Advances in the nonlinear dynamics of gaseous detonations

Paul Clavin

Institut de **R**echerche sur les **P**hénomènes **H**ors **É**quilibre
Aix-Marseille Université, CNRS & Centrale Marseille, France

Autumn Sciences Days at University of Almeria
in honor of Manuel Garcia VELARDE
September 24-27 2019

Understanding complex phenomena ?

Examples: combustion phenomena

Direct numerical simulations ?

A physicist approach: reduce the complexity
ending with simplified equations
to be solved analytically and compare with experiments

Hopefully gaseous detonations are not easy to initiate

What minimum energy should be deposited
by an external source
to initiate a gaseous detonation in an open space ?

Safety of nuclear power plant
Explosions…..supernovae….

Detonations = combustion supersonic waves

inert shock followed by an exothermal reaction zone

in gas at ordinary conditions: $1800-3400$ m/s, $15-30$ bar, $2500-3700$ K



Deflagration = combustion subsonic waves

reaction-diffusion waves

Old scientific topic (end of 19th - extensively studied since the mid 20th)

Comprehensible explanation of the multidimensional geometry and complex dynamics of the wave fronts has been elusive. Understanding is recent (nonlinear analyses)

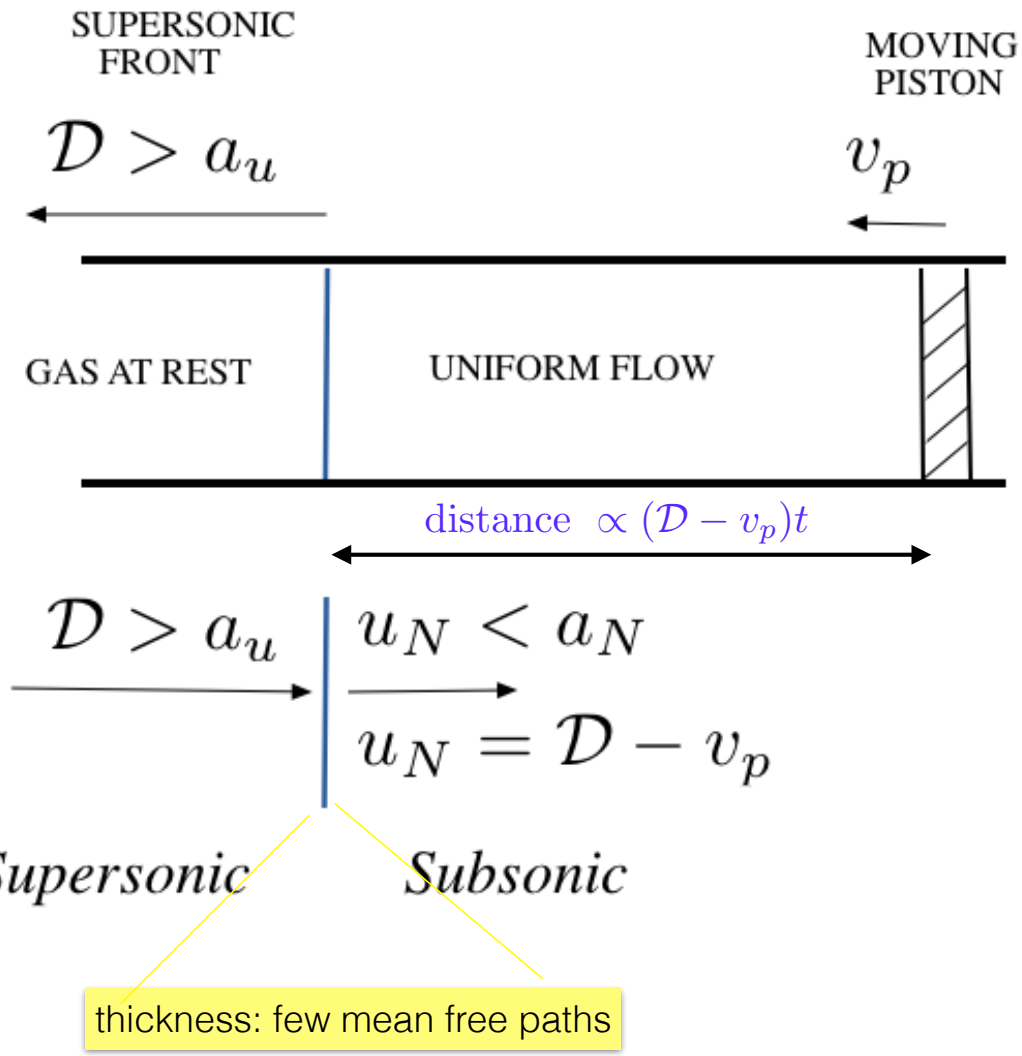
Reactive Euler equations

Back to school

Background in compressible fluids

Planar shock waves and detonations
1860-1940

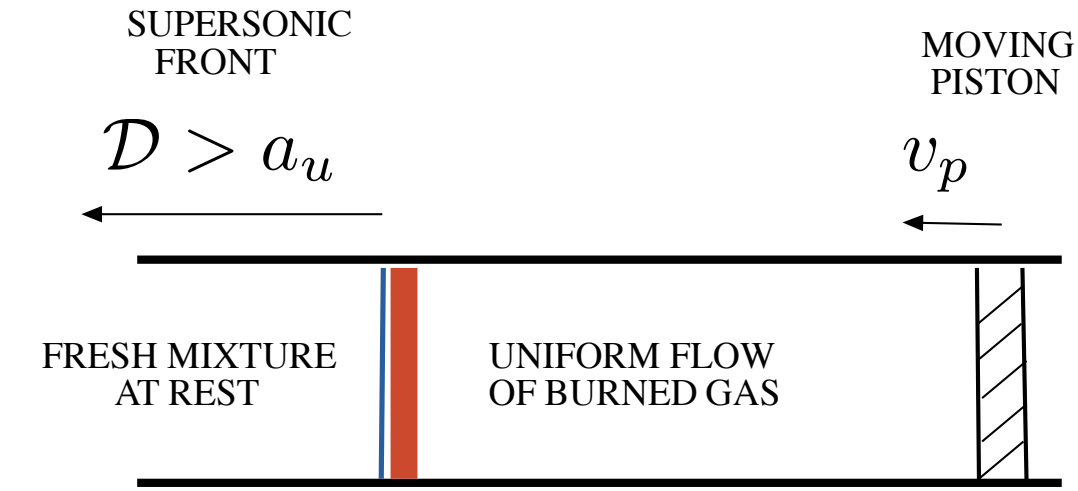
PLANAR SHOCK WAVE
INERT GAS

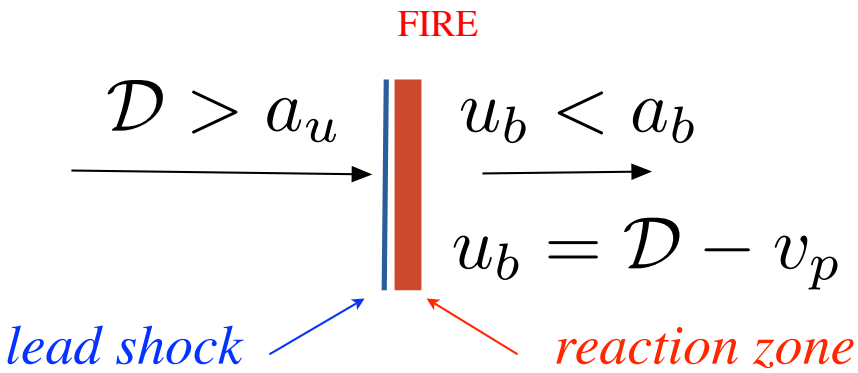


Poisson 1808, Stokes 1848, **Riemann** 1860, Rankine 1869, **Hugoniot** 1889, Rayleigh 1910

OVERDRIVEN DETONATION REACTING GAS

PISTON SUPORTED SUPERSONIC WAVE





Abel 1870, Berthelot et Vielle 1881, Mallard et Le Chatelier 1881, **Mikhel'son** 1893, Chapman 1899, Jouguet 1904, Vielle 1900, **Zel'dovich** 1940, von Neumann 1942, Döring 1943,

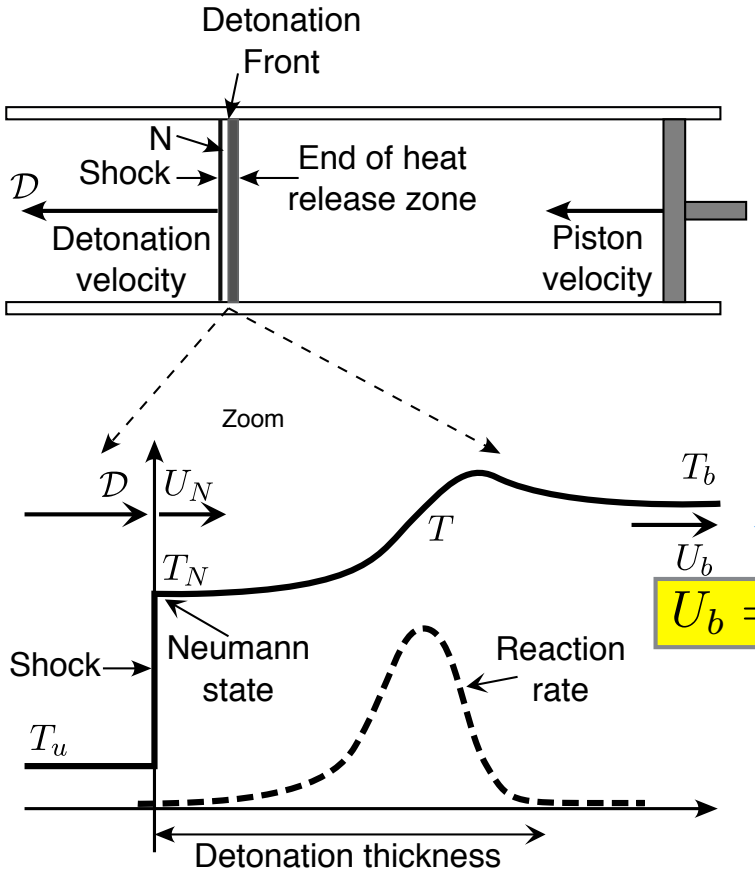
Planar detonation

Overdriven regime / Self sustained wave

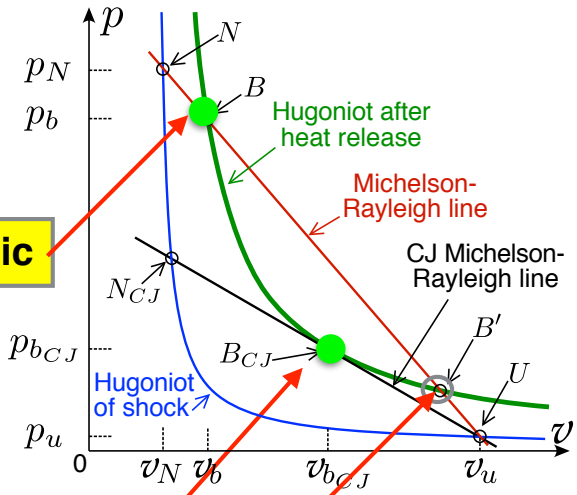
Marginal solution

the so called Chapman-Jouguet wave

Mikhel'son (1893)



$U_b = a_b$



subsonic

supersonic without shock
non physical
under ordinary conditions

thickness ≈ few mms

Arrhenius law e^{-E/k_BT}

$$reaction\ rate \approx \frac{e^{-E/k_BT}}{\tau_{coll}} \qquad \frac{E}{k_BT} \approx 10$$

τ_{coll} : *elastic collisions*

Sonic condition

Planar detonation
(inner structure in steady state)

