0$ $\qquad$ { $D_f(t) \searrow a_u$

$r_f(t) \nearrow \infty$

(Detonation = discontinuity) $\Rightarrow$ no criticality !
no length scale $\qquad$ no ignition failure

(Korobeinikov 1971, Liñan et al. 2012)

$D_f(t) \searrow \mathcal{D}_{CJ}$ $\boxed{\forall\, E}$ at $r_f \approx r_f^*$ and $t \approx t^*$ corresponding to $\rho_u r_f^{*3} \mathcal{D}_{CJ}^2 \approx E,\ t^* \approx r_f^*/\mathcal{D}_{CJ}$

The inner structure of detonation, d_{CJ}, should play an essential role in ignition failure

Order of magnitude estimate: Zeldovich criterion (1956)

criticality : $\tau_{CJ}^* = \tau_{N_{CJ}}$ $\qquad$ $\tau_{N_{CJ}} \approx d_{CJ}/u_{N_{CJ}}$ $\qquad$ $\mathcal{D}_{CJ}/u_{N_{CJ}} \approx (\gamma+1)/(\gamma-1)$

the time of the blast wave velocity to reach $\mathcal{D}_{CJ}$ = reaction time at the Neumann state of the CJ wave, $\tau_{N_{CJ}}$

$$\tau_{CJ}^* \approx (E/\rho_u)^{1/3} (\mathcal{D}_{CJ})^{-5/3} = d_{CJ}/u_{N_{CJ}} \approx \frac{\gamma+1}{\gamma-1} d_{CJ} (\mathcal{D}_{CJ})^{-1}$$

$$(E_c/\rho_u)^{1/3} \approx \frac{\gamma+1}{\gamma-1} d_{CJ} \mathcal{D}_{CJ}^{2/3}$$

$\mathcal{D}_{CJ}^2 \approx 2(\gamma^2 - 1) q_m$

strong CJ wave $\Rightarrow$ $\boxed{E_c \approx 2\rho_u q_m \dfrac{(\gamma+1)^4}{(\gamma-1)^2} d_{CJ}^3}$

Comparison with experimental data (Lee 1984)
many orders of magnitude smaller 10^{-5} - 10^{-6}

the critical energy is related to the chemical energy in a sphere of radius d_{CJ} ?

Curvature induced modifications to the structure of the planar CJ detonation is essential for estimating E_c

Critical energy

He Clavin (1994)

Nonlinear curvature effect of a spherical CJ detonation $\quad \nabla.\mathbf{j} = \frac{1}{r^2}\frac{\partial(r^2 j)}{\partial r} = \frac{\partial j}{\partial r} + \frac{2}{r}j$

reference frame of the lead shock $\quad x = r_f(t) - r \quad u = \mathcal{D} - v \quad \mathrm{d}r_f(t)/\mathrm{d}t = \mathcal{D} \quad \partial/\partial r \to -\partial/\partial x \quad \partial/\partial t \to \partial/\partial t + \mathcal{D}\partial/\partial x$

Euler eqs.

$$\boxed{\cancel{\frac{\partial \rho}{\partial t}} + \frac{\partial(\rho u)}{\partial x} + \frac{2}{r_f - \cancel{x}}\rho(\mathcal{D}-u) = 0}$$

$$\left(\frac{\partial}{\partial t} + u\frac{\partial}{\partial x}\right)u = -\frac{1}{\rho}\frac{\partial p}{\partial x} + \frac{\mathrm{d}\mathcal{D}}{\mathrm{d}t} \qquad \times\rho \Rightarrow$$

Conservation of energy

$$\left[\frac{\partial}{\partial t} + u\frac{\partial}{\partial x}\right](c_pT - q_m\psi) - \frac{1}{\rho}\left[\frac{\partial}{\partial t} + u\frac{\partial}{\partial x}\right]p = 0 \quad \Rightarrow$$

$$\boxed{\begin{array}{l} \cancel{\frac{\partial(\rho u)}{\partial t}} + \frac{\partial(\rho u^2 + p)}{\partial x} + \frac{2}{r_f - \cancel{x}}\rho(\mathcal{D}-u)u = \cancel{\rho\frac{\mathrm{d}\mathcal{D}}{\mathrm{d}t}} \\ \left[\cancel{\frac{\partial}{\partial t}} + u\frac{\partial}{\partial x}\right]\left(\underbrace{c_pT}_{\frac{\gamma}{\gamma-1}\frac{p}{\rho}} + \frac{u^2}{2} - q_m\psi\right) - \cancel{\frac{1}{\rho}\frac{\partial p}{\partial t}} - u\cancel{\frac{\mathrm{d}\mathcal{D}}{\mathrm{d}t}} = 0 \end{array}}$$

Quasi-steady state approximation $\qquad$ Large radius $\boxed{\epsilon \equiv d_{CJ}/r_f \ll 1}$

detonation thickness
curved detonation

Integration across the inner structure $x = 0:$ Neumann state, $\rho_N u_N = \rho_u \mathcal{D}$, $\qquad x = d:$ bunrt gas

First order approximation

unperturbed planar solution : $\overline{\rho}(x)\overline{u}(x) = \rho_u\mathcal{D}$

$$\boxed{\begin{array}{l} \frac{(\rho_b u_b - \rho_u\mathcal{D})}{\rho_u\mathcal{D}} \approx -I_1 \\ \frac{(\rho_b u_b^2 + p_b) - (\rho_u\mathcal{D}^2 + p_u)}{\rho_u\mathcal{D}^2} \approx -I_2 \end{array}}$$

$$I_1 \approx 2\epsilon\int_0^d\left(\frac{\overline{\rho}(x)}{\rho_u} - 1\right)\frac{\mathrm{d}x}{d_{CJ}} \qquad \left(\frac{\gamma}{\gamma-1}\frac{p_b}{\rho_b} + \frac{u_b^2}{2}\right) \approx \left(\frac{\gamma}{\gamma-1}\frac{p_u}{\rho_u} + \frac{\mathcal{D}^2}{2} + q_m\right)$$

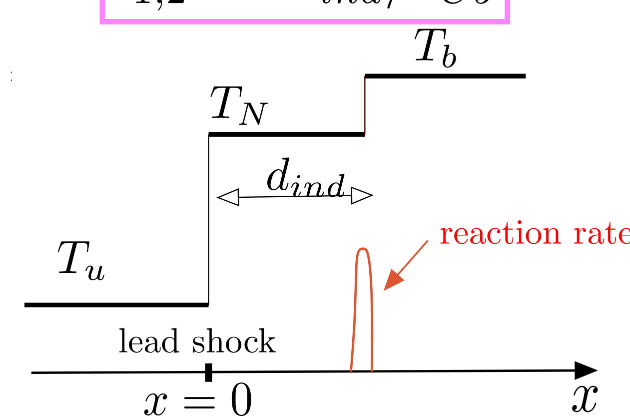
$$I_2 \approx 2\epsilon\int_0^d\left(1 - \frac{\rho_u}{\overline{\rho}(x)}\right)\frac{\mathrm{d}x}{d_{CJ}}$$

Square-wave model: thickness of the reaction zone $\ll$ thickness of the induction zone d_{ind}, $\quad \boxed{\begin{array}{l} d \approx d_{ind}, \\ I_{1,2} \propto \epsilon\, d_{ind}/d_{CJ} \end{array}}$

