

# Lagrangian particles evolution through RRE, RRR and BPR refraction structures

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# Outline

- 1 Reminder of the different refraction structures
- 2 Regular Refraction with reflected Expansion (RRE)
  - RRE - Theory and equations : gas dynamics
  - RRE - Results given by the inert gas dynamics theory
  - RRE - Use of CHEMKIN II to compute chemistry calculus
  - RRE - Results of the chemical calculus
- 3 Regular Refraction with Reflected Shock (RRR)
  - RRR - Theory and equations : gas dynamics
  - RRR - Results given by the inert gas dynamics theory
  - RRR - Results of the chemical calculus

# Reminder of the different refraction structures

From Henderson 1976 and 1978

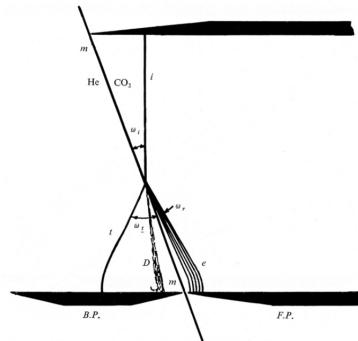
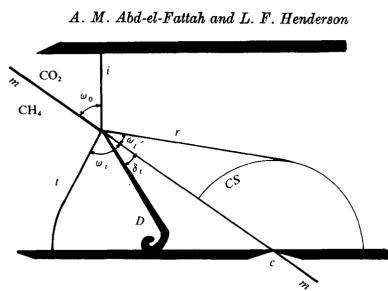


FIGURE 9. Regular refraction of a plane shock at a contaminated carbon dioxide-helium interface. For symbols see caption to figure 3.

(a) RRE struture



(b) RRR struture

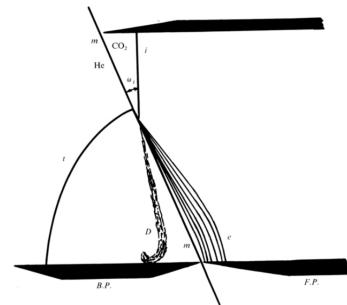


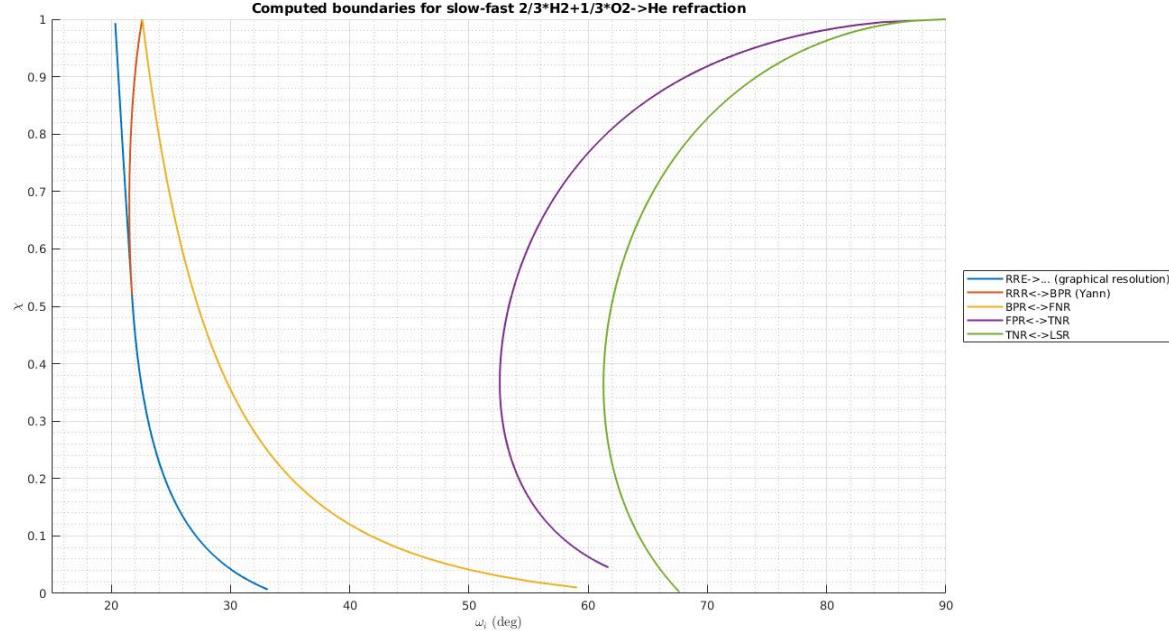
FIGURE 13. Bound-precursor irregular refraction of a plane shock at a contaminated carbon dioxide-helium interface. For symbols see captions to figures 3 and 10.