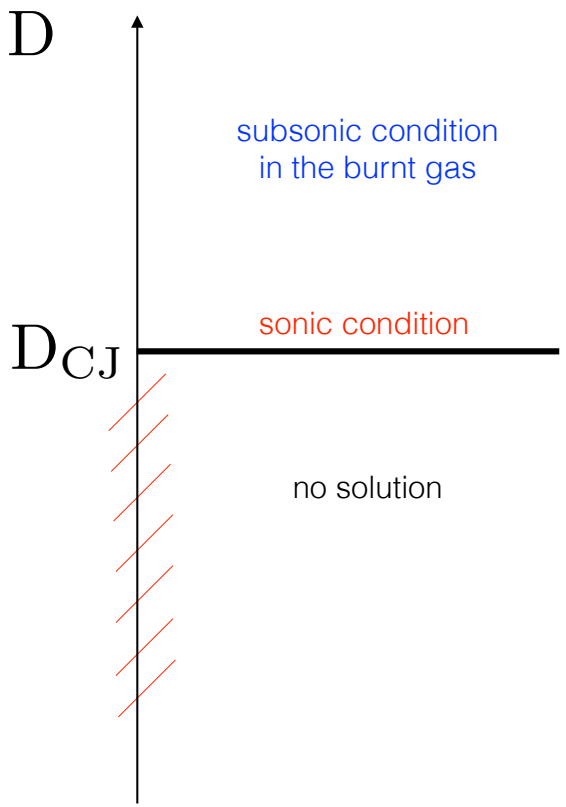
propagation velocity

supersonic overdriven wave

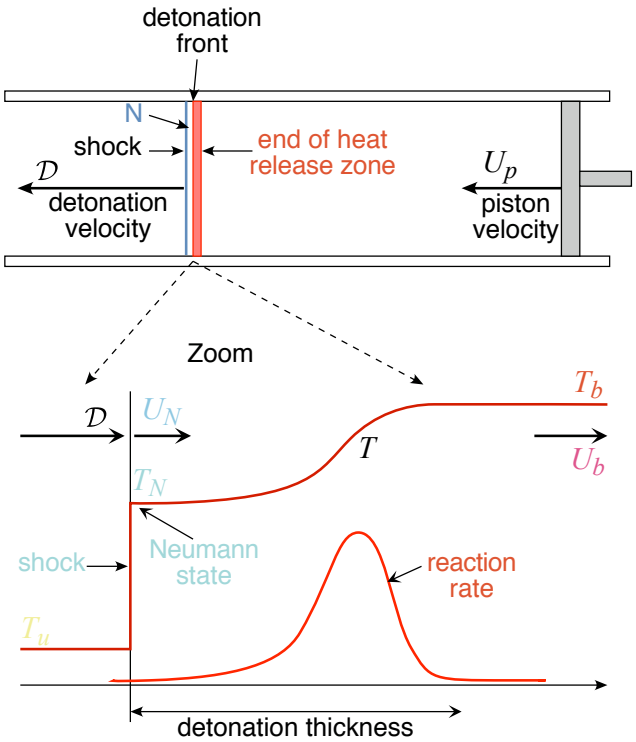
$$\mathrm{D} > a_u$$

self sustained supersonic wave

$$\frac{q_m}{c_p T_u} \gg 1 \quad \Rightarrow \quad \frac{\mathrm{D_{CJ}}}{a_u} \approx 2\sqrt{\frac{\gamma+1}{2}\frac{q_m}{c_p T_u}} > 1$$



Negligible heat conduction and viscosity



$$l = U_N \times t_r(T_N)$$

$U_N \approx a$ flow velocity/shock sound speed

reaction time $t_r \approx t_{coll} \times \mathrm{e}^{\mathcal{E}/k_b T} \gg t_{coll}$

$\mathcal{E}/k_b T \approx 10$

Reynolds nb $\dfrac{U_N\, l}{\nu} \approx \dfrac{a^2 \times t_r}{\nu} \approx \dfrac{t_r}{t_{coll}} \approx \mathrm{e}^{\mathcal{E}/k_b T} \gg 1$

$$\nu \approx a^2 \times t_{coll}$$

Back to our problem !

What minimum energy should be released
by an external source
to initiate a gaseous detonation in open space (3D) ?

Zeldovich criterion (1956)

$$\text{critical energy} \approx \frac{\text{chemical energy}}{\text{unit volume}} \times (\text{detonation thickness})^3$$

Wrong ! Under estimated by a factor 10^6–10^8

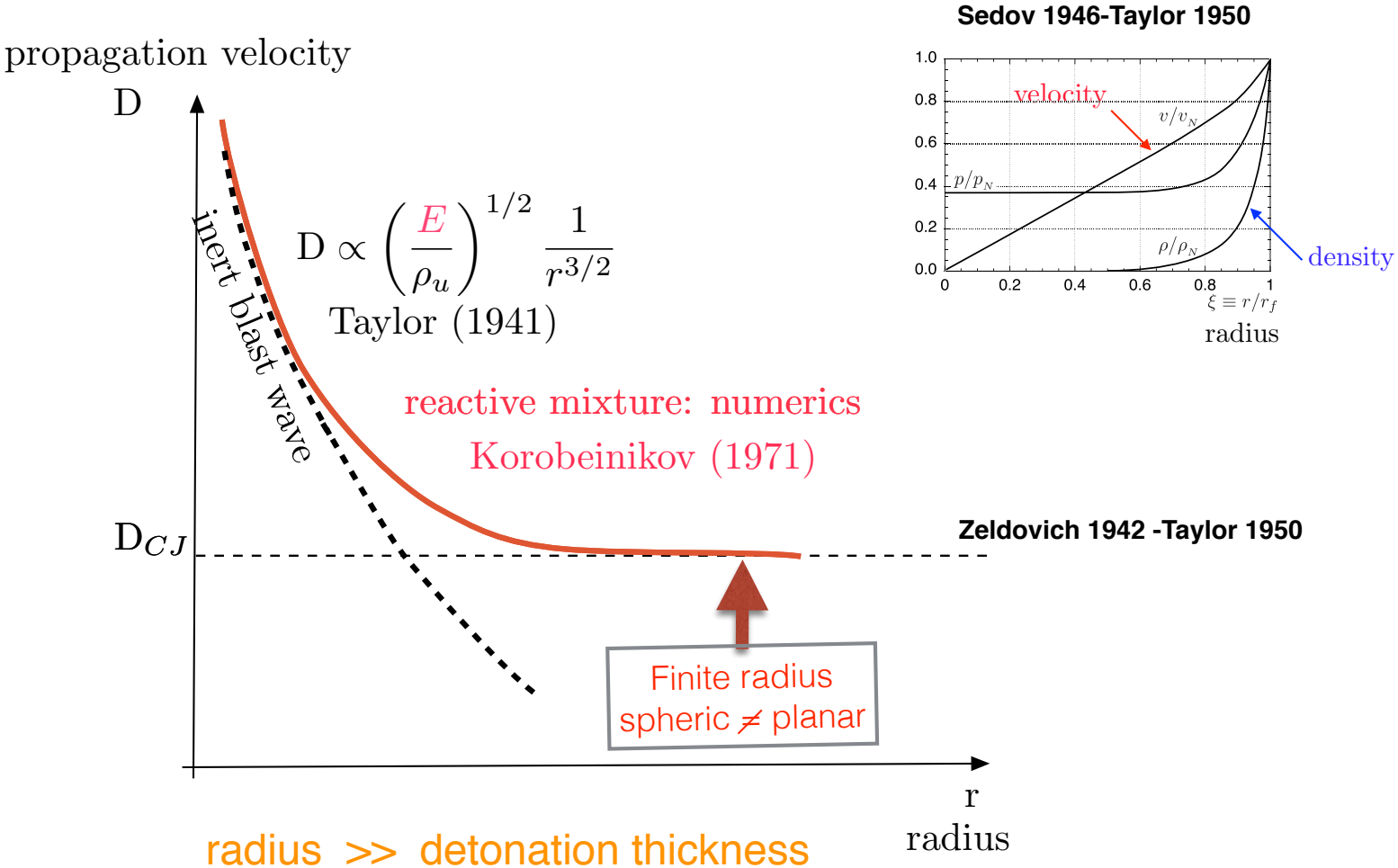
Experiments (1975)-(1980)

Numerics in spherical geometry

Korobeinikov (1971)
Detonation = discontinuity

(zero detonation thickness)

No critical energy !