Arrhenius law $\Rightarrow \beta_N \equiv \frac{E}{k_B T_{N_{CJ}}} \gg 1$, $\quad \boxed{d_{ind} = d_{CJ}\exp\left[-2\beta_N\frac{(\mathcal{D}-\mathcal{D}_{CJ})}{\mathcal{D}_{CJ}}\right]} \quad \frac{(\mathcal{D}-\mathcal{D}_{CJ})}{\mathcal{D}_{CJ}} = O(1/\beta_N)$

$$(\gamma-1)M_u^2 \gg 1 \Rightarrow \frac{\rho_u}{\rho_N} \approx \frac{\gamma-1}{\gamma+1}, \quad \frac{T_N}{T_u} \approx 2\gamma M_u^2\frac{(\gamma-1)}{(\gamma+1)^2}, \quad \frac{T_N}{T_{N_{CJ}}} \approx \left(\frac{\mathcal{D}}{\mathcal{D}_{CJ}}\right)^2$$

$$\boxed{I_1(\mathcal{D}) \approx \frac{4}{\gamma-1}\frac{d_{CJ}}{r_f}\exp\left[-2\beta_N\frac{(\mathcal{D}-\mathcal{D}_{CJ})}{\mathcal{D}_{CJ}}\right], \qquad I_2 \approx \frac{\gamma-1}{\gamma+1}I_1}$$



Small modification of the burnt gas state

$$d_{CJ}/r_f = O(1/\beta_N) \qquad \delta\mathcal{D}/\mathcal{D}_{CJ} \equiv (\mathcal{D}-\mathcal{D}_{CJ})/\mathcal{D}_{CJ} = O(1/\beta_N) \quad \Rightarrow \quad I_1 = O(1/\beta_N) \qquad I_2 = O(1/\beta_N)$$

$$\Rightarrow \quad \delta u_b(\mathcal{D})/a_{b_{CJ}} = O(1/\beta_N), \qquad \delta\rho_b(\mathcal{D})/\rho_{b_{CJ}} = O(1/\beta_N), \qquad \delta p_b(\mathcal{D})/p_{b_{CJ}} = O(1/\beta_N)$$

$$\delta u_b \equiv u_b - a_{b_{CJ}}, \qquad \delta\rho_b \equiv \rho_b - \rho_{b_{CJ}}, \qquad \delta p_b \equiv p_b - p_{b_{CJ}}$$

Small variations of the continuity eq, the Euler eqs and the energy eq yield

$$\frac{\delta\rho_b}{\rho_{b_{CJ}}} + \frac{\delta u_b}{a_{b_{CJ}}} = \frac{\delta\mathcal{D}}{\mathcal{D}_{CJ}} - I_1 \qquad \frac{1}{\gamma}\frac{\delta p_b}{p_{b_{CJ}}} + \frac{\delta\rho_b}{\rho_{b_{CJ}}} + 2\frac{\delta u_b}{a_{b_{CJ}}} = \left(\frac{\mathcal{D}_{CJ}}{a_{b_{CJ}}}\right)\left(2\frac{\delta\mathcal{D}}{\mathcal{D}_{CJ}} - I_2\right) \qquad \frac{1}{\gamma-1}\frac{\delta p_b}{p_{b_{CJ}}} - \frac{1}{\gamma-1}\frac{\delta\rho_b}{\rho_{\rho_{CJ}}} + \frac{\delta u_b}{a_{b_{CJ}}} = \left(\frac{\mathcal{D}_{CJ}}{a_{b_{CJ}}}\right)^2\frac{\delta\mathcal{D}}{\mathcal{D}_{CJ}}$$

Sonic condition in the burnt gas : $\quad u_b^2 = \gamma p_b/\rho_b \quad \Rightarrow \quad \dfrac{\delta p_b}{p_{b_{CJ}}} - \dfrac{\delta\rho_b}{\rho_{\rho_{CJ}}} - 2\dfrac{\delta u_b}{a_{b_{CJ}}} = 0$

$$\frac{(\rho_b u_b - \rho_u\mathcal{D})}{\rho_u\mathcal{D}} \approx -I_1$$

$$\frac{(\rho_b u_b^2 + p_b) - (\rho_u\mathcal{D}^2 + p_u)}{\rho_u\mathcal{D}^2} \approx -I_2$$

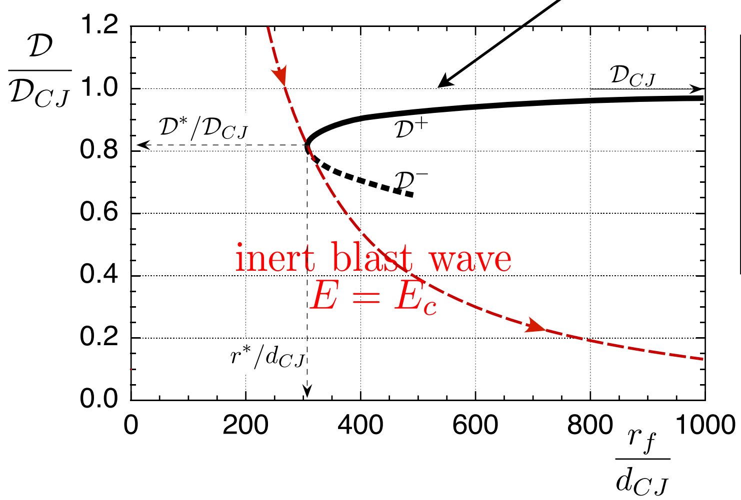
$$\left(\frac{\gamma}{\gamma-1}\frac{p_b}{\rho_b} + \frac{u_b^2}{2}\right) \approx \left(\frac{\gamma}{\gamma-1}\frac{p_u}{\rho_u} + \frac{\mathcal{D}^2}{2} + q_m\right)$$

$$\left\{\frac{\gamma+1}{\gamma}\left[1 + \frac{\gamma-1}{\gamma+1}\left(\frac{\mathcal{D}_{CJ}}{a_{b_{CJ}}}\right)^2\right] - 2\frac{\mathcal{D}_{CJ}}{a_{b_{CJ}}}\right\}\frac{\delta\mathcal{D}}{\mathcal{D}_{CJ}} = \frac{\gamma+1}{\gamma}I_1(\mathcal{D}) - \frac{\mathcal{D}_{CJ}}{a_{b_{CJ}}}I_2(\mathcal{D})$$

$$\frac{\mathcal{D}_{CJ}}{a_{CJ}} \approx \frac{\gamma+1}{\gamma}$$

$$I_1(\mathcal{D}) \approx \frac{4}{\gamma-1}\frac{d_{CJ}}{r_f}\exp\left[-2\beta_N\frac{(\mathcal{D}-\mathcal{D}_{CJ})}{\mathcal{D}_{CJ}}\right], \qquad I_2 \approx \frac{\gamma-1}{\gamma+1}I_1 \quad \Rightarrow \quad \boxed{2\beta_N\left(\frac{\mathcal{D}_{CJ}-\mathcal{D}}{\mathcal{D}_{CJ}}\right)\mathrm{e}^{-2\beta_N\left(\frac{\mathcal{D}_{CJ}-\mathcal{D}}{\mathcal{D}_{CJ}}\right)} = \frac{16\gamma^2}{\gamma^2-1}\beta_N\frac{d_{CJ}}{r_f}}$$

