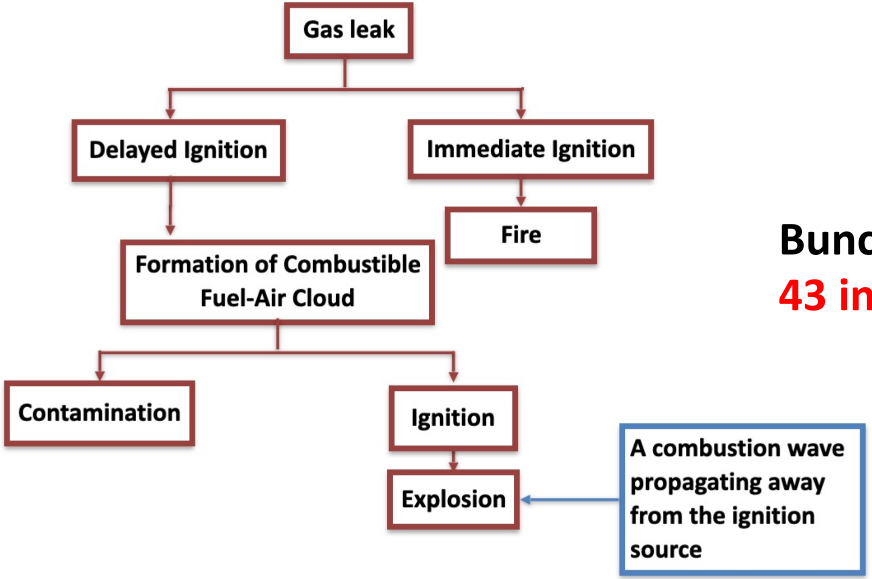
CENTRE EUROPÉEN DE RECHERCHE ET DE FORMATION AVANCÉE EN CALCUL SCIENTIFIQUE

# From Deflagration to Detonation

O. Dounia, CERFACS

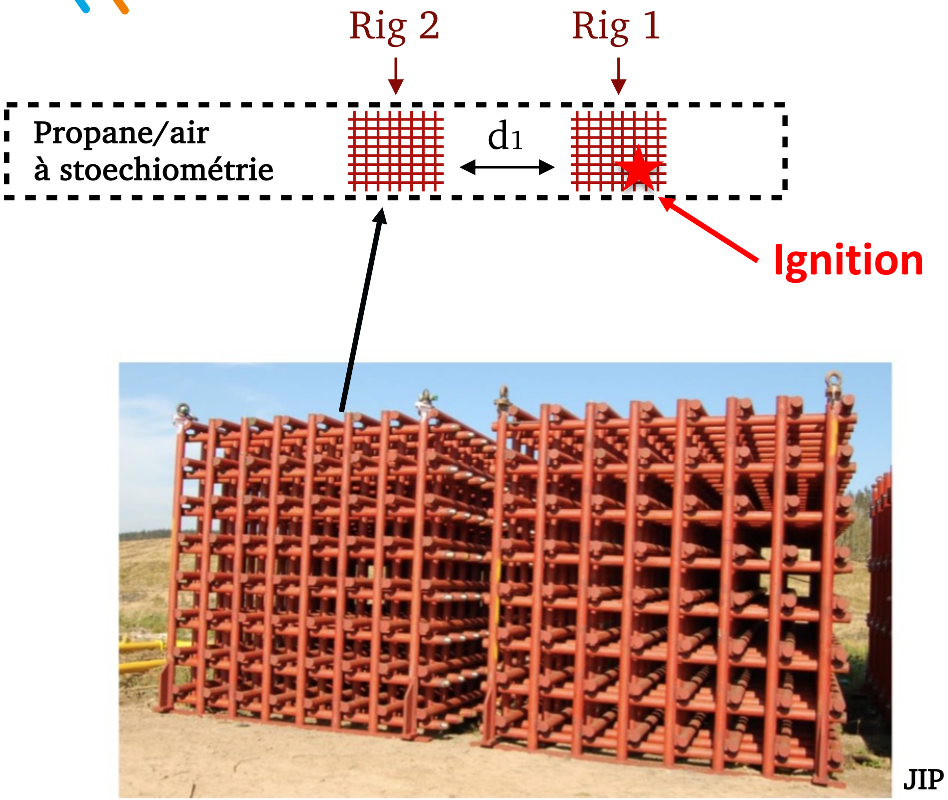
# Explosion events, tragic scenarios



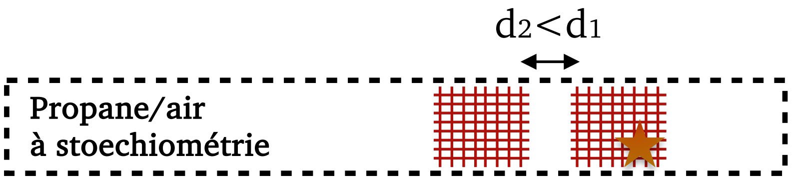

**Taijin, 2015**
**173 fatalities,**
**43 injuries**

**Buncefield, 2005**
**43 injuries**

# 2 regimes of explosions

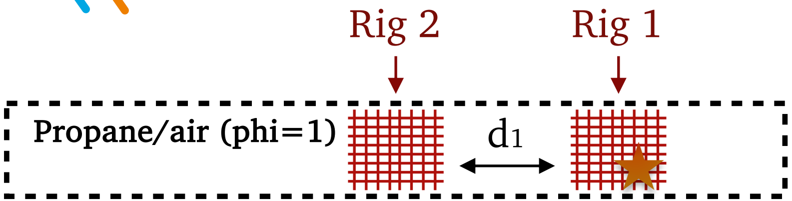


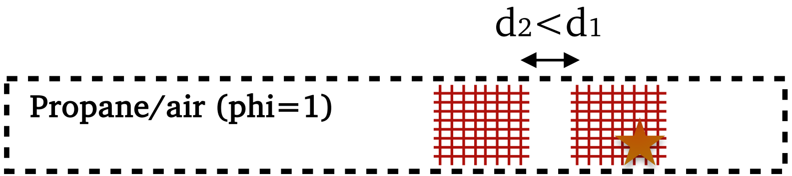

JIP MEASURE [1]




[1] Masri et al., IECR 2012

# 2 regimes of explosions






- Small changes in setup => **extreme escalation of the explosion scenario**
- Could suggest a change in "combustion regime"
  - Safety : Necessity to understand the triggering mechanisms of this transition

[1] Masri et al., IECR 2012

# Specificities of H2

- Safety : Necessity to understand the triggering mechanisms of DDT

- True for any fuel …

  … **BUT particularly true for H2**

  **H2 has some specificities that challenge many safety strategies**

  **High tendency to: leak, ignite and "detonate"**

| Properties | | Hydrogen | Methane | Gasoline | |
|---|---|---|---|---|---|
| **Minimum ignition energy in air (MIE)** | (mJ) | **0,02** | 0,29 | 0,24 | |
| **Flammability limits in air** | (vol. %) | **4 - 75** | 5,3 - 15 | 1,0 - 7,6 | |
| **Detonation limits in air** | (Vol. %) | **13 - 65** | 6,3 - 13,5 | 1,1 - 3,3 | *[1,2]* |

*Accidentology involving hydrogen, BARPI report, 2007*
*A.E. Dahoe, JLPPI 2005*

# Disclaimer

- We assume the conditions for direct detonation initiation are not met
  - i.e. the scenario never starts with the violent regime of explosion
  - Requirements too strong (strong blast decay):
    - $E_c \geq 10^4\ (H_2);\ 10^5\ (C_2H_4); 10^6\ (C_3H_8)$ [J] [1]
  - Consistent with observations from industrial accidents