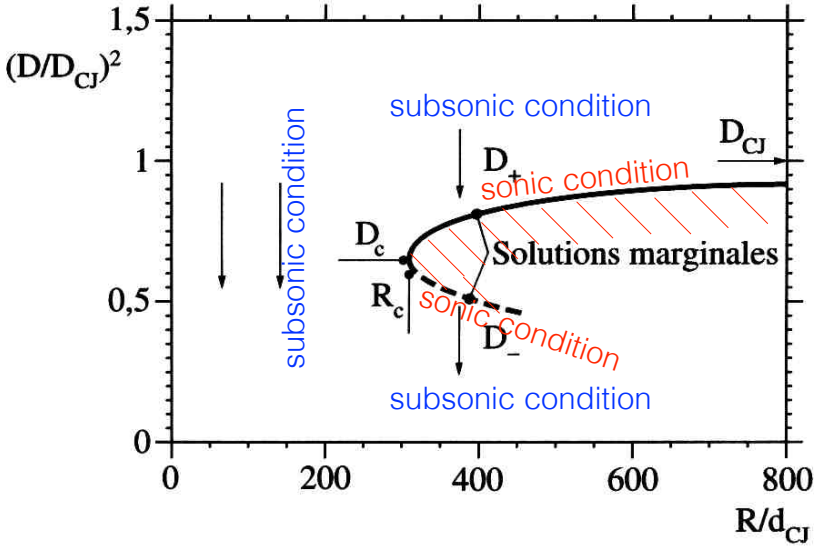
Conclusion: the critical energy is due to small modifications of the inner structure !

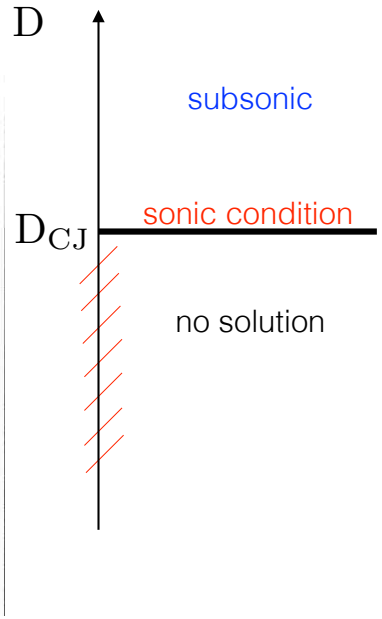
Curvature effect (steady state approximation)

L. He & P.C (1994)

Marginal CJ condition in the parameter space «radius-velocity »

Turning point

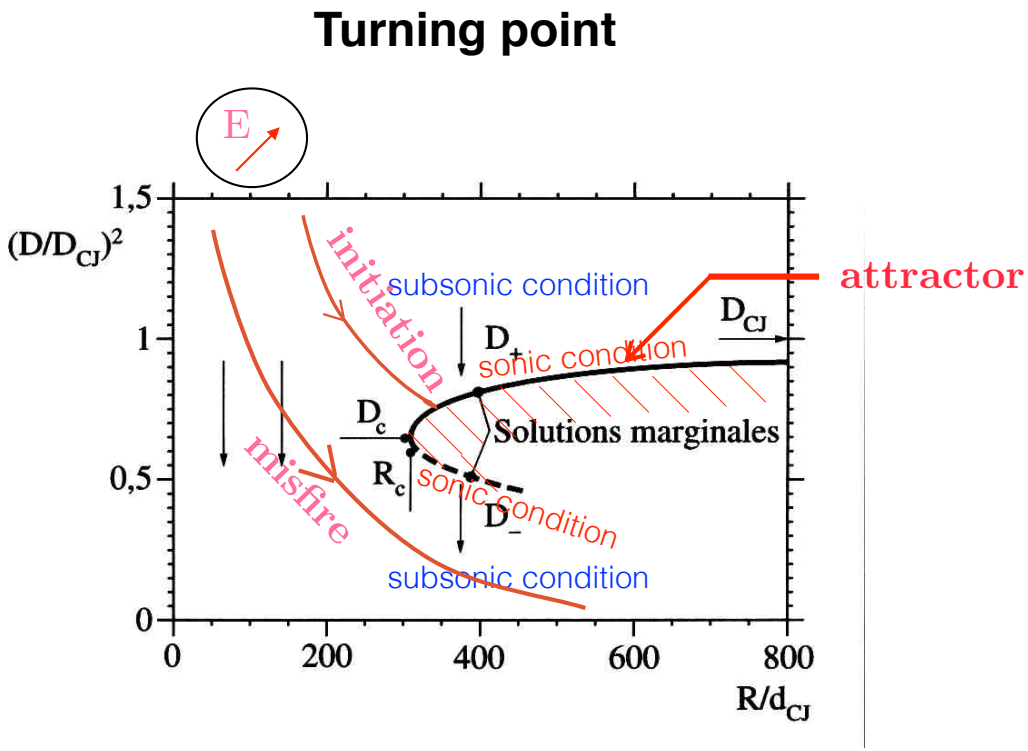




$$\frac{\text{critical radius}}{\text{detonation thickness}} \propto \frac{8}{\gamma - 1} e^{E/k_B T_N} \approx 10^2$$

Arrhenius factor

Curvature effect (steady state approximation)

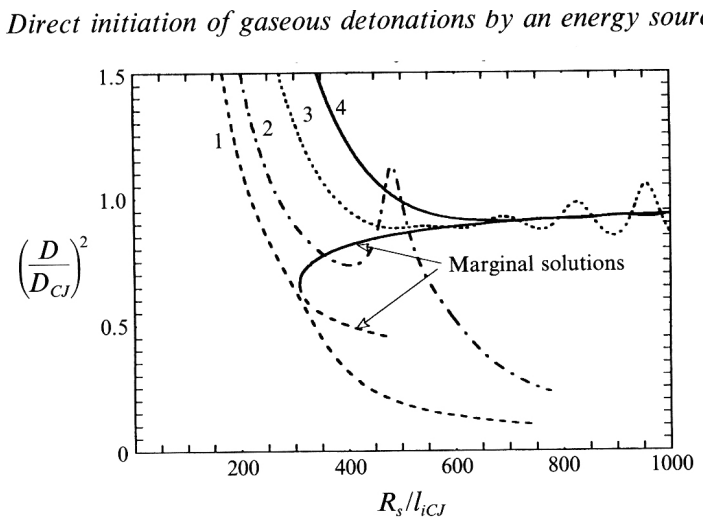


$$\frac{\text{critical radius}}{\text{detonation thickness}} \approx 10^2 \quad \Rightarrow \quad \frac{\text{critical energy}}{\text{Zeldovich value}} \approx 10^6$$