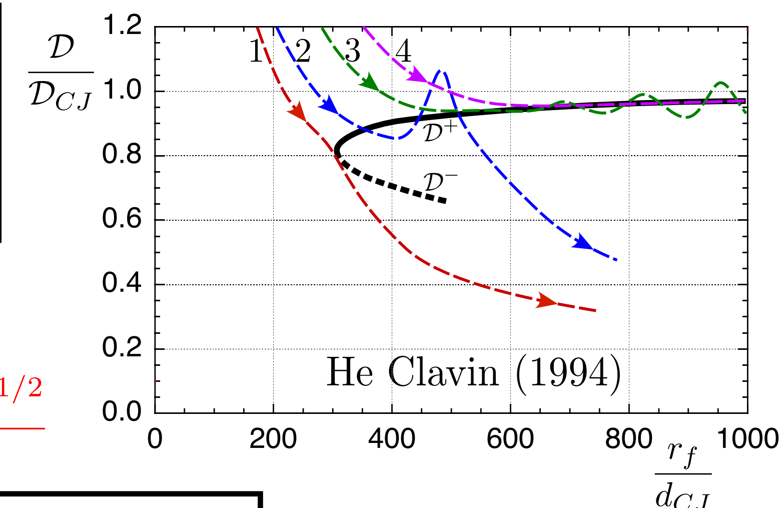
$\left(\dfrac{\mathcal{D}_{CJ}-\mathcal{D}}{\mathcal{D}_{CJ}}\right)$ vs $\dfrac{d_{CJ}}{r_f}$ is a C-shaped curve with a turning point at $\boxed{r^* = \dfrac{16\,\mathrm{e}\,\gamma^2}{\gamma^2-1}\beta_N\,d_{CJ}, \qquad \mathcal{D}^* = \left(1 - \dfrac{1}{2\beta_N}\right)\mathcal{D}_{CJ}}$



there is no spherical CJ detonation with a radius $r_f < r^*$
$r_f^*/d_{CJ} \approx 10^3$

inert blast wave $\quad D \propto \dfrac{(E/\rho_u)^{1/2}}{r^{3/2}}$

marginal blast wave $\quad D_{CJ} \propto \dfrac{(E_c/\rho_u)^{1/2}}{r^{*3/2}}$



$$\boxed{Ec \approx (5/2)^2\rho_u\mathcal{D}_{CJ}^2 r^{*3} = (5^2/2)(\gamma^2-1)q_m\rho_u r^{*3} \approx 10^8 \text{ - } 10^9 \times \text{Zeldovich value (1956)}}$$

ok with DNS of He Clavin (1994)
ok with the experiments of Lee (1984)

Limitations of the analysis: Square-wave model. Quasi-steady state

No change in order of magnitude

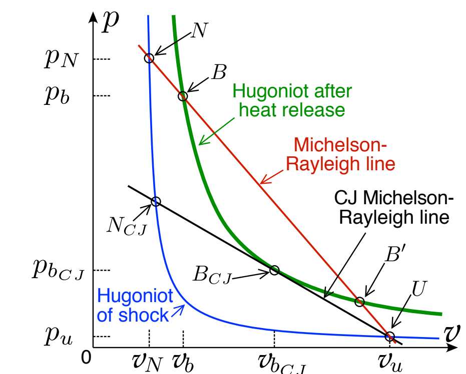
XI-2) Spontaneous initiation and quenching

Spontaneous initiation of detonation at high temperature

Zeldovich (1970-1980) Lee (1978)

Gaseous detonations are difficult to ignite: a large increase of pressure is required $p_{N_{CJ}} \approx 30-50$atm

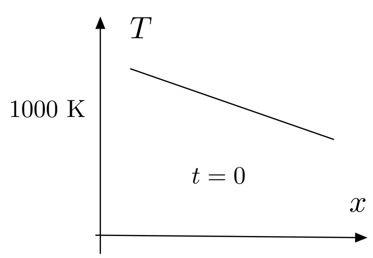
Not possible with an homogeneous explosion of a gaseous pocket at constant volume $(\Delta p/p < 10)$



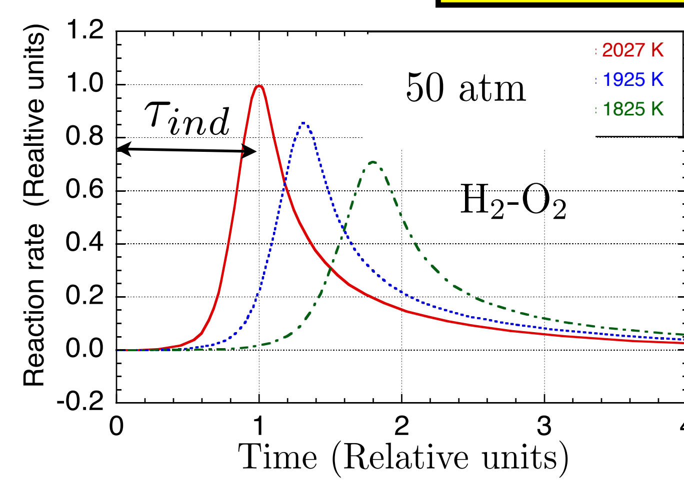
Possible with gradients of T

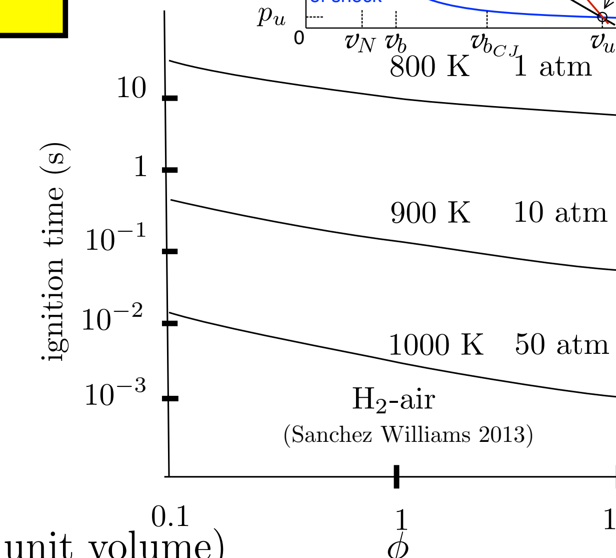
Induction delay (Ignition time) $\tau_{ind}(T,p)$ is highly sensitive to T $\boxed{\tau_{ind} \searrow \quad T \nearrow}$

$t=0$: initial gradient of T $\Rightarrow$ gradient of τ_{ind}



$\boxed{\tau_{ind}(x)}$





1-D : hot slides ignite before cold slides $\dot{q}_v = q_v \varpi \left(t - \tau_{ind}(x)\right)$ (rate of heat release per unit volume)

dimension of $\varpi =$ (reaction time)$^{-1}$

$\Rightarrow$ propagation of an induction front at a speed $\approx (\mathrm{d}\tau_{ind}/\mathrm{d}x)^{-1}$