(c) BPR structure

Figure 1: Three of the already known refraction structures : RRE and BPR schemes are from Henderson, Abd-el-Fattah & Lozzi 1976; RRR scheme is from Henderson & Abd-el-Fattah 1978.

# Reminder of the different refraction structures

## Refraction with reflected Expansion



**Figure 2:** Boundaries of the different structures in the  $\chi - \omega$  plane, for a  $H_2 - O_2 // He$  system

Strength of the shock  $\chi$  is related to Mach number of the shock  $M_{sh}$ .

# Regular Refraction with reflected Expansion (RRE)

Relation between strength  $\chi$  and Mach number  $M_{sh}$

$$\chi = 1/\xi_i$$

$$\xi_i = \frac{1 - \gamma_I + 2\gamma_I M_{sh}}{\gamma_I + 1}$$

where  $\gamma_I$  is the heat ratio of phase I and  $M_{sh}$  is the normal component of the Mach number of the shock (see figure 5, slide 10). It is equal to  $M_{1n}$  the normal component of the Mach number of the incident flow. It is related to the Mach number of the flow by the following relation :

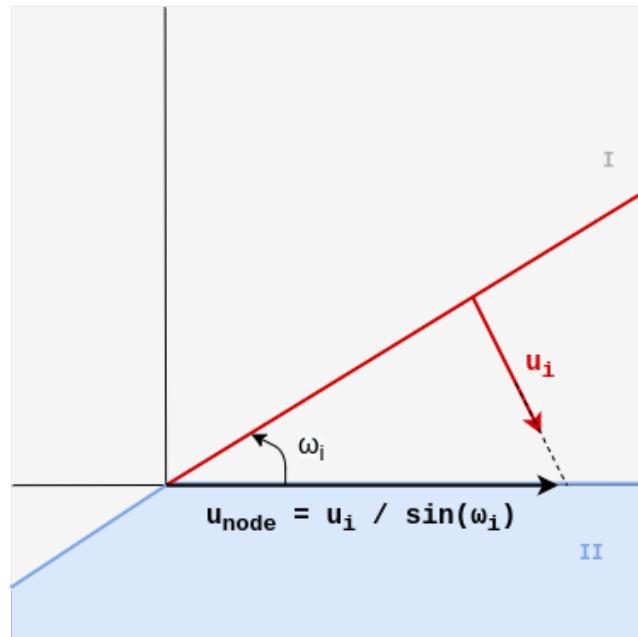
$$M_{sh} = \frac{M_1}{\sin(\omega_i)}$$

which finally leads to (with  $\omega_i = 14.5^\circ$ ):

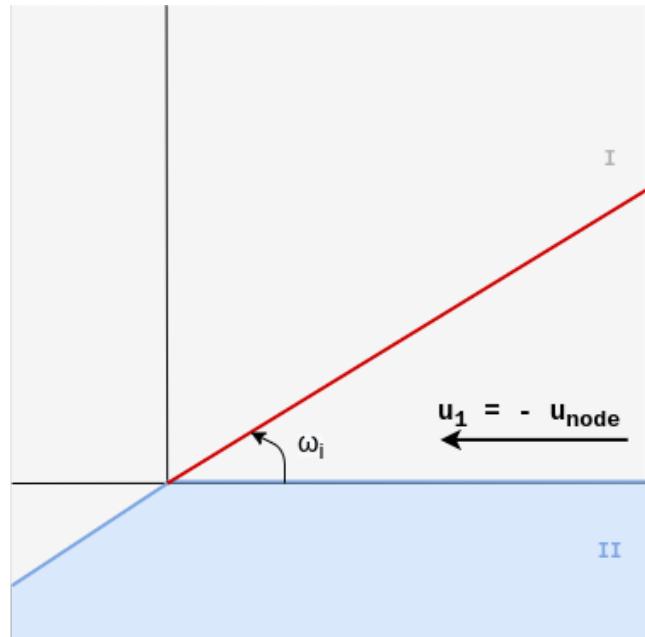
$$\chi \in [0.01; 1] \iff M_{sh} \in [1; 2.95] \iff M_1 \in [4; 11.78] \quad (1)$$