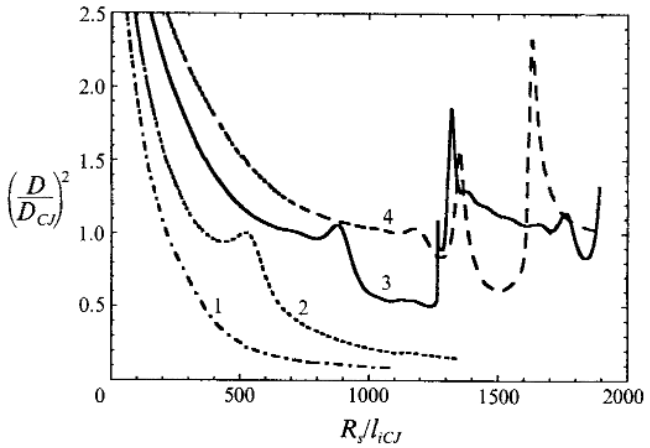
Arrhenius factor

Role of unsteadiness of the inner structure ?
Dynamics close to the critical radius ?

Experiments and DNS show a sensitivity to details



unsteadiness promotes failure
trajectory 2



unsteadiness promotes re-ignition
trajectory 3

The analysis is in progress

1D dynamics in planar geometry

PC & F.A. Williams (2002-2009)

1-D dynamics of the inner structure of planar detonations

Constitutive equations

$$\frac{1}{\rho}\frac{D}{Dt}\rho + \frac{\partial u}{\partial x} = 0, \qquad \frac{D}{Dt}u = -\frac{1}{\rho}\frac{\partial p}{\partial x} \qquad p/\rho = (c_p - c_v)T$$

$$\frac{D}{Dt} \equiv \frac{\partial}{\partial t} + u\frac{\partial}{\partial x}$$

Entropy wave:

energy

progress variable

$$\frac{D}{Dt}\left[\ln T - \frac{(\gamma-1)}{\gamma}\ln p\right] = \frac{q_m}{c_p T}\frac{\dot{\mathrm{w}}}{t_r}, \qquad \frac{D}{Dt}Y = \frac{\dot{\mathrm{w}}}{t_r}$$

$\dot{\mathrm{w}}(Y,T)$

heat released/mass

reaction rate

$$\frac{D^{\pm}}{Dt} \equiv \frac{\partial}{\partial t} + (u \pm a)\frac{\partial}{\partial x}$$

$$\frac{1}{\gamma}\frac{D^{\pm}}{Dt}\ln p \pm \frac{1}{a}\frac{D^{\pm}}{Dt}u = \frac{q_m}{c_p T}\frac{\dot{\mathrm{w}}(Y,T)}{t_r}$$

Hyperbolic equations: Eqs. of the characteristics

Nonlinear acoustic waves generated by an exothermal reaction

1-D compressible, inviscid and reactive gas mixture

+ energy eq. for T — heat release per unit mass — progress variable

$$\left(\frac{\partial}{\partial t}+u\frac{\partial}{\partial r}\right)\left[\ln T-\frac{(\gamma-1)}{\gamma}\ln p\right]=\frac{q_m}{c_pT}\frac{\dot{w}(T,Y)}{t_r}$$

$$\left(\frac{\partial}{\partial t}+u\frac{\partial}{\partial r}\right)Y=\frac{\dot{w}(T,Y)}{t_r}$$

entropy wave — $\dot{w}$: non-dimensional reaction rate — chemical kinetics

Newtonian approximation

acoustic waves — heat release rate

$$\frac{1}{\gamma p}\left[\frac{\partial}{\partial t}+(u\pm a)\frac{\partial}{\partial x}\right]p\pm\frac{1}{a}\left[\frac{\partial}{\partial t}+(u\pm a)\frac{\partial}{\partial x}\right]u=\frac{q_m}{c_pT}\frac{\dot{w}}{t_r}$$

sound speed $a\equiv\sqrt{(\gamma-1)c_pT}$

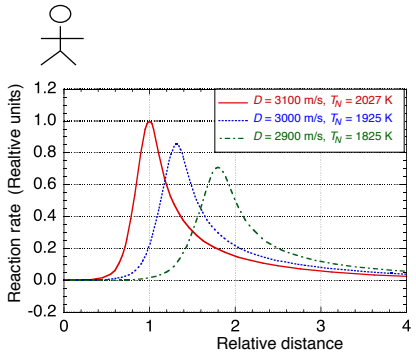
small heat release: $a\approx \mathrm{cst}.$

3 nonlinear modes: Entropy wave + 2 acoustic waves

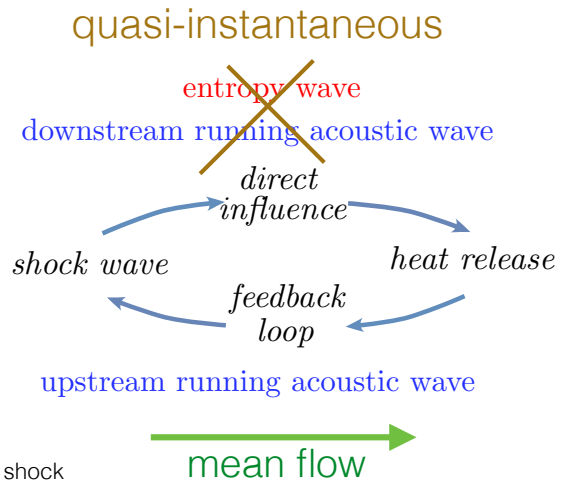
4 nonlinear equations & 4 unknowns: $p,\ T,\ u,\ Y$

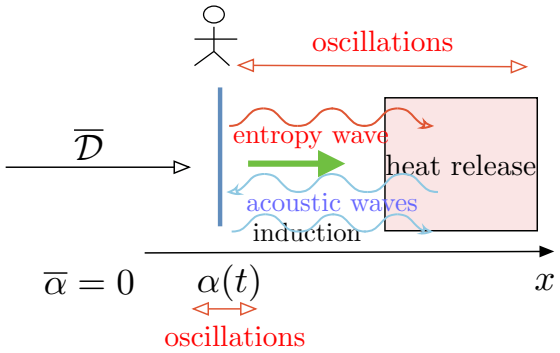
too complicated system for a general analytical solution

1-D dynamics of the inner structure of planar detonations
Set of feedback loops



distribution of the rate of heat release for different velocity of the leading shock





Threshold of the planar instability of the CJ regime:

Small heat release $\Rightarrow$ Transonic flow

3rd simplification:

Two-time scales: The upstream running acoustic wave controls the loops

The two other modes involves much shorter time lags

Integral equation for the propagation velocity $\dot{a}_t(t)$

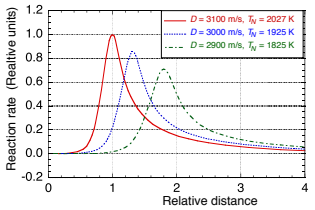
Unperturbed flow velocity of burnt gas (intrinsic dynamics):

velocity of the lead shock

time lag / upstream running acoustic wave

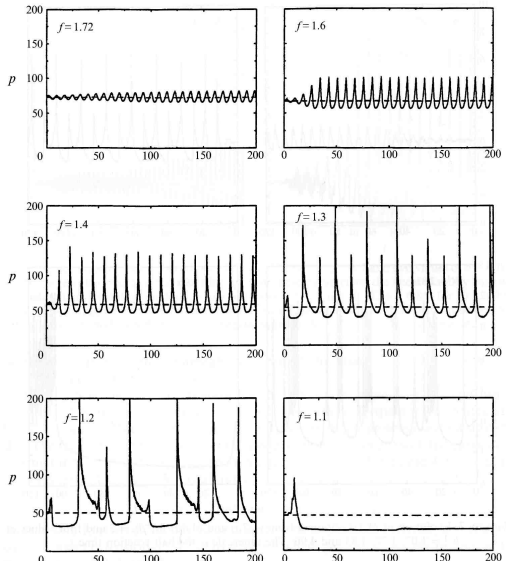
$$2\dot{a}_t(t) = \int_{-\infty}^{0} G(z', \dot{a}_t(t + z'))dz'$$

distributions in steady state for different $\dot{a}_t$



$G(z, \dot{a}_t)$: distribution of the rate of heat release for $\dot{a}_t$ (constant)

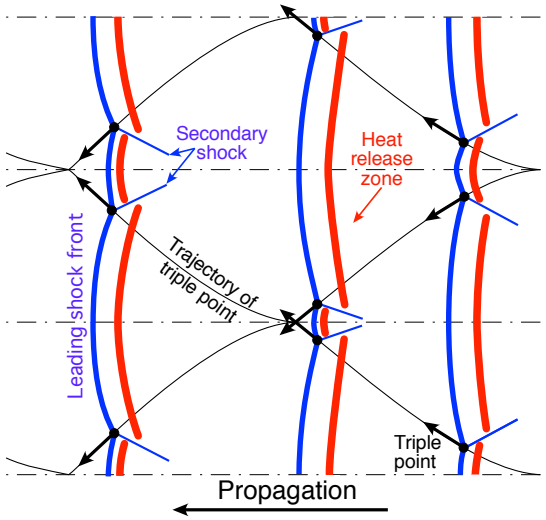
Typical solution for the dynamics when increasing the activation energy



period doubling

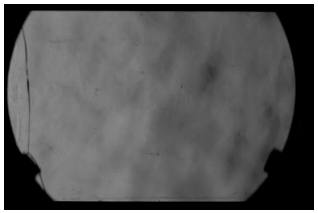
intermittency

Theoretical analyses of cellular structures 1996-2017



1-D oscillatory instability + transverse propagation and Mach stem formation

one-dimensional instability 1996-2002

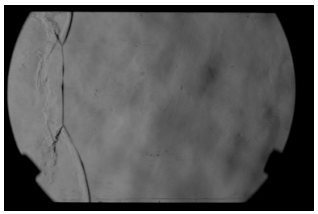


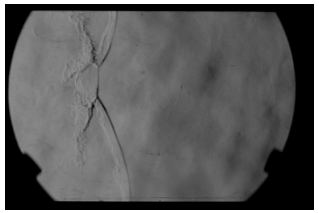
B.Maxwell, R.Bhattacharjee, S. Lau-Chapelaine, S.Falle, G. Sharpe and M. Radulescu

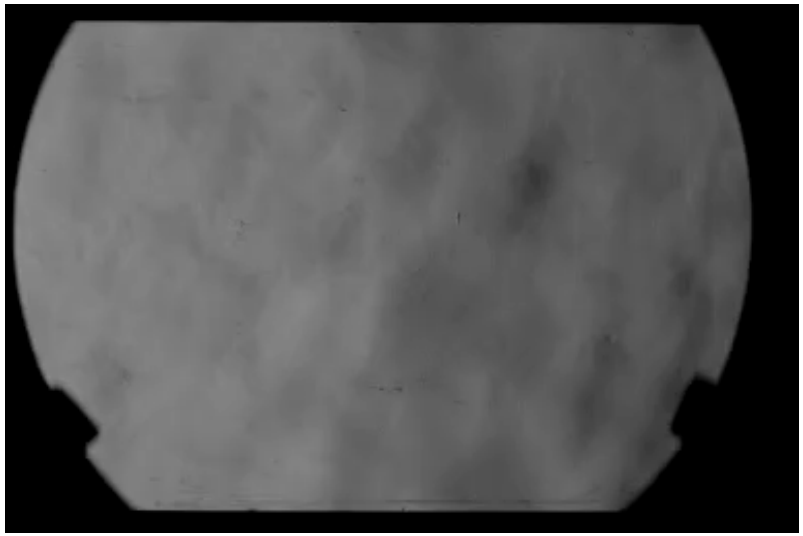
Journal of Fluid Mechanics 2017

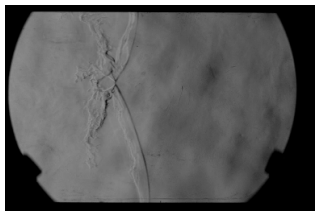
$\mathrm{CH_4} + 2\mathrm{O_2} \quad p = 3.5kP_a \quad$ 2D geometry experiment