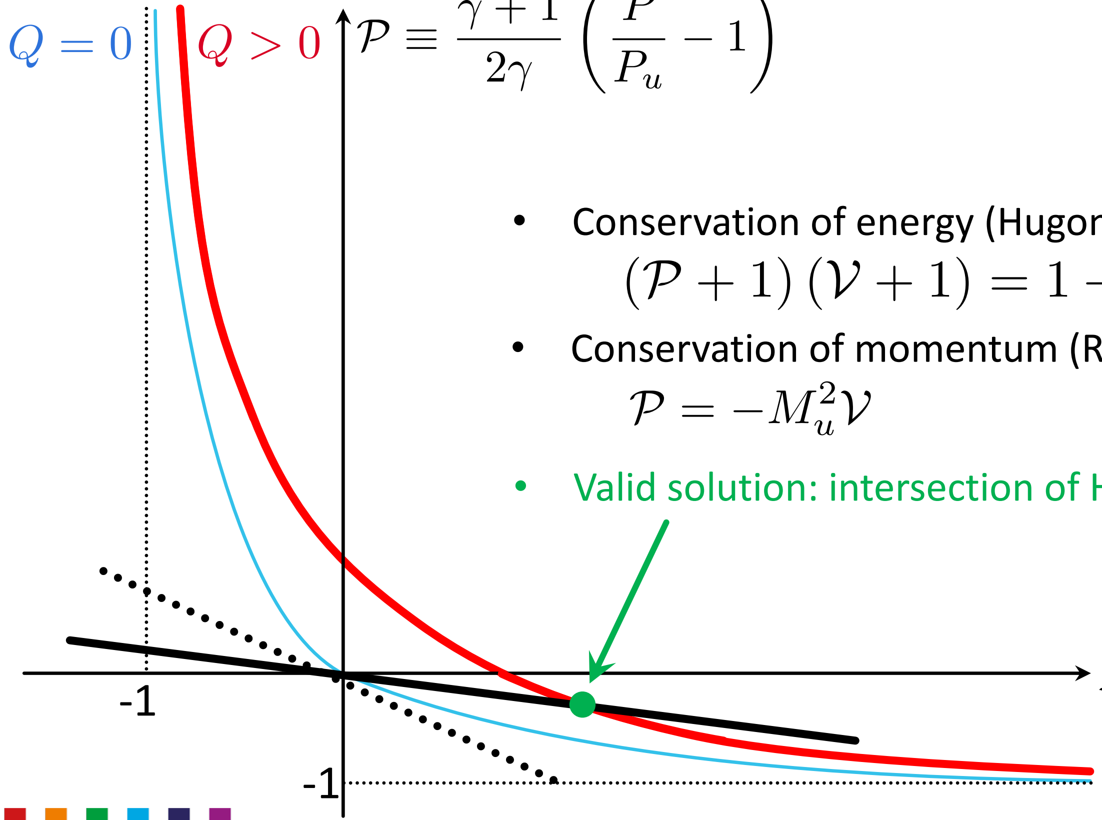
[1] G. Ciccarelli and S. Dorofeev, PECS, 2008

# Existence of two regimes of combustion:
# Based on conservation laws

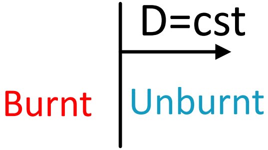
# Generalized Rankine-Hugoniot relations

- Set of thermodynamic relations that planar exothermic waves must satisfy

$$\mathcal{P} \equiv \frac{\gamma+1}{2\gamma}\left(\frac{P}{P_u}-1\right)$$




$$\mathcal{V} \equiv \frac{\gamma+1}{2}\left(\frac{\rho_u}{\rho}-1\right)$$




- Conservation of energy (Hugoniot curve)

$$(\mathcal{P}+1)(\mathcal{V}+1) = 1 + Q$$

$$Q \equiv \frac{\gamma+1}{2}\left(\frac{q_m}{c_p T_u}\right)$$

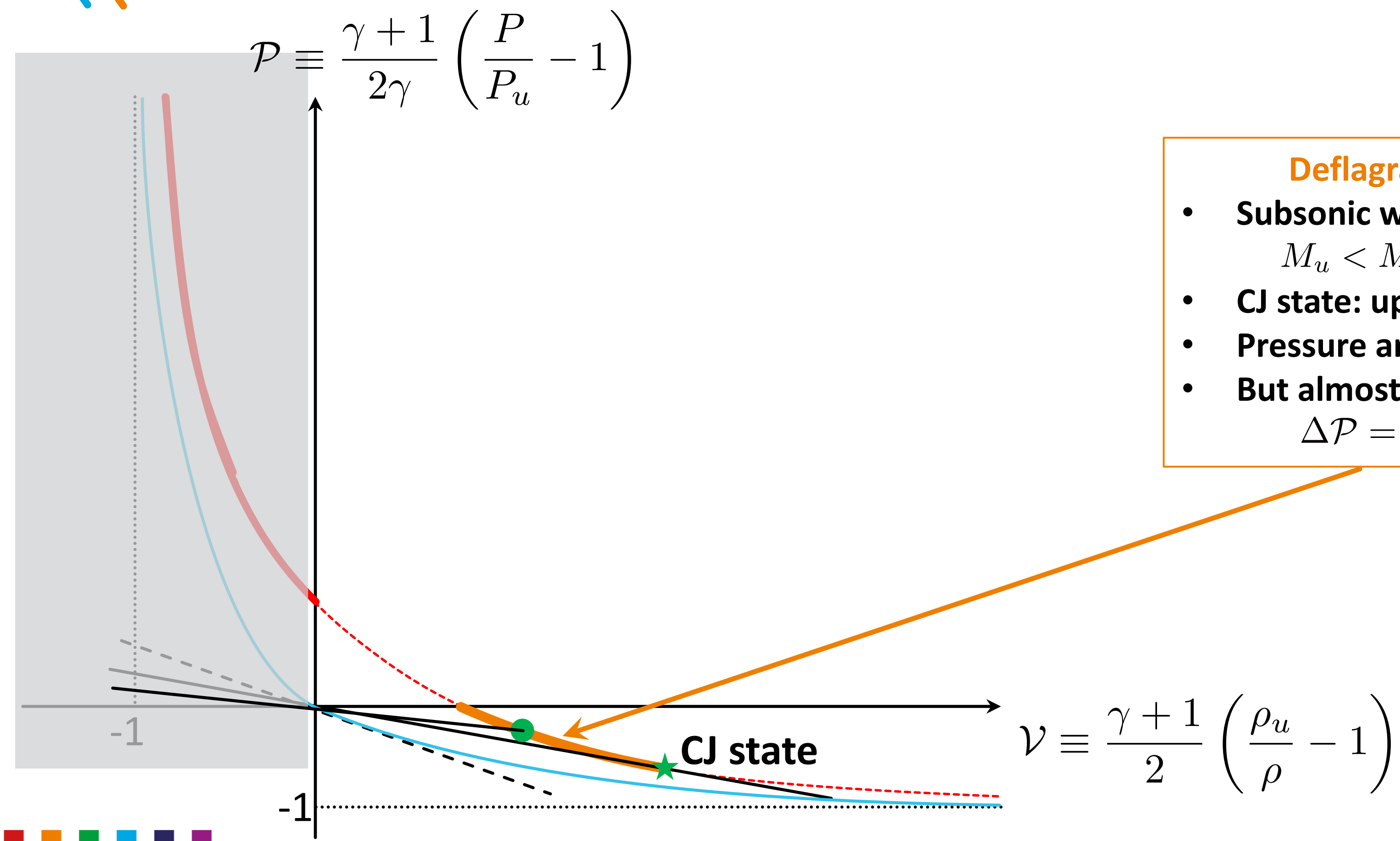
- Conservation of momentum (Rayleigh-Michelson line)