# RRE - Theory and equations : gas dynamics

## Change and rotation of frame of reference



(a) Frame of reference of the tube : shock is moving at  $u_i$



(b) Frame of reference of the shock : flow is moving at  $u_1$

Figure 3: Change of frame of reference (see legend on next slide)

# RRE - Theory and equations : gas dynamics

## Useful symbols

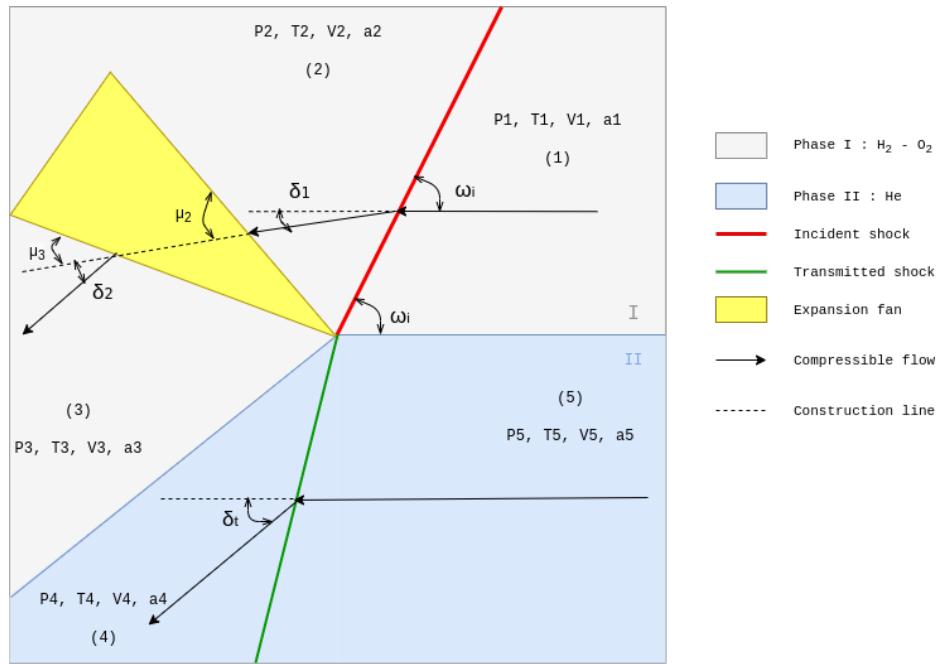


Figure 4: Symbols, zones and angles for computation

# RRE - Theory and equations : gas dynamics

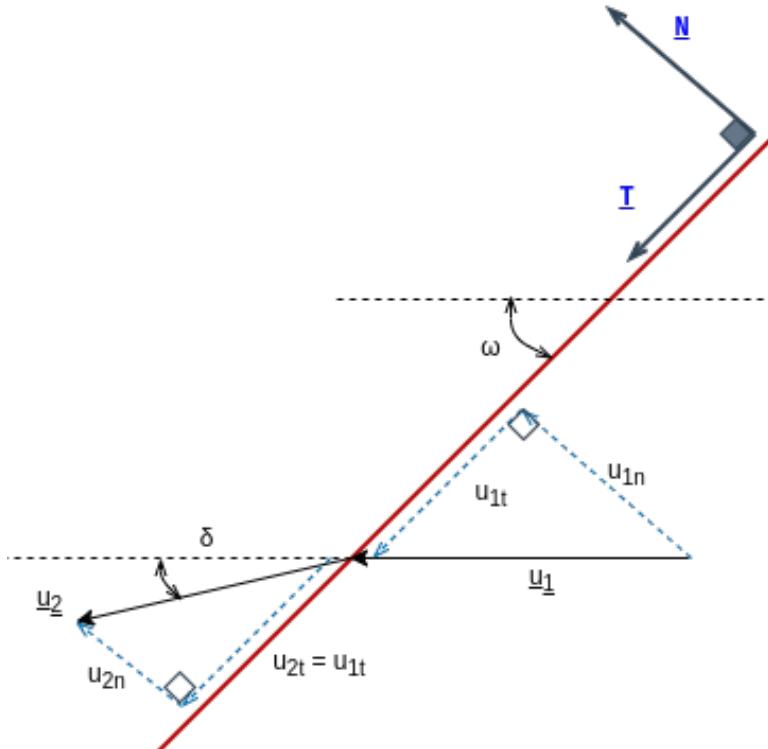
## Initial conditions in zone (1)