High activation energy: Irregular structure and transient phenomena

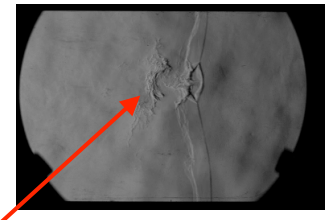


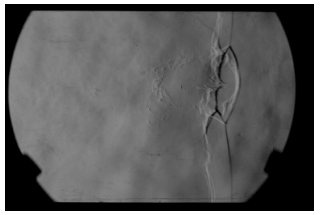


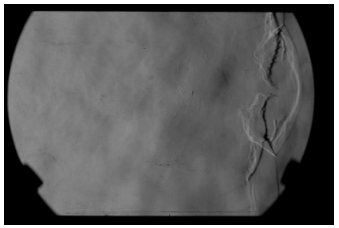




Schlieren images







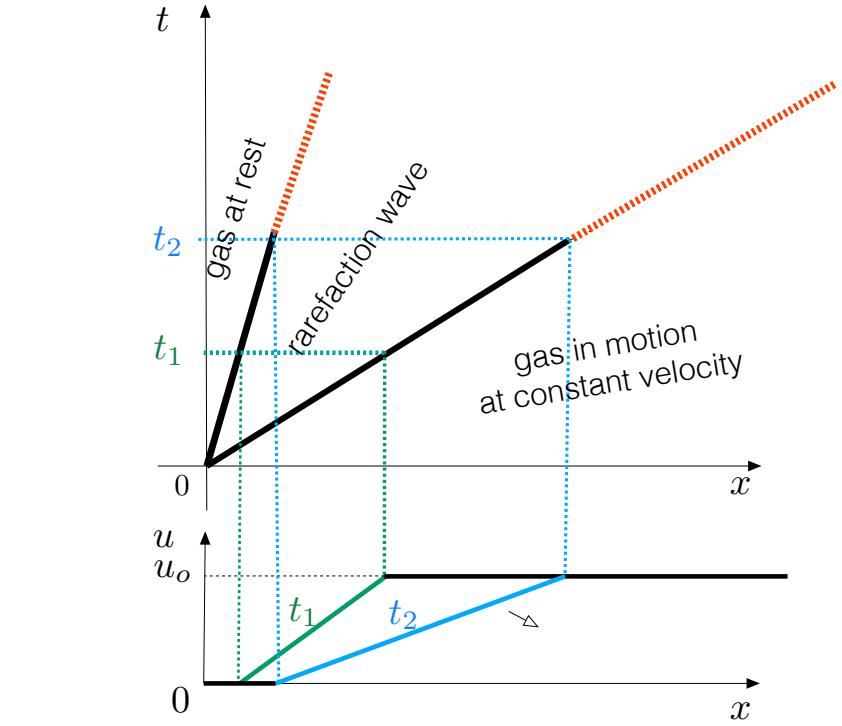
Intermittent formation
of
burning pockets of fresh mixture
engulfed in the burned gas

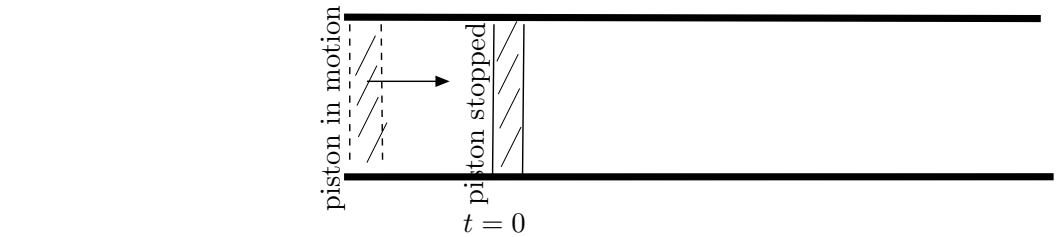
Successive frames $11\mu s$ apart

The role of unsteadiness in the decay to the CJ regime when the piston is brought to instantaneous halt

PC & B. Denet (2018)

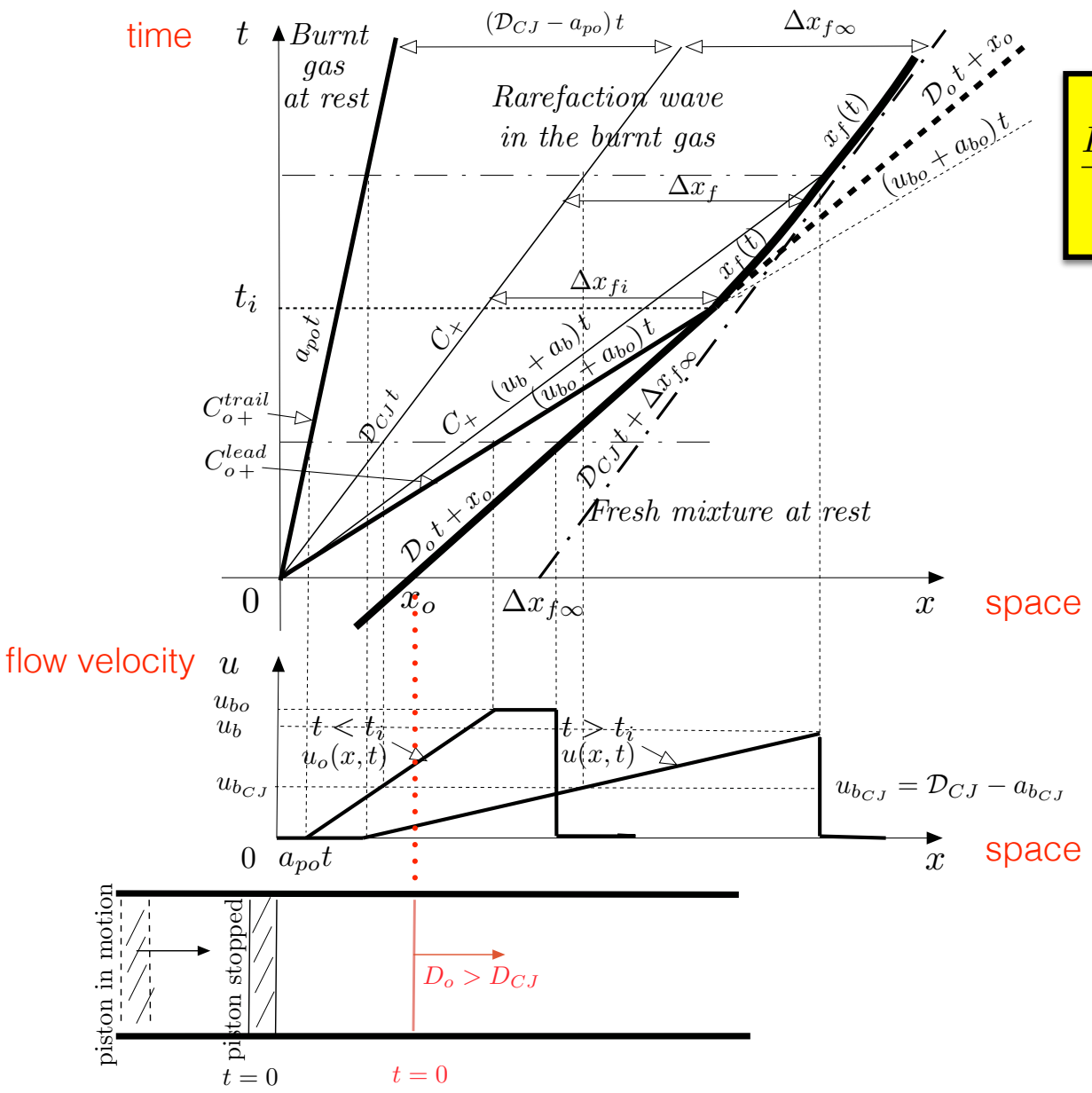
1-D (planar) centered rarefaction wave when the piston is suddenly arrested





Selection mechanism of the self sustained propagation (CJ wave) by the rarefaction wave in the burnt gas (**planar** geometry and inner structure of the detonation in **steady state**)