$$\mathcal{P} = -M_u^2 \mathcal{V}$$

$$M_u = \frac{D}{a_u}$$

- Valid solution: intersection of Hugoniot and Rayleigh-Michelson

# The deflagration branch

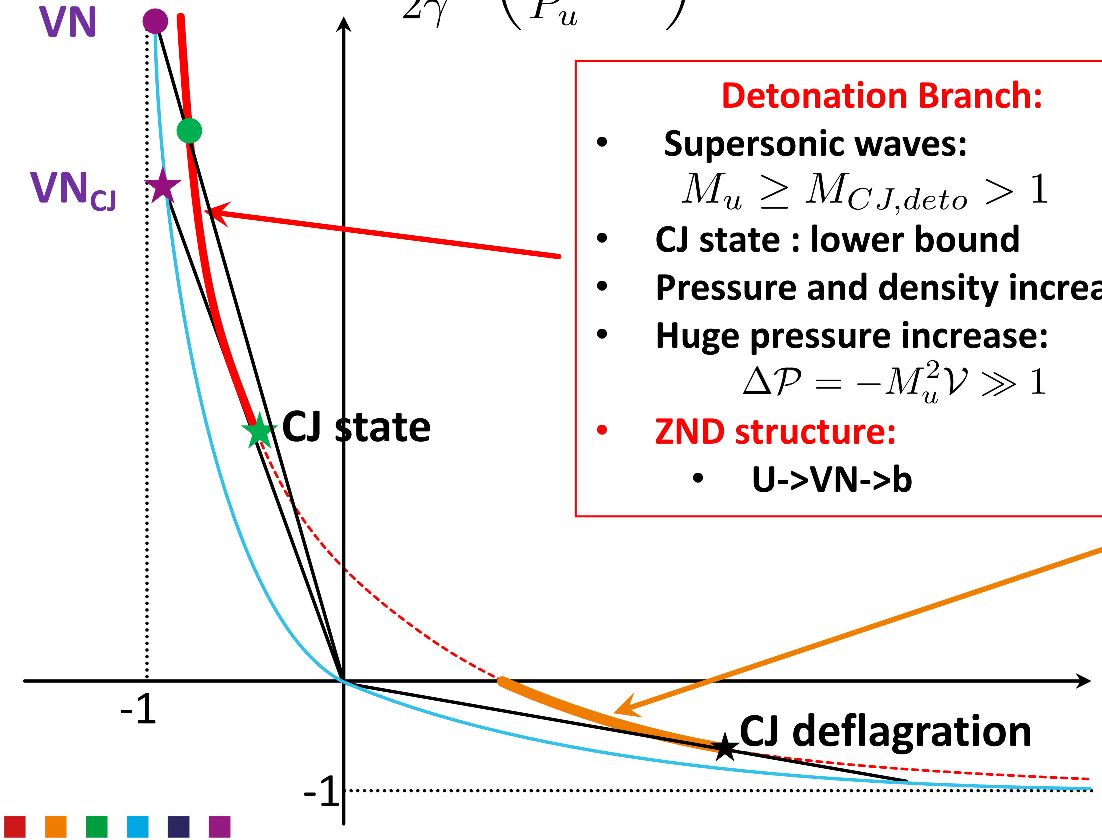



**Deflagration Branch:**

- **Subsonic waves:**
  $$M_u < M_{CJ,deflag} \ll 1$$
- **CJ state: upper bound**
- **Pressure and density decrease**
- **But almost isobaric:**
  $$\Delta\mathcal{P} = -M_u^2\mathcal{V} \ll 1$$

# The detonation branch

$$\mathcal{P} \equiv \frac{\gamma+1}{2\gamma}\left(\frac{P}{P_u}-1\right)$$




$$\mathcal{V} \equiv \frac{\gamma+1}{2}\left(\frac{\rho_u}{\rho}-1\right)$$

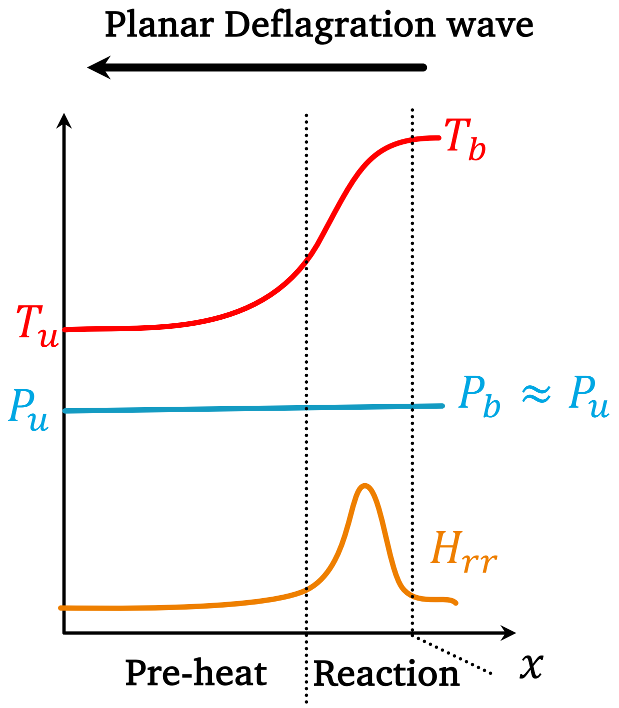
**Detonation Branch:**

- **Supersonic waves:**
  $$M_u \geq M_{CJ,deto} > 1$$
- **CJ state : lower bound**
- **Pressure and density increase**
- **Huge pressure increase:**
  $$\Delta\mathcal{P} = -M_u^2\mathcal{V} \gg 1$$
- **ZND structure:**
  - **U->VN->b**

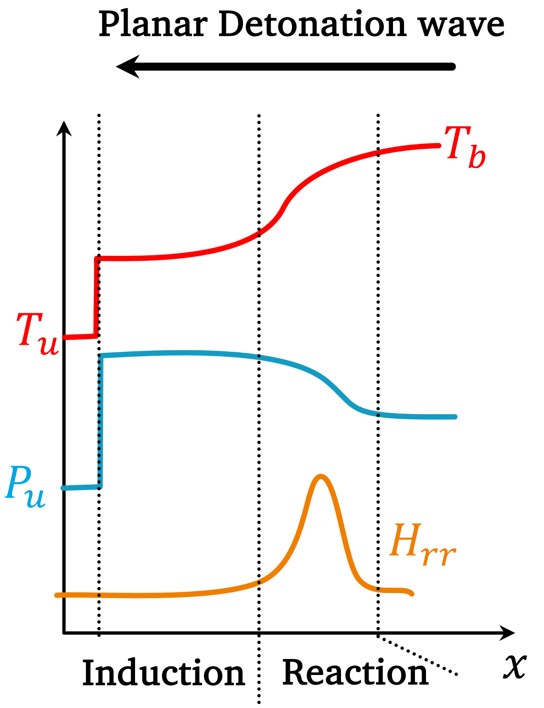
**Deflagration Branch:**

- **Subsonic waves:**
  $$M_u < M_{CJ,deflag} \ll 1$$
- **CJ state: upper bound**
- **Pressure and density decrease**
- **But almost isobaric:**
  $$\Delta\mathcal{P} = -M_u^2\mathcal{V} \ll 1$$

# Internal structure of deflagration and detonation waves

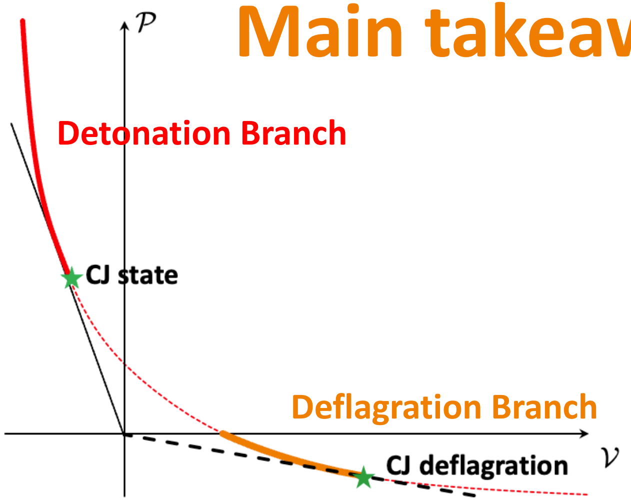



Propagation by diffusion




Propagation by reaction-assisted shock

# Main takeaway




## Huge safety concern

**Deflagration Branch:**
- **Relatively slow,** $M_u \leq 10^{-2}$
- **Almost isobaric** $P \approx cst$

**Detonation Branch:**
- **Supersonic** $M_u \geq 4-5$
- **Huge pressure increase:** $P_b > 10P_u; P_{VN} > 20P_u$

**Gap in acceptable solutions**

0.01 — 0.1 — 1

$$M_u = \frac{D}{a_u}$$

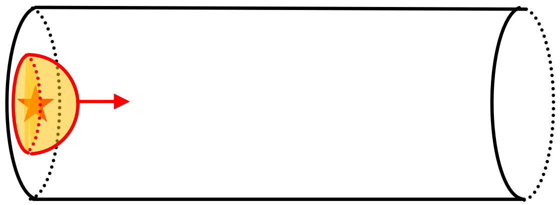
**Relative velocities**

- Conservation laws predict a huge gap in acceptable solutions
- A naïve conclusion:
  "If my scenario starts with a deflagration, I am safe"