Mechanism spontaneous initiation: combustion $\Rightarrow$ pressure pulses that propagate with about the speed of sound a

synchronisation : $\boxed{(\mathrm{d}\tau_{ind}/\mathrm{d}x)^{-1} = a}$

$\mathrm{d}\tau_{ind}/\mathrm{d}x \approx$ cst. $\Rightarrow \tau_{ind}(x) \approx \tau^o_{ind} + x(\mathrm{d}\tau_{ind}/\mathrm{d}x)$ $\quad \dot{q}_v = q_v \varpi \left(t - \tau^o_{ind} - x(\mathrm{d}\tau_{ind}/\mathrm{d}x)\right) \approx q_v \varpi \left(t - \tau^o_{ind} - x/a\right)$

$\partial^2 p/\partial t^2 - a^2 \partial^2 p/\partial x^2 = (\gamma - 1)\partial \dot{q}_v/\partial t$ $\quad$ simple wave : $\quad \dfrac{\partial}{\partial t}\delta p + a\dfrac{\partial}{\partial x}\delta p = (\gamma-1) q_v \varpi \left(t - \tau^o_{ind} - x/a\right)$

run away (secular solution) $\quad \delta p = t(\gamma - 1) q_v \varpi \left(t - \tau^o_{ind} - x/a\right)$

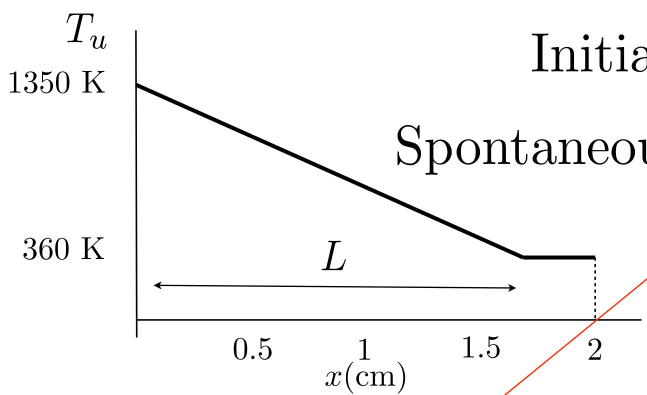
The amplitude of the pressure pulse increases linearly with time at the rate of the reaction rate

$$\boxed{(\mathrm{d}\tau_{ind}/\mathrm{d}x)^{-1} = a}$$

Zeldovich & Lee criterion for spontaneous initiation (1970-1980) has been observed in numerics and experiments
Zeldovich et al. (1970), Kapila et al. (2002) Lee (1978)

Spontaneous quenching

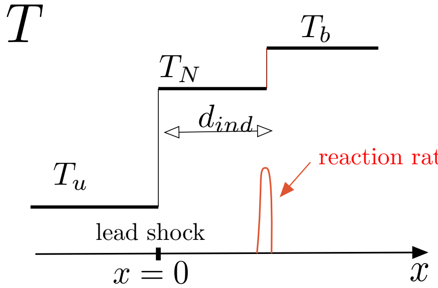
(He Clavin 1992-1994)



Initiation in a uniform cold mixture from a nonuniform hot pocket

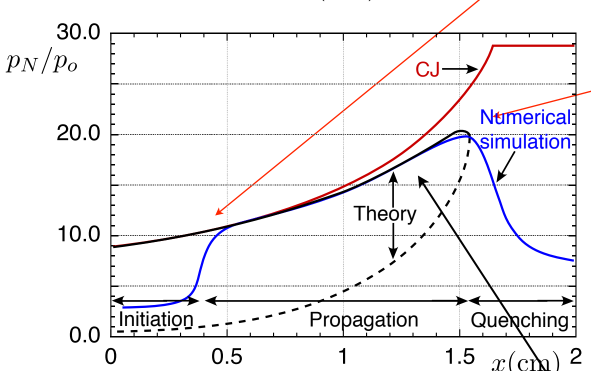
before reaching the uniform cold mixture

Spontaneous ignition at high T may be followed by sudden quenching at lower T

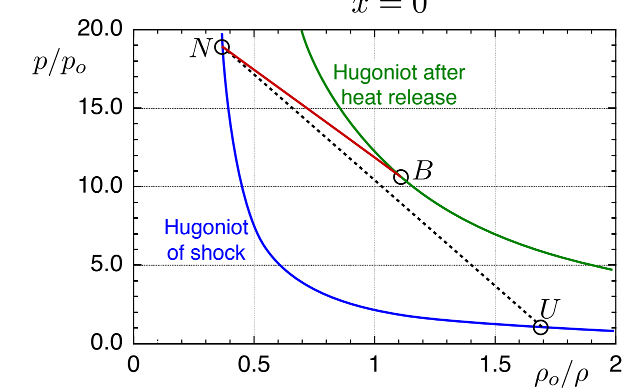


Theoretical analysis:

- square-wave model
- quasi-steady induction zone : $d_{ind}/\overline{d}_{ind} \approx \mathrm{e}^{-2\beta_N \frac{(\mathcal{D}-\overline{\mathcal{D}})}{\overline{\mathcal{D}}}}$
- $\mathrm{d}d_{ind}/\mathrm{d}t \neq 0 \Rightarrow$ mass flux in reaction zone $\neq \rho_u \mathcal{D}$



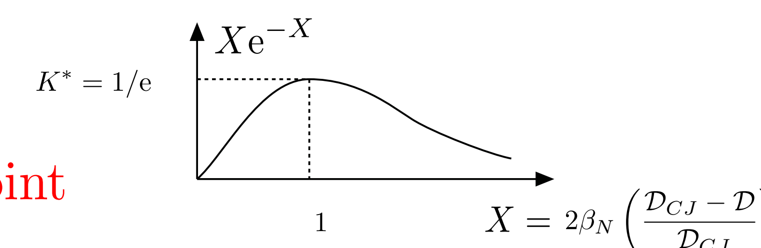
$$\frac{\delta D_{CJ}}{D_{CJ}} \approx (2M_{u_{CJ}}^2)^{-1}\frac{\delta T_u}{T_u} \Rightarrow \boxed{\frac{\mathrm{d}}{\mathrm{d}t}d_{ind} \propto \mathrm{e}^{-2\beta_N \frac{(\mathcal{D}-\overline{\mathcal{D}})}{\overline{\mathcal{D}}}} L \frac{\mathrm{d}\mathcal{D}}{\mathrm{d}x}}$$



geometrical construction:

difference of mass flux = difference of slopes of UN and $NB \propto (\mathcal{D}-\overline{\mathcal{D}})/\overline{\mathcal{D}}$ $\quad$ ($(\gamma-1)M_u^2 \gg 1$)

$$(\gamma-1)M_u^2 \gg 1 : \quad \boxed{\frac{\mathrm{d}}{\mathrm{d}t}d_{ind} \propto \overline{u}_N \frac{(\mathcal{D}-\overline{\mathcal{D}})}{\overline{\mathcal{D}}}}$$