Measure (unit)	Symbol	Value
Pressure (Pa)	$P_1$	101 325
Temperature (K)	$T_1$	600
Specific Volume	$V_1$	$V_1 = R_I * T_1 / P_1$
Mach number	$M_1$	6
Angle of incidence (deg)	$\omega_i$	14.5
Normal mach number	$M_{1n}$	$M_{1n} = M_1 \sin(\omega_i)$
Speed of sound (m/s)	$a_1$	$a_1 = \sqrt{\gamma_I R_I T_1}$

Table 1: Initial conditions

# RRE - Theory and equations : gas dynamics

## Definition of normal Mach number



$$\begin{aligned} M1_n &= \frac{u1_n}{a_1} \\ &= \frac{u1 \sin(\omega_i)}{a_1} \\ &= M1 \sin(\omega_i) \end{aligned}$$

$$\xi_i = \frac{1 - \gamma_I + 2\gamma_I M1_n}{\gamma_I + 1}$$

Figure 5: Geometry associated with the oblique shock

# RRE - Theory and equations : gas dynamics

From zone (1) to zone (2): oblique shock

$$M1_n = M1 \sin(\omega_i)$$

$$\frac{V2}{V1} = \frac{(\gamma_I + 1) M1_n^2}{2 + (\gamma_I - 1) M1_n^2}$$

$$M2_n^2 = \frac{1 + \frac{\gamma_I - 1}{2} M1_n^2}{\gamma_I M1_n^2 - \frac{\gamma_I - 1}{2}}$$

$$\frac{P2}{P1} = 1 + \frac{2\gamma_I}{\gamma_I + 1} (M1_n^2 - 1)$$

$$M2 = \frac{M2_n}{\sin(\omega_i - \delta_1)}$$

$$\frac{T2}{T1} = \frac{P2}{P1} \frac{V2}{V1}$$

where  $\delta_1$  is the angle of deflection behind the incident shock.

$$\tan(\delta_1) = 2 \cot(\omega_i) \frac{M1_n^2 - 1}{M1^2(\gamma_I + \cos 2\omega_i) + 2}$$

# RRE - Theory and equations : gas dynamics

From zone (5) to zone (4) : oblique shock of unknown angle

$$M5_n = M5 \sin(\omega_t)$$

$$\frac{V4}{V5} = \frac{(\gamma_{II}+1)M5_n^2}{2+(\gamma_{II}-1)M5_n^2}$$

$$M4_n^2 = \frac{1 + \frac{\gamma_{II}-1}{2} M5_n^2}{\gamma_{II} M5_n^2 - \frac{\gamma_{II}-1}{2}}$$

$$\frac{P4}{P5} = 1 + \frac{2\gamma_{II}}{\gamma_{II}+1} (M5_n^2 - 1)$$

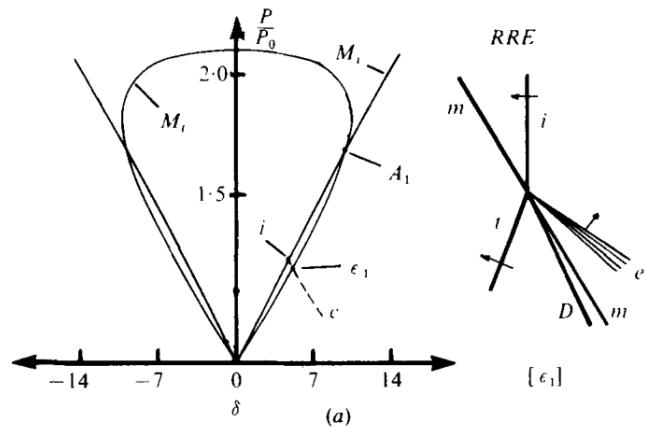
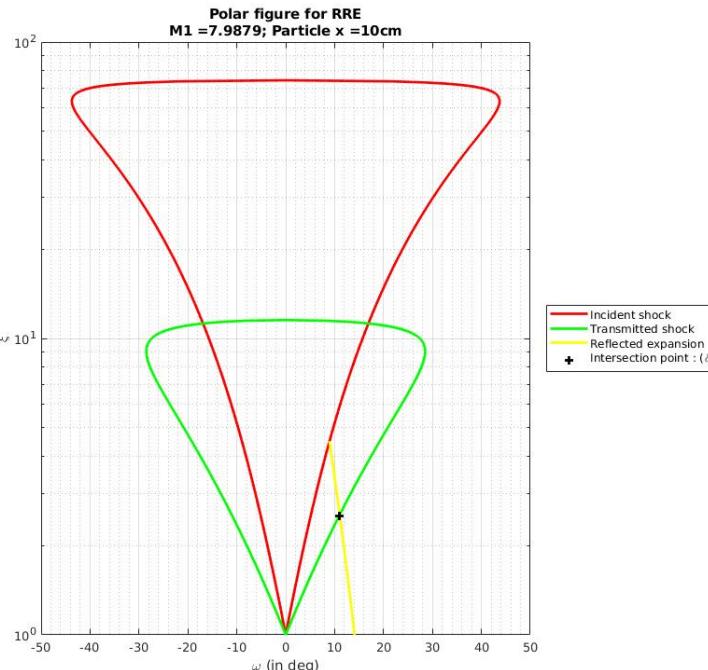
$$M4 = \frac{M4_n}{\sin(\omega_t - \delta_t)}$$