# DDT in lab-scale experiments: Observations

# Experimental observations

- Typical experiment:
  - Closed tube or channel filled with reactive mixture (obstacles optional)
  - Ignite on one end
  - Flame kernel formation and propagation in the mixture



Objective:

Evolution of the **self-propagating** flame inside the tube/channel

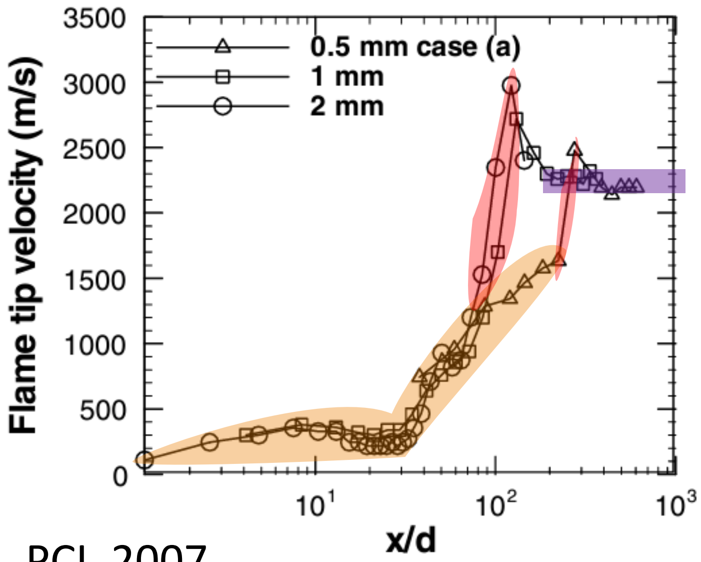
Key variable: **flame propagation velocity** (laboratory frame of reference)

# 3 phases of DDT scenarios

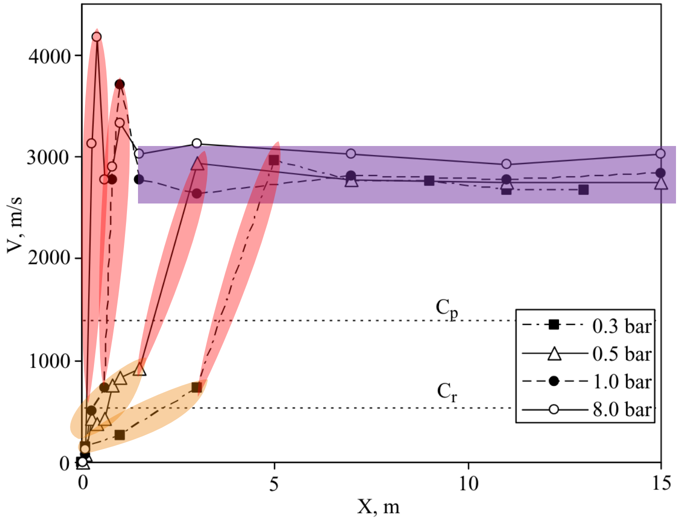
1) Flame acceleration (FA) : precursor of DDT

2) Sudden acceleration: DDT

3) Detonation propagation: Relax to a Cst speed (when possible)
   - Remarkably close to the Generalized Rankine-Hugoniot




Wu et al, PCI, 2007




Kuznetsov et al, Shock Waves, 2005

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# A recipe for strong FA

- Flames are intrinsically unstable reaction waves
- Many mechanisms can accelerate a flame front (coupling possible)

- The following is a recipe for a very efficient FA

**WARNING**
**Safety engineer discretion is advised**

# First FA following ignition

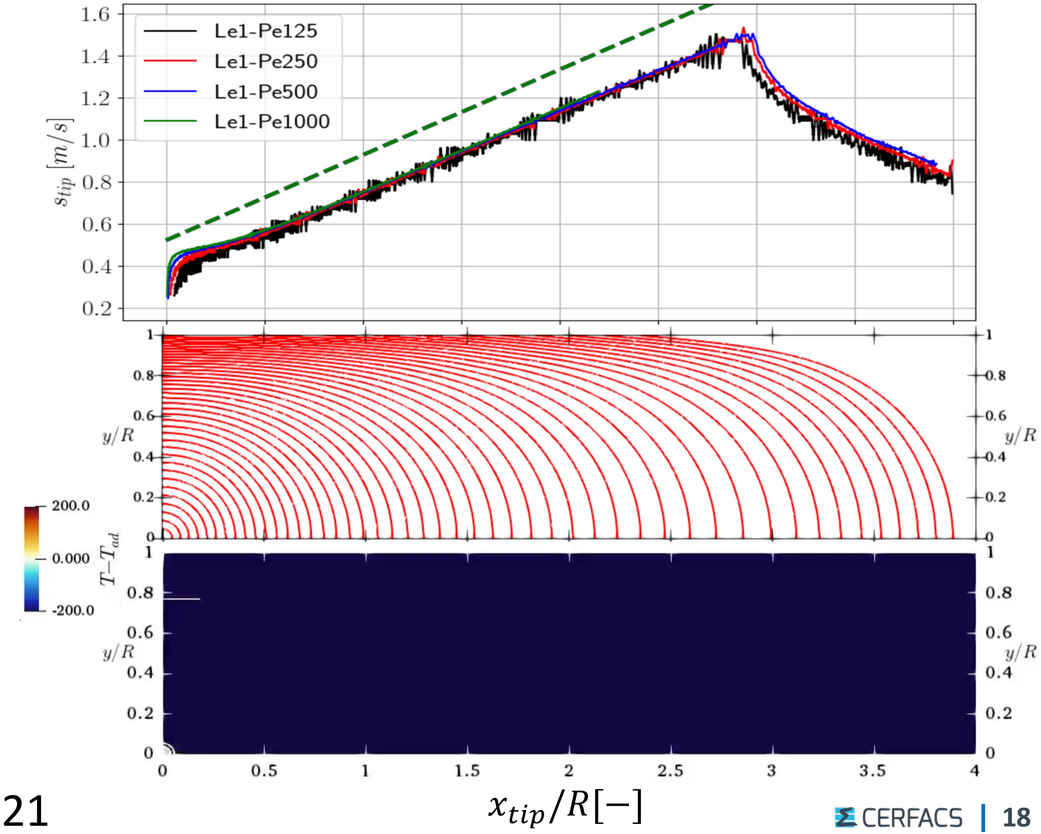
Recipe for a strong FA:
1) 1 table spoon of confinement

- Finger-shaped flame
- FA Exponential in time

$$\frac{dX_{tip}}{dt} = \sigma s_L^0 + (\sigma - 1) s_L^0 (X_{tip}/R) \qquad \sigma \equiv \rho_u/\rho\_b$$