C-shaped curve $\mathcal{D}$ vs $\mathrm{d}T_u/\mathrm{d}x$ with a turning point

$$\boxed{2\beta_N\left(\frac{\mathcal{D}_{CJ}-\mathcal{D}}{\mathcal{D}_{CJ}}\right)\mathrm{e}^{-2\beta_N\left(\frac{\mathcal{D}_{CJ}-\mathcal{D}}{\mathcal{D}_{CJ}}\right)} = K}$$

where $\quad K \equiv 4\beta_N^2 \tau_{ind}(T_{N_{CJ}})\left(-\frac{\mathrm{d}\mathcal{D}_{CJ}}{\mathrm{d}x}\right) = O(1)$

critical condition for sudden quenching $\quad K^* = 1/\mathrm{e}$ $\quad \left(\frac{\mathcal{D}_{CJ}-\mathcal{D}^*}{\mathcal{D}_{CJ}}\right) = \frac{1}{2\beta_N}$ $\quad$ ok with DNS

A CJ detonation cannot survive to a strong temperature gradient at low temperature $\quad (K > 1/\mathrm{e}) \quad \frac{\mathrm{d}K}{\mathrm{d}T_u} < 0$

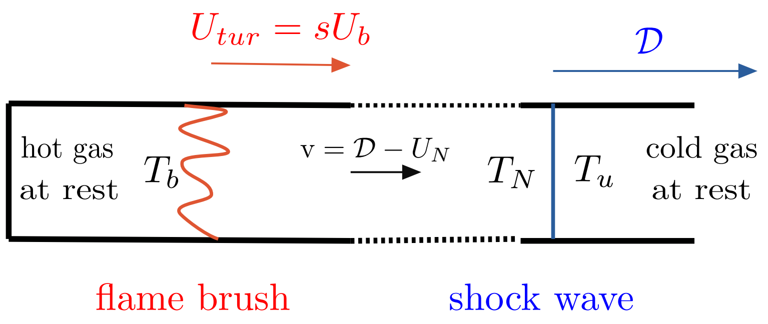
The non-uniform pocket of hot gas should hav hape for initiating a detonation

XI-3) Deflagration-to-detonation transition (DDT)

DDT is not observed in free space (without confinement or obstacle). Supernovae ?
explosions $\neq$ detonations

Basic ingredients for DDT in tubes

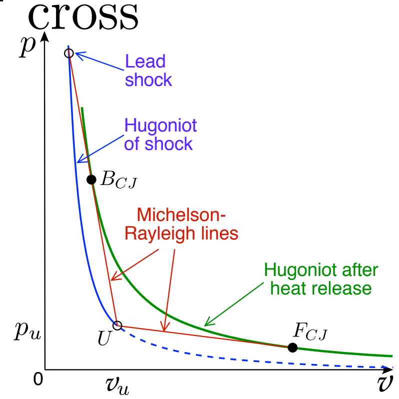
-1) Piston effect: fresh gas put in motion ahead of the flame
-2) Flame acceleration through an increase of the flame surface area
-3) Heating of the fresh mixture by compressible effects
(through a shock wave or a compression wave and/or viscous dissipation)



Experiments

Shchelelkin, Troshin (1965), Oppenheim et al (1966-1973), Lee et al (1977-2008),..

For turbulent flames in energetic mixtures ($U_L \approx 10$ m/s) DDT is observed in tubes of few 10 cm^2 cross section when the turbulent flame speed approaches sufficiently large values $U_{tur} \gtrsim 300$ m/s
(Lee 1977)



Obstacles facilitate DDT

Obstacles may also generate turbulent chocked regime, $U_{tur} \approx 600-1000$, m/s without DDT
(Lee Berman 1997)

DDT may result from localized explosions (Zeldovich mechanism) ahead of a fast turbulent flame
(Oppenheim et al 1966-1973)

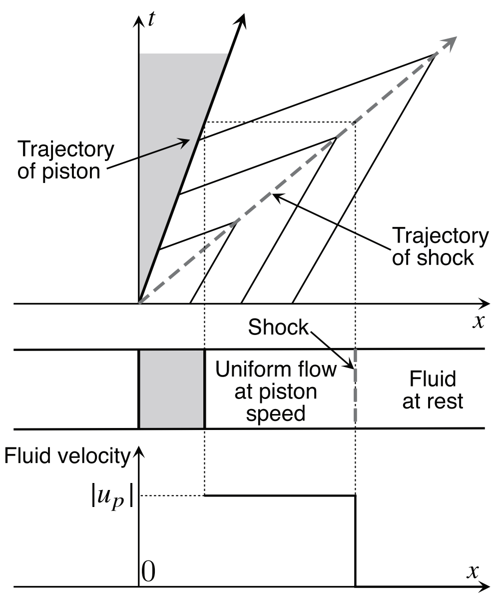
In fuel-air mixture ($U_L \approx 40$ cm/s), DDT is not observed in tubes at laboratory scale
it is observed in large scale experiments (coal mines) (Oran et al. 2014)

DDT is observed in energetic mixtures ($U_L \approx 10$ m/s) in smooth-walled capillary tube
(Wu et al 2007-2011)

Runaway phenomenon (Deshaies Joulin 1989)

1-D self-similar solution of a shock wave generated by a flame brush propagating at a constant velocity U_{turb} from the closed end of a tube

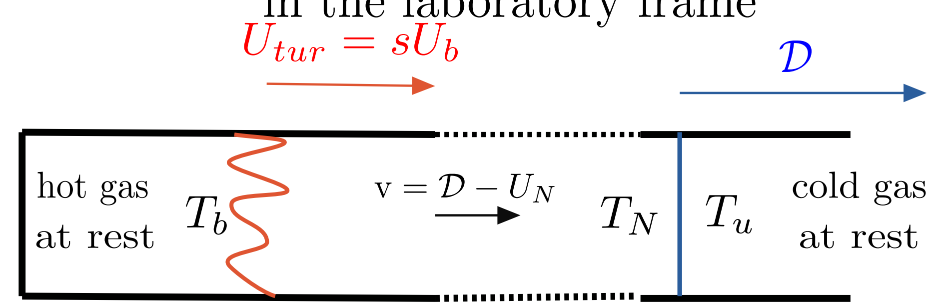
$$U_{turb} = sU_b \qquad s \text{ degree of folding}$$



Flame $\equiv$ semi-permeable piston

$$\mathrm{v} = s(U_b - U_L)$$

in the laboratory frame



flame brush　　shock wave

in the reference frame of the wave

$\mathrm{v} = s(U_b - U_L)$　　$\mathrm{v} = \mathcal{D} - U_N$

flow velocity in the lab frame

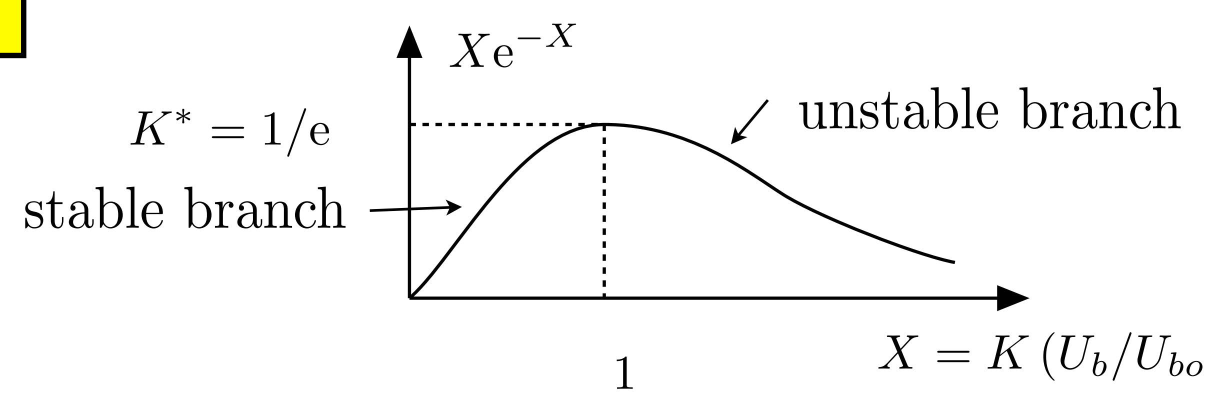
Look for the nonlinear relation $\mathcal{D} - U_{turb}$ $(\mathcal{D} - s)$

key relations: $\boxed{U_b/a_o \propto \mathrm{e}^{-\frac{E}{2k_B T_b}} \quad \left(\frac{T_b}{T_u} - 1\right) \propto s\frac{U_b}{a_u}}$