$$\frac{T4}{T5} = \frac{P4}{P5} \frac{V4}{V5}$$

where  $\delta_t$  is the angle of deflection behind the transmitted shock.  
Unfortunately,  $\omega_t$ , the angle between the transmitted shock and the flow in zone (5), remains unknown.

# RRE - Theory and equations : gas dynamics

Membrane equilibrium between zone (4) and zone (3)



$$\delta_t = \delta_1 + \delta_2$$

$$P3 = P4$$

Figure 6: Polars for RRE structure, reference from Henderson et al. 1978 on the right

# RRE - Theory and equations : gas dynamics

From zone (2) to zone (3) : Prandtl-Meyer expansion

Thanks to the polars of the shock,  $\delta_t$  and  $\xi_t$  can be determined (intersection of expansion and transmitted shock polar).  $P4$  thus  $P3$  are known and so  $M3$  thanks to Prandtl-Meyer relations.  $\nu$  is the Prandtl-Meyer function, depending on the heat ratio of the gas at stake.

$$\nu(M3) = \delta_2 + \nu(M2)$$

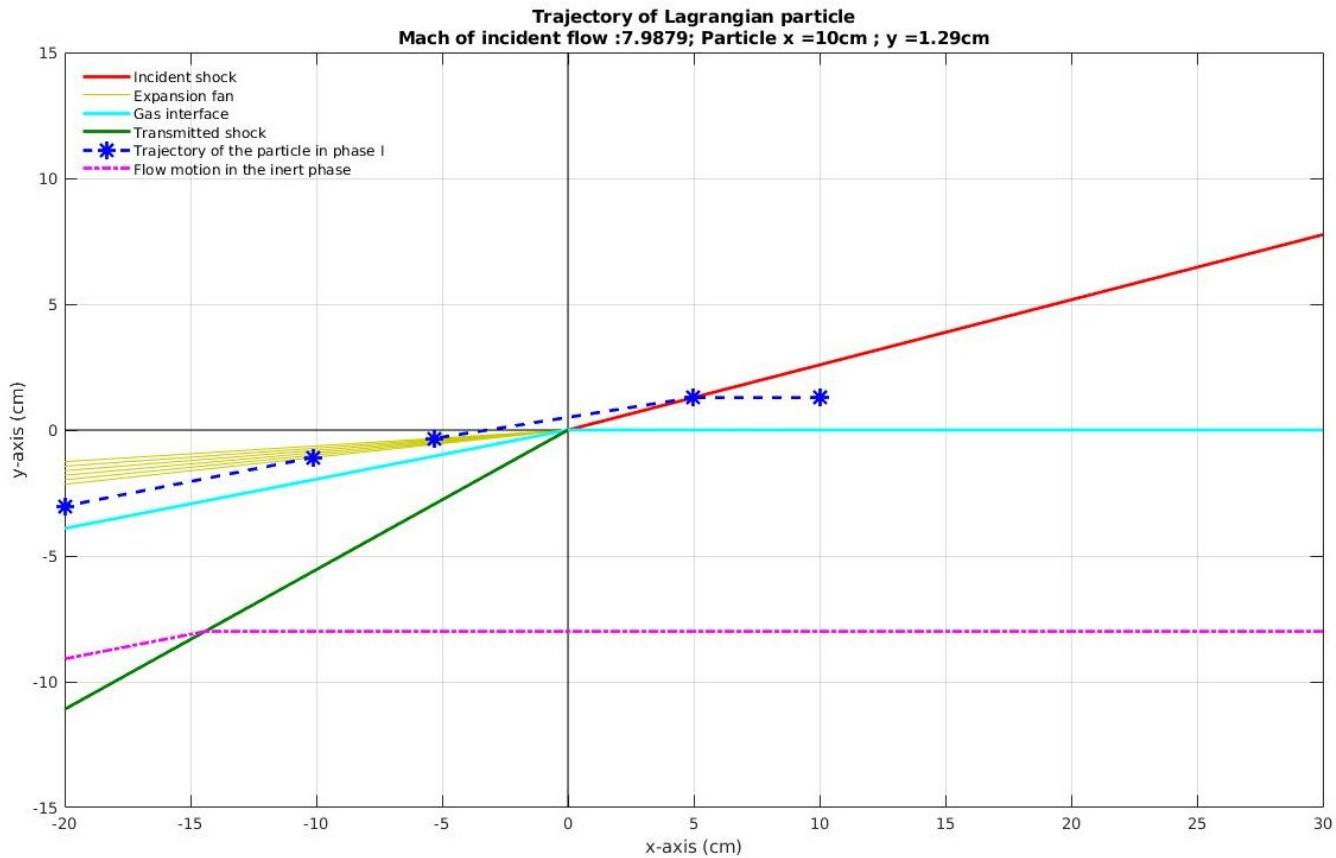
$$P3 = P4 = P5 \times \xi_t$$

$$T3 = T2 \left( \frac{P3}{P2} \right)^{\frac{\gamma_I - 1}{\gamma_I}}$$

$$V3 = R_I \frac{T3}{P3}$$

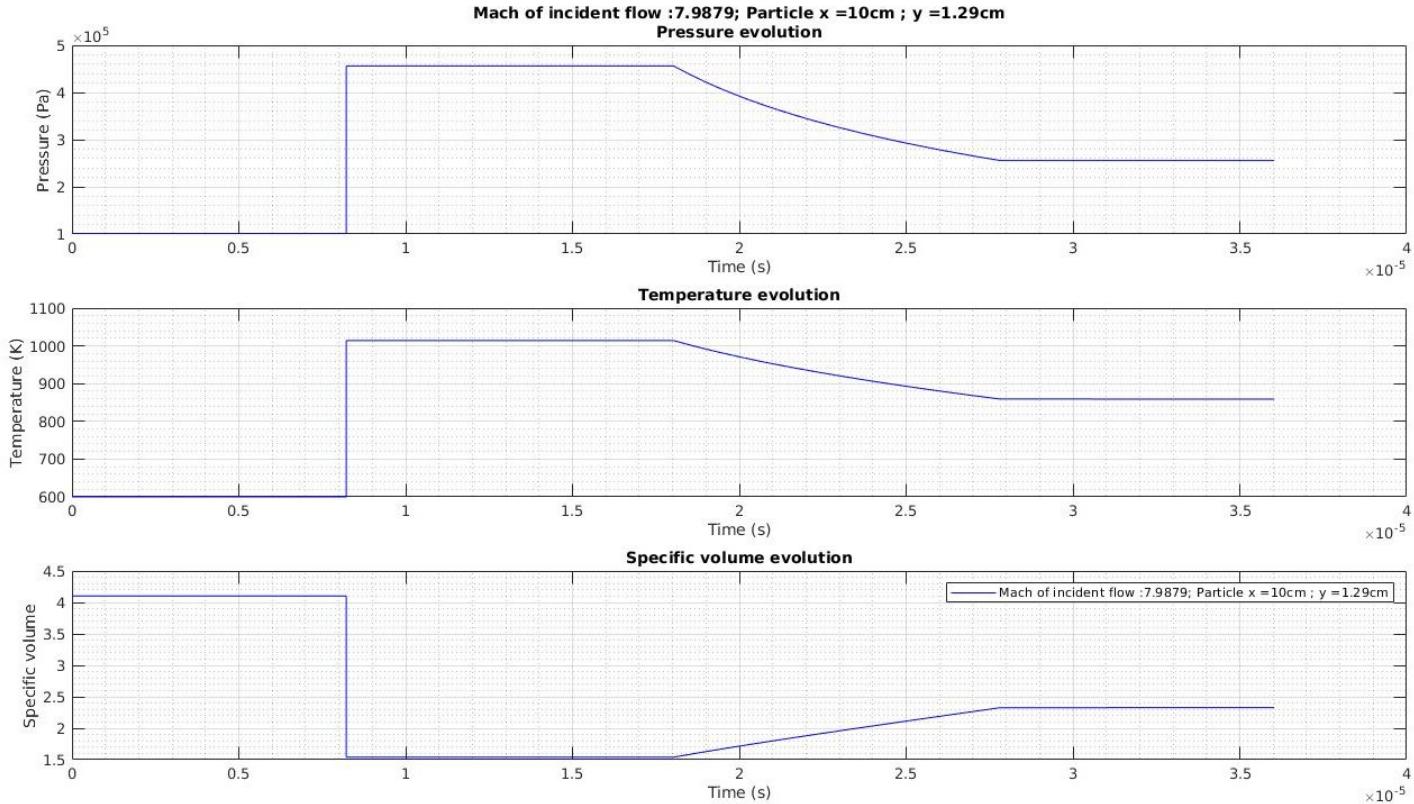
# RRE - Results given by the inert gas dynamics theory