- BUT limited in time

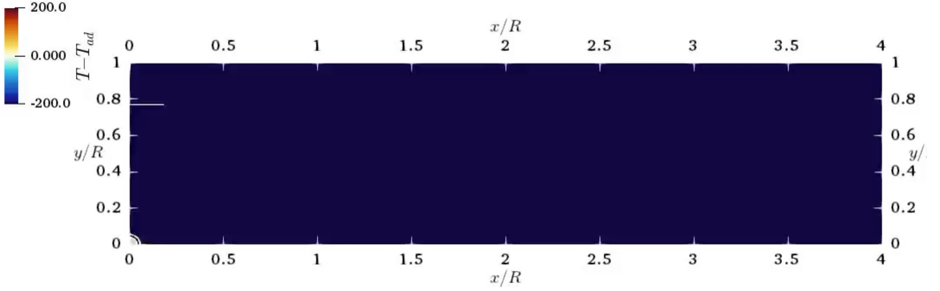
H2/air, $\phi = 0.36, P = 1atm, T_u = 300K, Le_{eff} = 1$ [1]

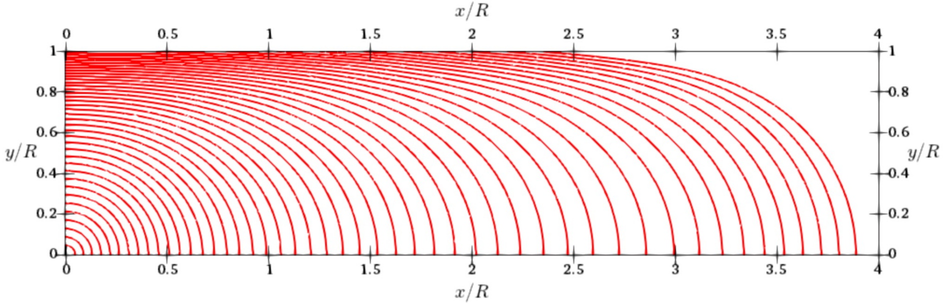



[1] J. J. Hok, et al., ICDERS 2021

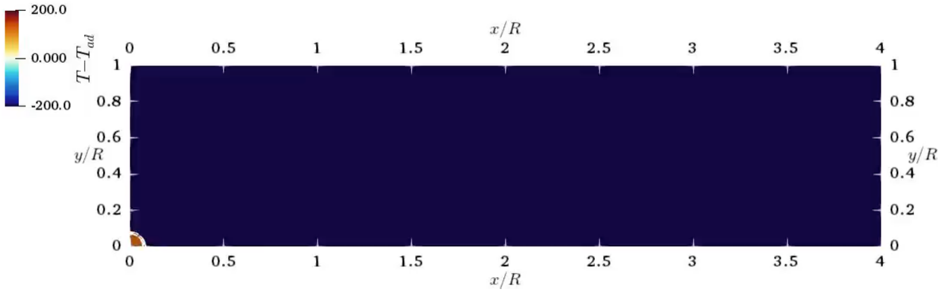
# Flame instabilities

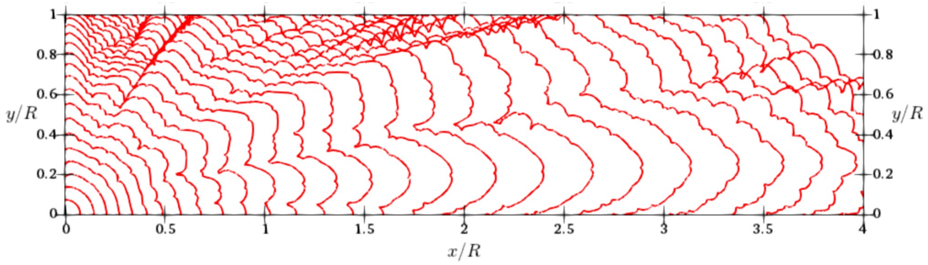
Typical finger flame acceleration: H2/air, $\phi = 0.36, P = 1atm, T_u = 300K, Le_{eff} = 1$ [1]




Thermo-diffusively unstable flames: H2/air, $\phi = 0.36, P = 1atm, T_u = 300K, Le_{eff} = 0.3$ [1]

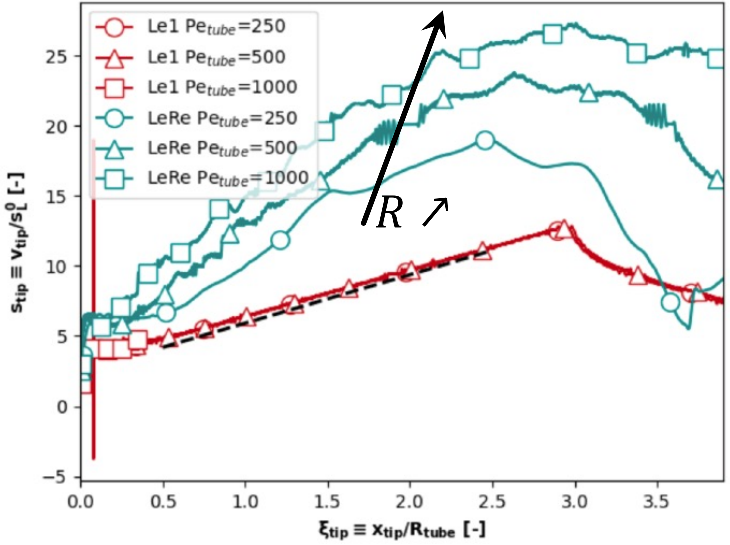


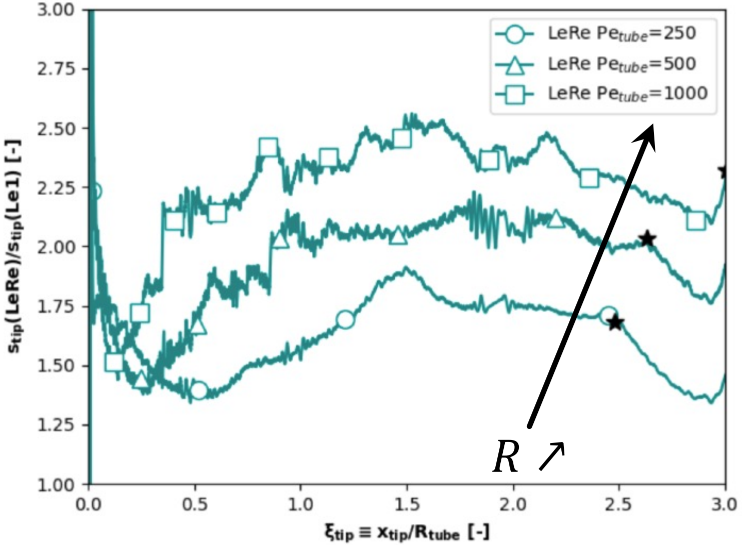

[1] J. J. Hok, et al., ICDERS 2021

# Early stages of flame acceleration

Coupling between thermo-diffusive effects and geometrical acceleration




Additional contribution of TD Depends on confinement (R)