$\mathrm{v} = s(U_b - U_L) = \mathcal{D} - U_N$ and $(T_b - T_{bo}) \approx (T_N - T_u)$

$\boxed{X\mathrm{e}^{-X} = K}$　　$K \propto s(U_{Lo}/a_u)$　　$X \equiv K(U_b/U_{bo})$

K is linear in the folding s



No solution for $K > 1/\mathrm{e}$　i.e when the folding is too large $s > s^*$

If $s \nearrow s^*$: runaway at the critical condition $s = s^*$　DDT !

Runaway phenomenon (Deshaies Joulin 1989)

1-D self-similar solution of a shock wave generated by a flame brush propagating from the closed end of a tube

look for the solution of this nonlinear problem $\mathcal{D} - U_{turb}$

$U_{tur} \equiv sU_b$: subsonic velocity (/ lab frame) of the turbulent flame brush $\ll$ supersonic shock velocity $\mathcal{D}$

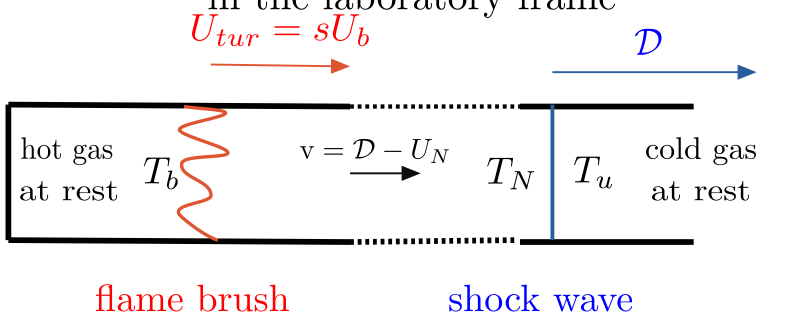
$\boxed{s \equiv \langle S \rangle / S_o}$ is the degree of folding $sU_b/a_u \ll 1 \;\Rightarrow$ weak shock : $(M_u - 1) \ll 1$ where $M_u = \mathcal{D}/a_u > 1$

ρ and T weakly modified $(T_N - T_u)/T_u = O(M_u - 1)$

Large activation energy $E/k_BT \gg 1$, $(M_u - 1) = O(k_BT_b/E) \Rightarrow U_b/U_{bo} = O(1)$

$U_b \propto \mathrm{e}^{\frac{E}{2k_BT_b}} \;\Rightarrow\; \boxed{U_b/U_{bo} \approx \mathrm{e}^{\frac{E}{2k_BT_{bo}}\left(\frac{T_b - T_{bo}}{T_{bo}}\right)}}$ U_{bo} and T_{bo} : without shock

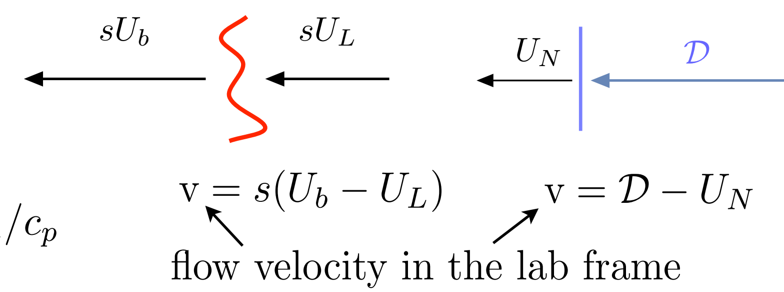
in the laboratory frame



Conservation of mass across the waves:

$$\left.\begin{aligned} &\rho_b U_b = \rho_u U_L \Rightarrow \mathrm{v} = s(U_b - U_L) = \left(1 - \frac{\rho_b}{\rho_u}\right) sU_b \\ &\rho_N U_N = \rho_u \mathcal{D} \Rightarrow \mathrm{v} = \mathcal{D} - U_N \end{aligned}\right\} \quad \boxed{\mathcal{D} - U_N = \left(1 - \frac{\rho_b}{\rho_u}\right) sU_b}$$

in the reference frame of the wave



Weak shock : $\dfrac{\mathcal{D} - U_N}{a_u} \approx \dfrac{2}{\gamma + 1}(M_u^2 - 1)$, $\quad \dfrac{T_N}{T_u} - 1 \approx \dfrac{2(\gamma - 1)}{\gamma + 1}(M_u^2 - 1)$

$$\boxed{\frac{T_N}{T_u} - 1 \approx (\gamma - 1)\frac{(\mathcal{D} - U_N)}{a_u} = (\gamma - 1)\left(1 - \frac{\rho_b}{\rho_u}\right) s\frac{U_b}{a_u} \ll 1}$$

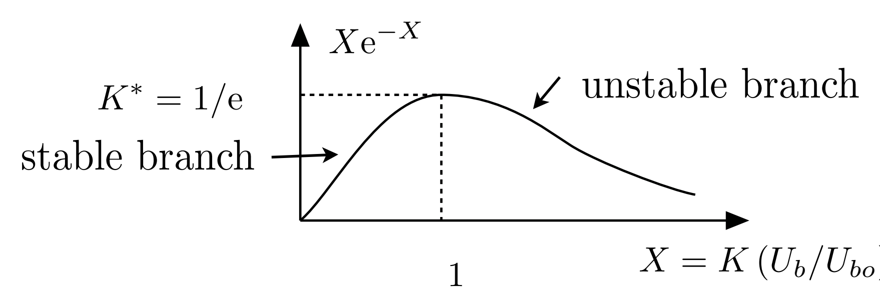
and $T_b \approx T_N + q_m/c_p \quad T_{bo} \approx T_u + q_m/c_p$

$(T_b - T_{bo}) \approx (T_N - T_u)$

$$\frac{T_b - T_{bo}}{T_u} \approx (\gamma - 1)\left(1 - \frac{\rho_b}{\rho_u}\right) s\frac{U_b}{a_u} \;\Rightarrow\; \boxed{\frac{E}{2k_BT_{bo}}\frac{(T_b - T_{bo})}{T_{bo}} = K\frac{U_b}{U_{bo}}} \quad \text{where} \quad \boxed{K \equiv (\gamma - 1)\frac{E}{2k_BT_b}\left(1 - \frac{\rho_b}{\rho_u}\right) s\frac{U_L}{a_u}}$$

equation for U_b/U_{bo} in terms of s $\quad (U_{bo}/U_L = T_{bo}/T_u)$ $\quad$ K is linear in the folding s

$\boxed{(U_b/U_{bo}) = \exp[K(U_b/U_{bo})]}$ $\qquad X\mathrm{e}^{-X} = K \quad$ where $\quad X \equiv K(U_b/U_{bo})$



Two solutions for $K < K^* \equiv 1/\mathrm{e}$: one is unstable the other stable

No solution for $K > 1/\mathrm{e}$ i.e when the folding is too large $s > s^*$

Assume that the degree of folding increases with time (instability, fingering, development of turbulence ..)