Levin & Chernyi (1967), P.C.& B.Denet (2017)



$$\frac{D(t) - D_{CJ}}{D_{CJ}} \propto \frac{1}{t^2}$$

Integral equation for the propagation velocity $\dot{a}_t(t)$

Unperturbed flow velocity of burnt gas

$$2\dot{a}_t(t) = \int_{-\infty}^{0} G(z', \dot{a}_t(t+z'))dz'$$

Relaxation to the CJ regime when the piston is suddenly stopped at $t = 0$ *:*

PC & B. Denet *JFM* (2018)

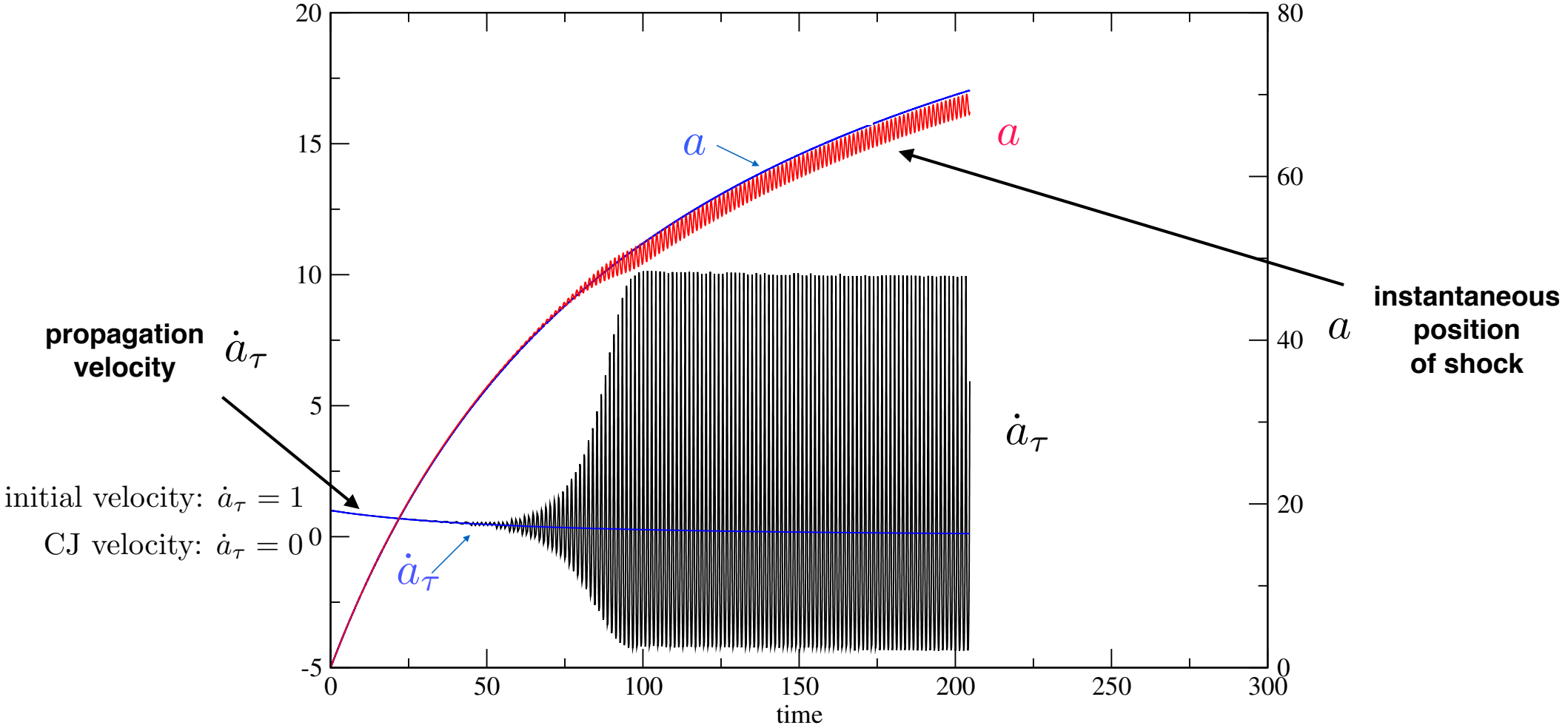
nonlinear response function: intrinsic dynamics

forcing term: rarefaction wave in the burnt gas

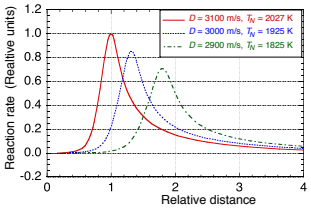
$$t \geqslant 0: \quad 2\dot{a}_t(t) = \int_{-\infty}^{0} G(z', \dot{a}_t(t+z'))dz' + (1 + t/\tau_i)^{-2}.$$

$$t \leqslant 0: \quad \dot{a}_t(t) = 1 \qquad \int_{-\infty}^{0} G(z', 1)dz' = 1$$

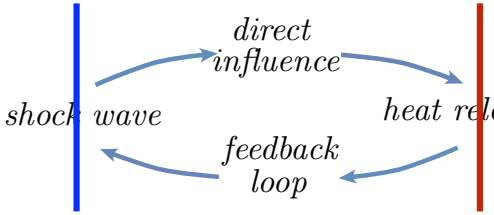
piston-supported detonation (overdriven regime)


20
15
10
5
0
-5
80
60
40
20
0
0
50
100
150
200
250
300
time
a
a
a
$\dot{a}_\tau$
$\dot{a}_\tau$
$\dot{a}_\tau$
propagation velocity
instantaneous position of shock
initial velocity: $\dot{a}_\tau = 1$
CJ velocity: $\dot{a}_\tau = 0$

distributions in steady state for different $\dot{a}_t$



lead shock end of reaction zone



rarefaction wave driven decay

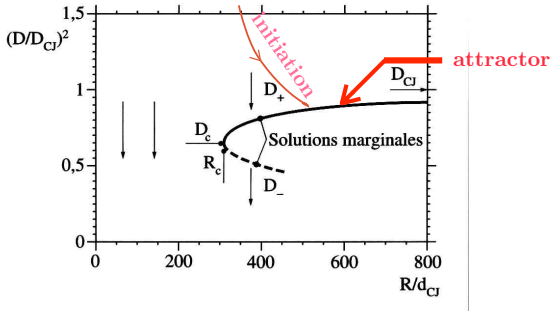
upstream running acoustic wave

mean flow

the upstream running mode controls the response

Transonic flow: divergence of the delay when approaching the CJ self-sustained regime

Solvability condition: selection of the family of the overdriven regimes approaching the CJ regime



This analysis presents a simple tool that can be extended for describing the chaotic dynamics around the critical radius controlling the initiation of detonations in free space.

Results are expected soon !

Thank you for your attention