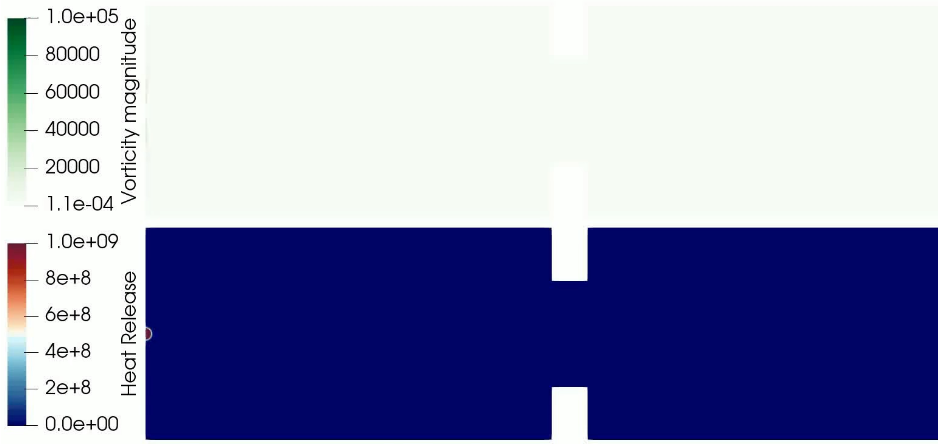

[1] J. J. Hok, et al., ICDERS 2021

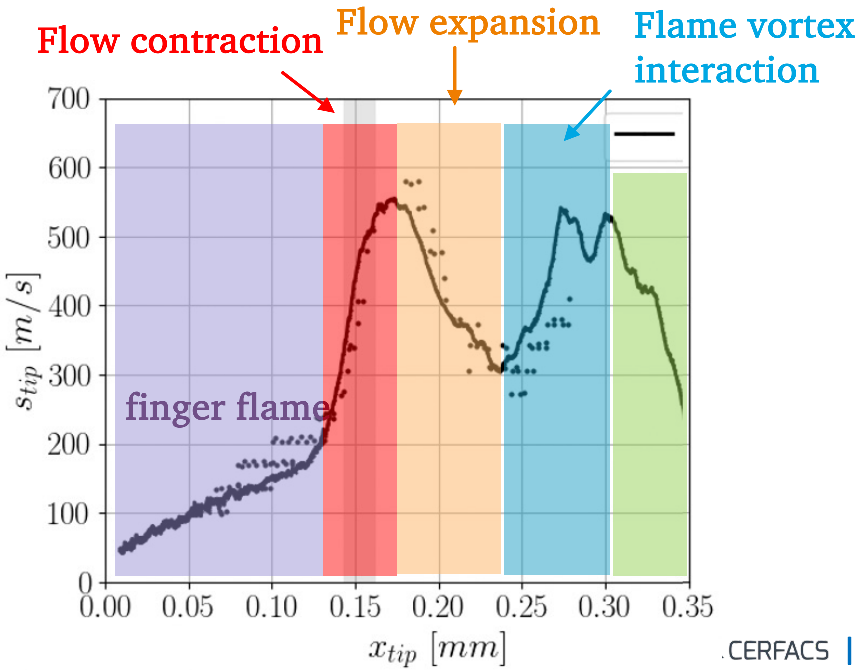
# Going beyond the early stages: obstacles

Recipe for a strong FA:
1) 1 table spoon of confinement
2) 1 pinch of obstruction

- Flame=semi-permeable piston (sets reactives in motion)
- Flame/obstacle interaction: strong FA
  - Depends on obstacle configuration (shape, BR)
- BUT also limited to the vicinity of the obstacle

$H_2/O_2, \phi = 1., P = 15kPa, T_u = 300K$ [1]



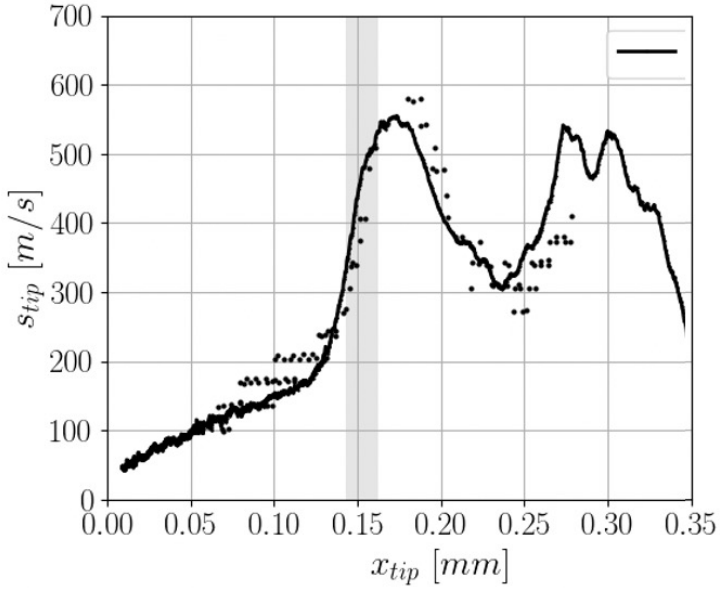

[1] B. Van Barsel, PhD thesis, 2024

# Going beyond the early stages: obstacles

$s_{tip}$

- Absolute speed on an iso-level surface
- Includes both burning and advection by the flow
- Not a burning velocity relative to fresh gases

The reaction wave is still subsonic relative to fresh gases (deflagration branch)

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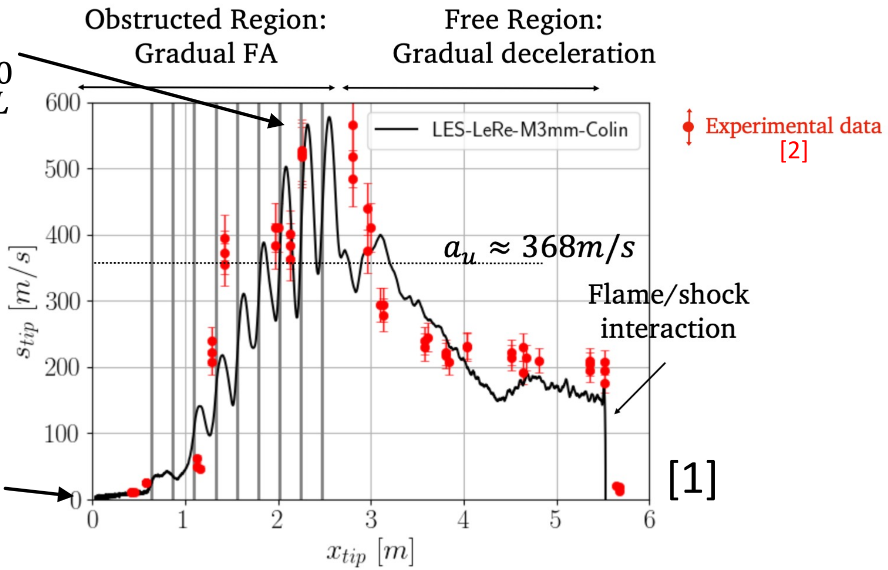
# The remarkable efficiency of repeated obstacles

$s_{tip} \approx 600\ m/s$
$\approx 1000\ \sigma\ s_L^0$

Recipe for a strong FA:
1) 1 table spoon of confinement
2) ~~1 pinch of obstruction~~
3) 1 gallon of obstruction

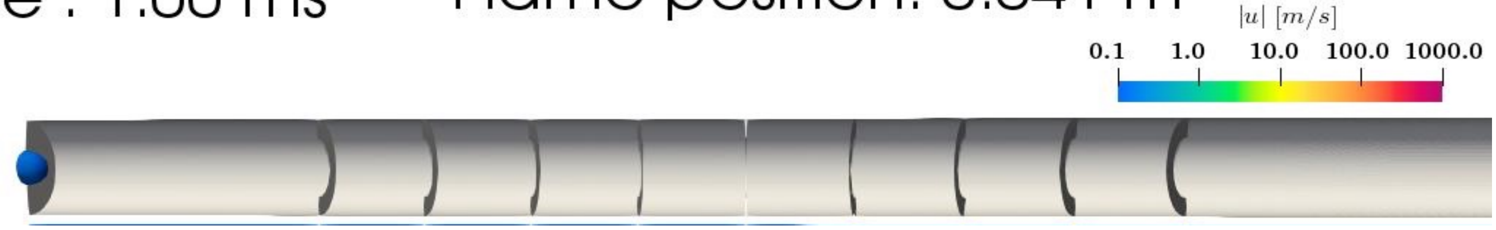
Strong sensitivity to obstacle configuration: spacing and BR

$\sigma s_L^0 \approx 0.6\ m/s$




[1]

Time : 1.00 ms Flame position: 0.041 m





[1] J. J. Hok, PhD 2024
[2] R. Gorsseuvres, PhD 2018

1) Flame acceleration (FA) : precursor of DDT

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3) Detonation propagation: Relax to a Cst speed (when possible)
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# Two classes of DDT mechanisms

- Many mechanisms to explain DDT

- Overall,  2classes to be distinguished:

**1) DDT involving shock waves**

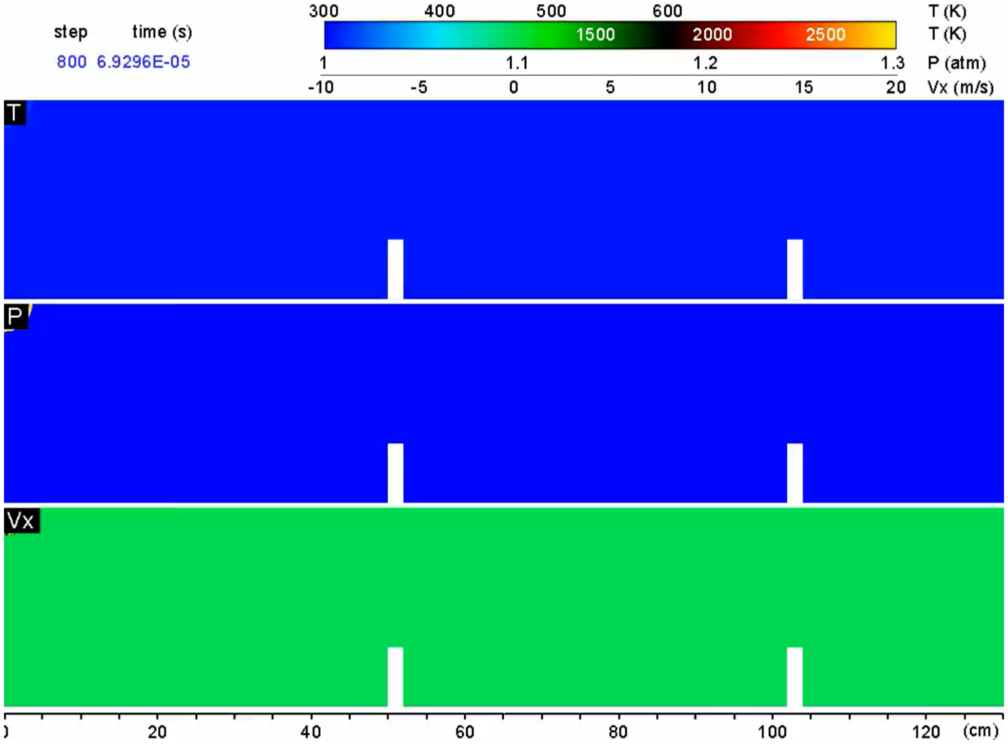
- Localised thermal explosion [1] (Zeldovich or SWACER mechanism)

→ Require a strong FA

→ Compressibility and shock formation

→ Bring the mixture to ignitable conditions (not a sufficient condition!!!)

Courtesy of Pr. E. Oran




[1] A. Oppenheim and R. Soloukhin, Ann. Rev FM, 1973

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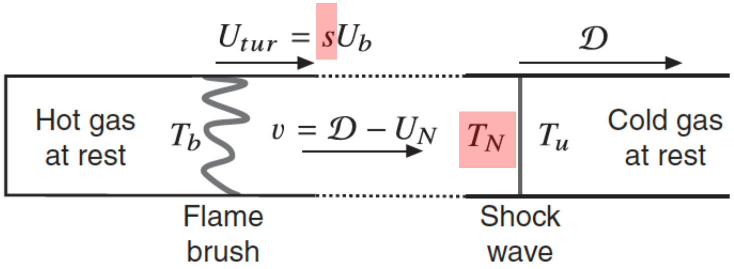
- Many mechanisms to explain DDT

- Overall,  2classes to be distinguished:

**1) DDT involving shock waves**

- Localised thermal explosion[1] (Zeldovich or SWACER mechanism)
- Thermal runaway [2,3]
  - Thermal sensitivity of the flame speed
    $U_b = f(T_N)$
  - Critical degree of flame folding $s^\star$
  - No self-similar solution above $s^\star$





[1] A. Oppenheim and R. Soloukhin, Ann. Rev FM, 1973
[2] B. Deshaies and G. Joulin, C&F, 1989
[3] L. Kagan and G. Sivashinsky, PCI, 2014

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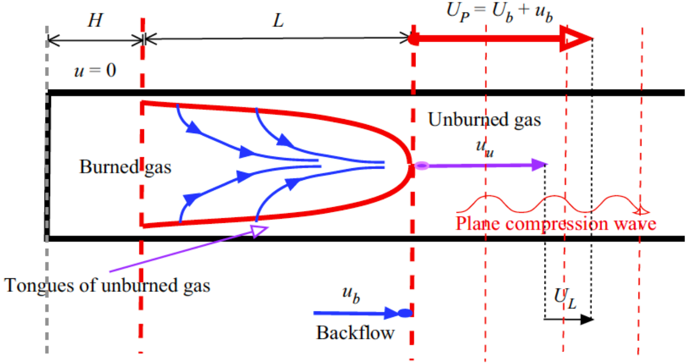
- Overall,  2classes to be distinguished:

## 1) DDT involving shock waves

  - Localised thermal explosion[1] (Zeldovich or SWACER mechanism)
  - Thermal runaway [2,3]

## 2) Shockless DDT

  - Friction induced adiabatic compression (hydraulic resistance) [4,5]
  - Pressure runaway of strongly elongated flames [6,8]





[1] A. Oppenheim and R. Soloukhin, Ann. Rev. FM, 1973
[2] B. Deshaies and G. Joulin, C&F, 1989
[3] L. Kagan and G. Sivashinsky, PCI, 2014
[4] I. Brailovsky and Sivashinsky, C&F, 2000
[5] I. Brailovsky, Sivashinsky et al, Philos. Trans. R.S., 2012
[6] P. Clavin, C&F, 2022
[7] P. Clavin, and M. Champion, CST, 2022
[8] P. Clavin, JFM, 2023

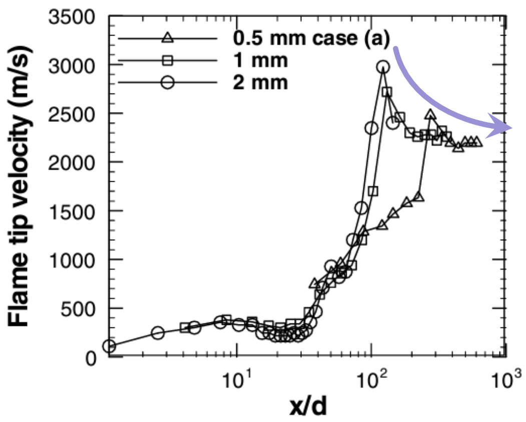
1) Flame acceleration (FA) : precursor of DDT

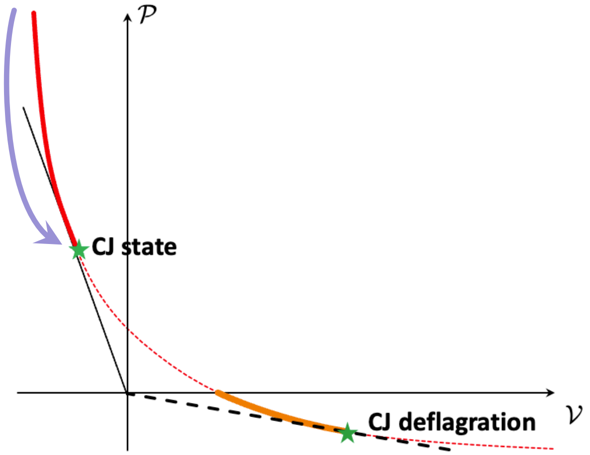
2) Sudden acceleration: DDT

3) Detonation propagation: Relax to a Cst speed (when possible)
    - Remarkably close to the Generalized Rankine-Hugoniot

# The specificity of the CJ detonation

- Experimental observation:
  - A decay to CJ detonation is often observed
  - Existence of a selection mechanism once detonations are formed
- The key point: the burnt gas state
  - Overdriven detonations: the flow post-reaction is subsonic (reference frame of the detonation)
  - CJ detonation: the flow post-reaction is **sonic**