If $s \nearrow s^*$: runaway at the critical condition $s = s^*$ DDT !

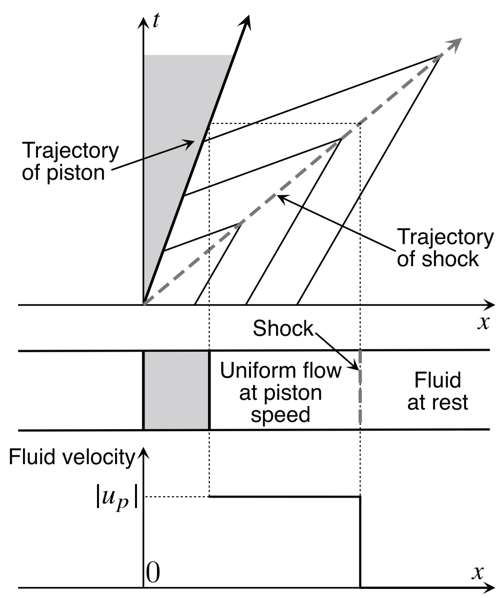
$$\mathrm{s}^* = \left[(\gamma - 1)\left(1 - \frac{\rho_b}{\rho_u}\right)\frac{E}{2k_BT_b}\frac{U_L}{a_u}\mathrm{e}\right]^{-1}$$

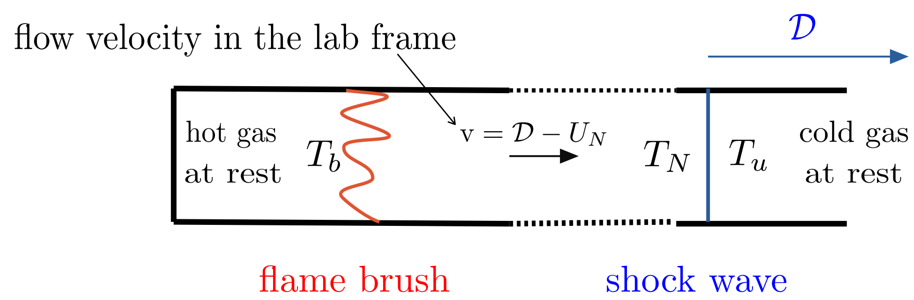
$\boxed{U_{turb}^* = s^* U_b^* \approx 500 \text{ m/s}}$ OK with experiments

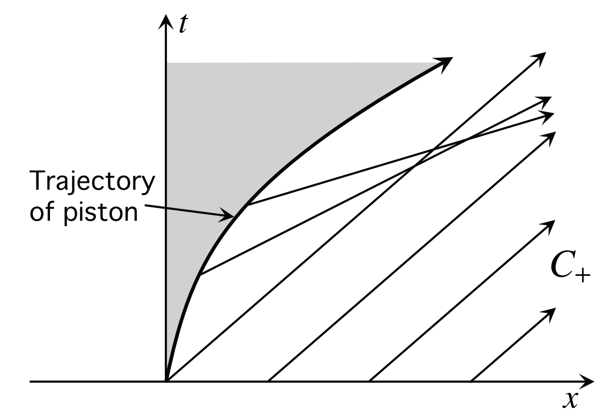
Constant flame velocity $\neq$ accelerating flame

self-similar solution

no self similar solution
multiple chocs formation







Reasoning for the run away is easily extended to the case of simple waves emitted from an accelerating front without considering the shock formation

Deshaies-Joulin (1989)

Riemann invariants $\quad C_+ : \dfrac{\mathrm{d}x}{\mathrm{d}t} = \mathrm{v} + a, \qquad C_- : \dfrac{\mathrm{d}x}{\mathrm{d}t} = \mathrm{v} - a$

transient regime $\neq$ standing wave
far upstream from the flame the gas is at rest

$$J_+ \equiv \frac{2}{\gamma-1}a + \mathrm{v} = \text{ cst sur } C_+ \qquad J_- \equiv \frac{2}{\gamma-1}a - \mathrm{v} = \text{ cst sur } C_- \Rightarrow \frac{2}{\gamma-1}a - \mathrm{v} = \frac{2}{\gamma-1}a_o$$

cst $\forall\,(x,t)$

value at the flame front for a simple (compression) wave:

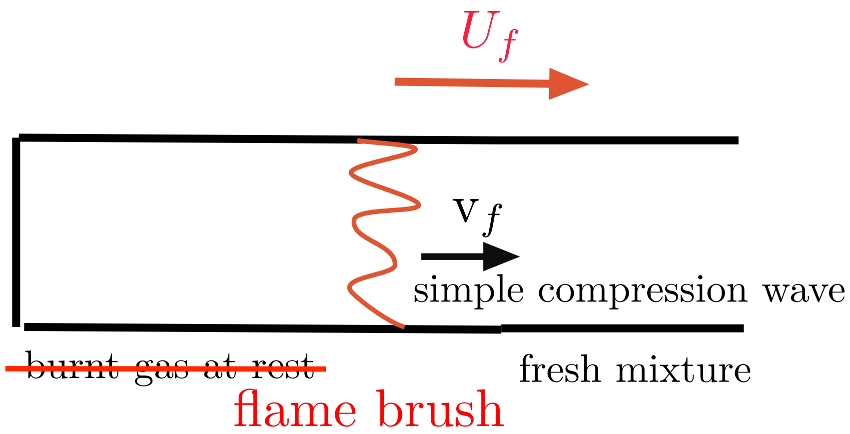
$$\boxed{\frac{2}{\gamma-1}(a_f - a_o) = \mathrm{v}_f} \qquad a_f/a_o = \sqrt{T_f/T_u} \qquad \Rightarrow \qquad \boxed{\begin{array}{c} \dfrac{T_f}{T_u} \approx 1 + (\gamma-1)\dfrac{\mathrm{v}_f}{a_o} \\ \mathrm{v}_f/a_o \propto U_f/a_o \propto \sqrt{\mathrm{e}^{-E/k_B T_f}} \end{array}}$$

piston effect $\qquad$ chemical kinetics

$U_f = sU_b$

same nonlinear solution for U_f as in the self-similar case

No solution for U_f above a critical value



$$T_f/T_u \approx 1 + (\gamma - 1)\mathrm{v}_f/a_o$$

simple compression wave

$$\Rightarrow \quad U_b/U_{bo} = \mathrm{e}^{\frac{\beta(\gamma-1)}{2}\frac{T_u}{T_{bo}}\frac{\mathrm{v}_f}{a_o}}$$