## Evolution of a Lagrangian particle in the $H_2 - O_2$ phase



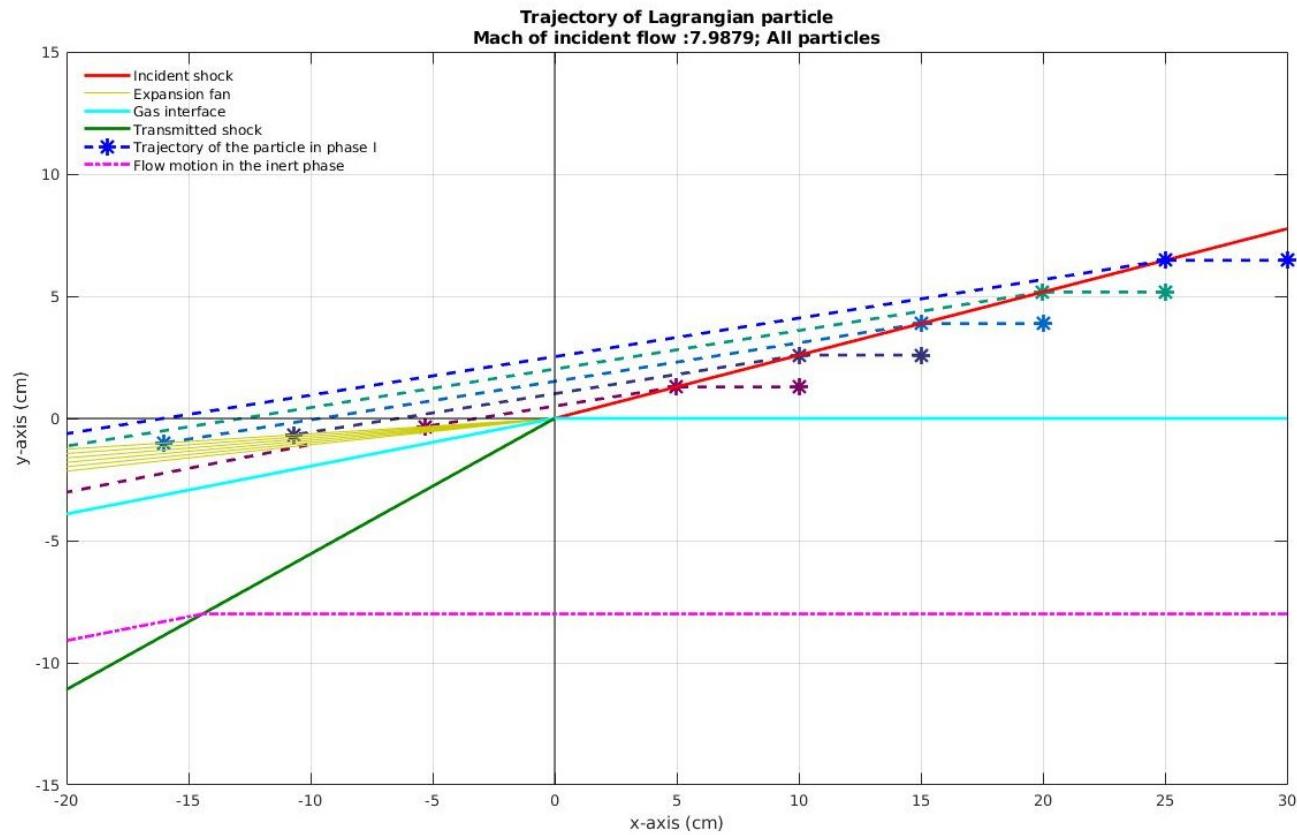
# RRE - Results given by the inert gas dynamics theory