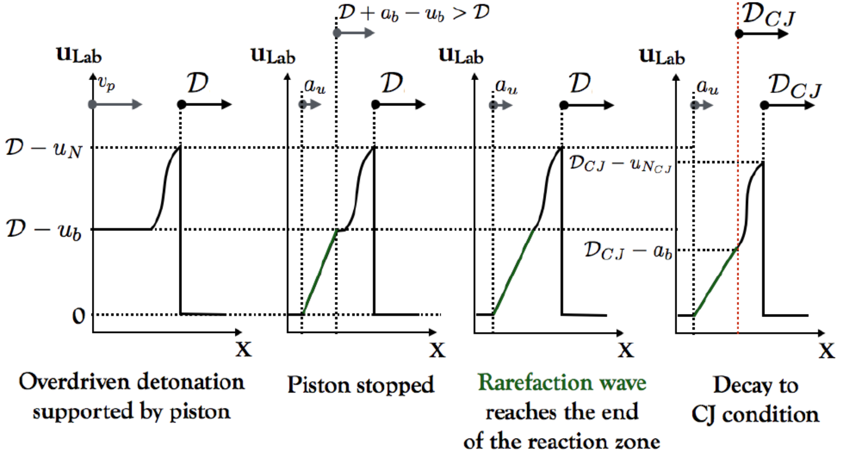


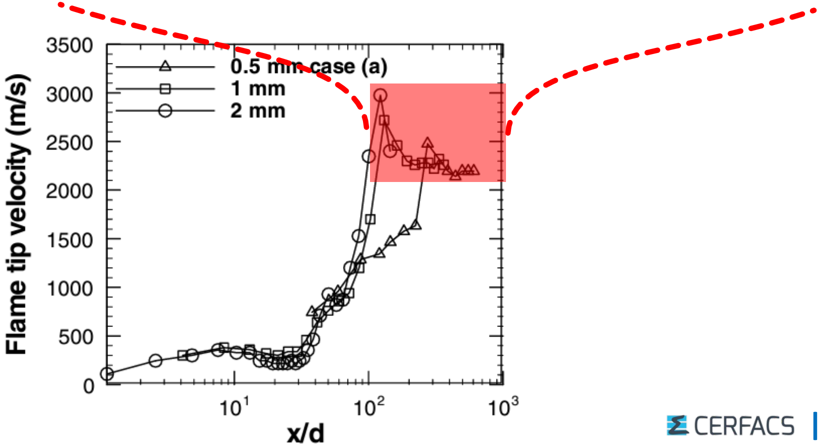



# Relax to CJ

- Overdriven detonations are unstable and can not self-propagate
- Overdriven detonations exist only when supported by a piston (local explosion)
- As soon as the piston support stops:
  - Decay to CJ
  - At CJ: detonation wave protected by the sonic plane
  - CJ solution is the only solution allowing autonomous detonation waves

Adapted from [1]





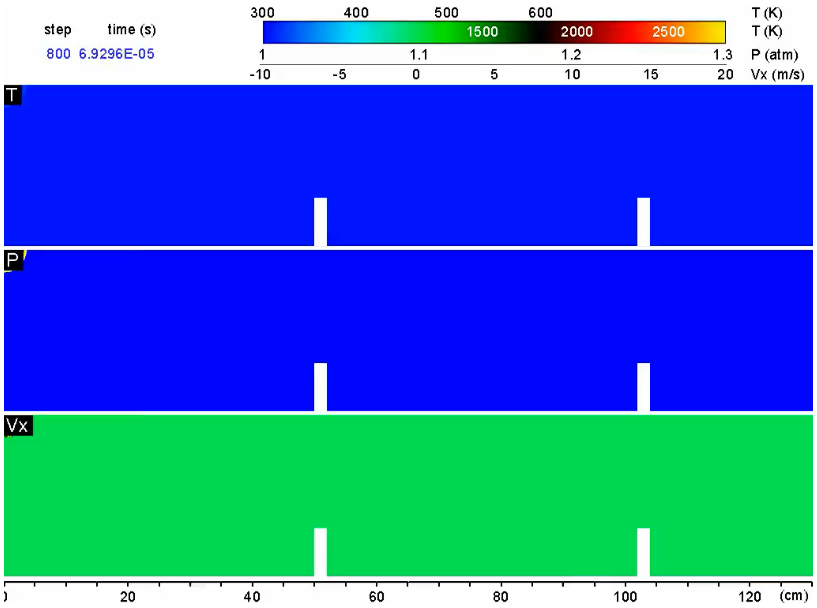
[1] P. Clavin and G. Searby, Cambridge University Press, 2016

# Concluding remarks

- No universal mechanism behind FA/DDT
- Often, combination of different mechanisms can explain FA/DDT

- Most experiments (even when well-instrumented) do not provide the details behind DDT

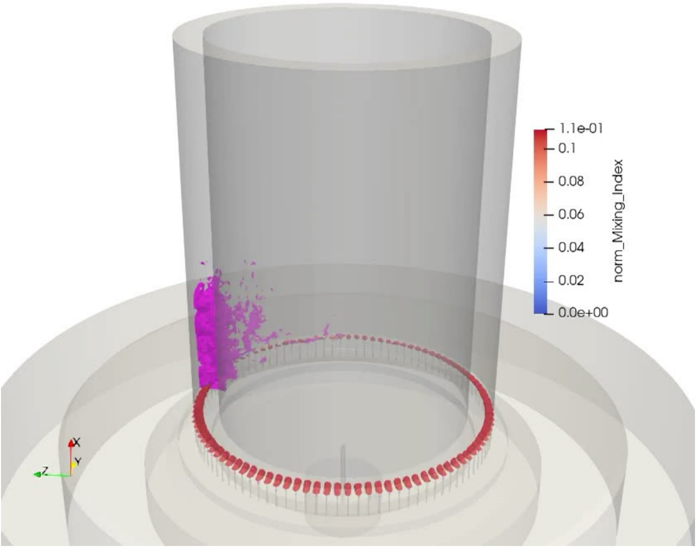
- High-fidelity simulations of FA/DDT at scales of industrial relevance is still a difficult task
  - the large range of scales at play
  - Constantly evolving



# Detonations can also be useful

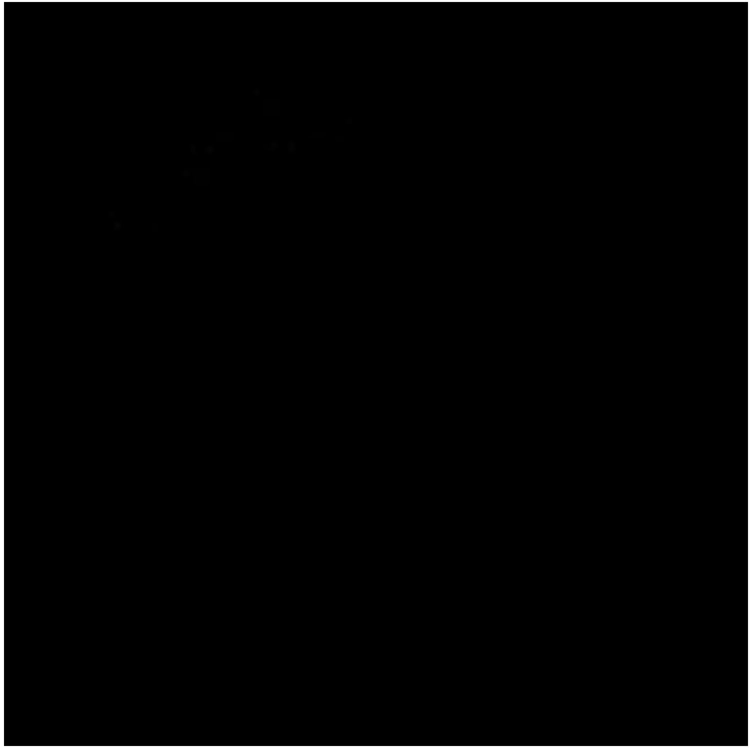
## RDE simulation

P. Stempfl, PhD, 2024




## RDE start-up

Credit: James Koch/University of Washington



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