$$T_b - T_{bo} = T_f - T_u \Rightarrow \; U_b/U_{bo} = \mathrm{e}^{\frac{\beta}{2}\frac{T_f - T_u}{T_{bo}}}$$

chemical kinetics

$$\cancel{\mathrm{v}_f = \left(1 - \frac{\rho_b}{\rho_u}\right)U_f} \quad + \quad \cancel{U_f = sU_b} \quad \Rightarrow \quad U_b/U_{bo} = \mathrm{e}^{\frac{\beta(\gamma-1)}{2}\left(1-\frac{\rho_b}{\rho_u}\right)\frac{\rho_b}{\rho_u}\frac{sU_b}{a_o}} = \mathrm{e}^{\left[\frac{\beta(\gamma-1)}{2}\left(1-\frac{\rho_b}{\rho_u}\right)\frac{U_L}{a_o}s\right]\frac{U_b}{U_{bo}}}$$

mass conservation across the flame brush — wrinkling

nonlinear relation $\boxed{U_b/U_{bo} = \mathrm{e}^{K(U_b/U_{bo})}}$

Response involving time-delay

Delay due to the propagation of acoustic waves in the burned gas: $\rho_b(u_f^{(a)} - U_f) = \rho_u(\mathrm{v}_f - U_f) = \rho_b s U_b$

Delay due to the transit time across the flamelets $\quad U_b(t + \Delta t)/U_{bo} = \mathrm{e}^{\frac{\beta}{2}\frac{T_f(t) - T_u}{T_{bo}}}$

Both delays are of the same order...

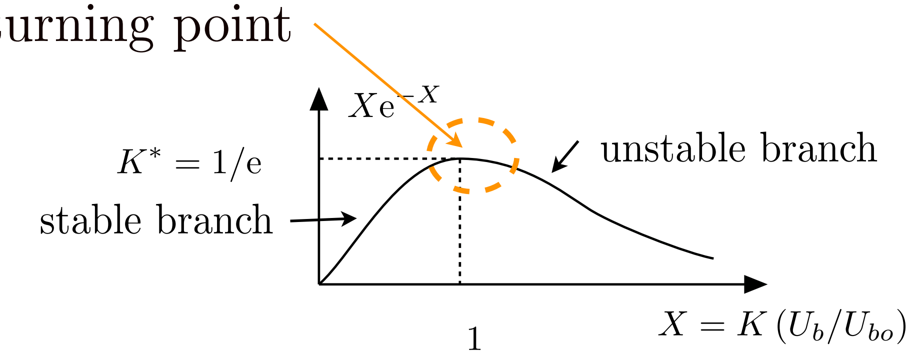
Dynamical model of runaway when the folding increases linearly with time

$$s = t/\tau_e + \mathrm{cst.}$$

Neglecting acoustic for simplicity

Fast response $\quad \Delta t \ll \tau_e, \quad U_b(t + \Delta t) \approx U_b(t) + (\Delta t)\mathrm{d}U_b/\mathrm{d}t$

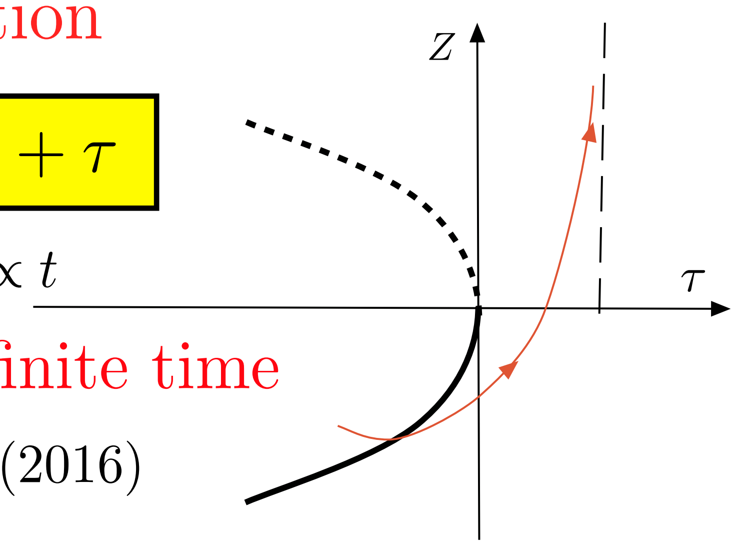
Near the turning point



Riccati equation

$$\boxed{\mathrm{d}Z/\mathrm{d}\tau = Z^2 + \tau}$$

$Z \propto U_f \qquad \tau \propto t$



Singularity after a finite time

Clavin (2016)

Mechanisms of DDT

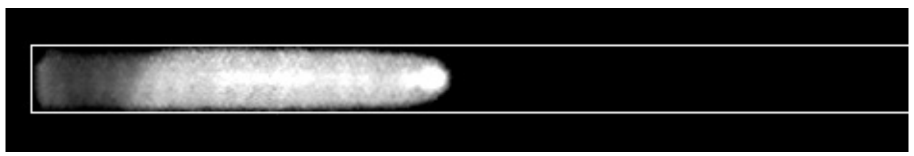
Acceleration mechanisms of the flame brush leading to DDT ?

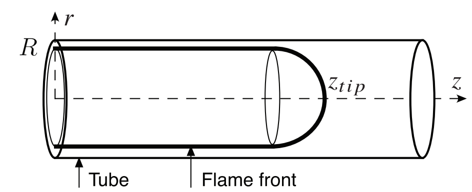
Turbulence induced DDT (Shchelkin 1940-1945)

turbulent flow of fresh mixture $\Rightarrow s\nearrow \Rightarrow U_{tur}\nearrow \Rightarrow$ flow velocity$\nearrow\Rightarrow$ turbulence intensity$\nearrow \Rightarrow s\nearrow \Rightarrow U_{tur}\nearrow$

(positive feedback)

Acceleration of an elongated flame (Clanet Searby 1996, Bychkov 2006)





$\left.\begin{array}{l}\text{lateral combustion}\\ \text{stick condtion at the wall}\end{array}\right\} \Rightarrow$ velocity of the tip $\propto \exp(t/\tau_a)$, $1/\tau_a \equiv 2(\rho_u/\rho_b)U_L/R \Rightarrow$ induced flow velocity$\nearrow \propto \mathrm{e}^{t/\tau_a}$

(runaway or positive feedback)

DDT induced by local explosions

(Oppenheim's experiments 1966-1973)

2 possibilities for heating: compression waves and viscous dissipation in the boundary layer at the wall

heating + boundary layer $\Rightarrow \nabla T \neq 0 \Rightarrow 1/|\nabla \tau_{ind}| = a$:

local explosion by the spontaneous initiation mechanism of Zeldovich

ignition: $T > T^* \approx 1000$ K $\Rightarrow$ vitesse de flamme/labo > 300 m/s

this is also the typical velocity of the flame brush for the runaway mechanism of Deshaies Joulin !!

Preheating by compression and viscous dissipation in narrow insulated tube

Kagan Sivashinsky (2003-2014)

piston like effect $\Rightarrow$ precursor flow $\Rightarrow$ compression+viscous dissipation $\Rightarrow T_b\nearrow\ U_b\nearrow\Rightarrow$ piston effect$\nearrow$

runaway mechanism similar to that of Deshaies Joulin (1989) (but folding is not necessary)