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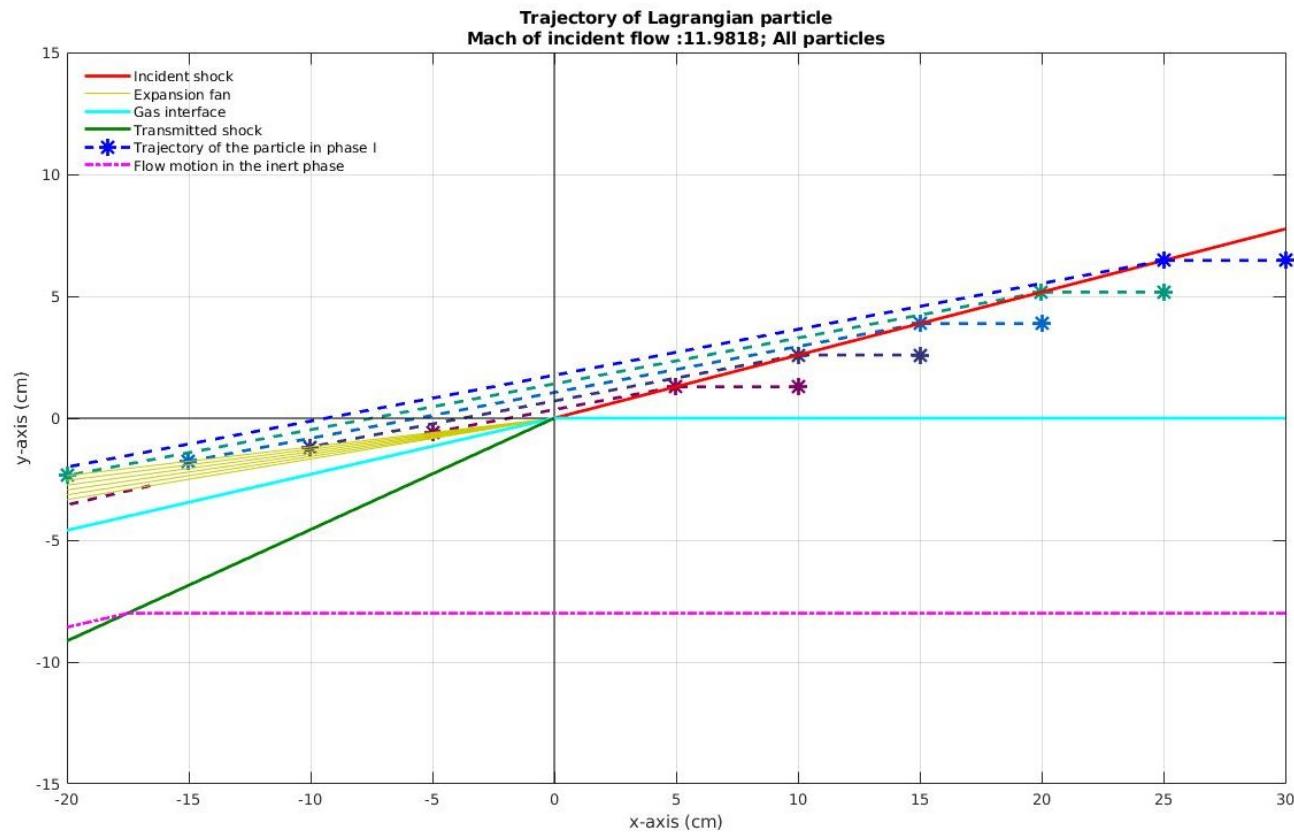
# RRE - Results given by the inert gas dynamics theory

Evolution depends on position of the particle...



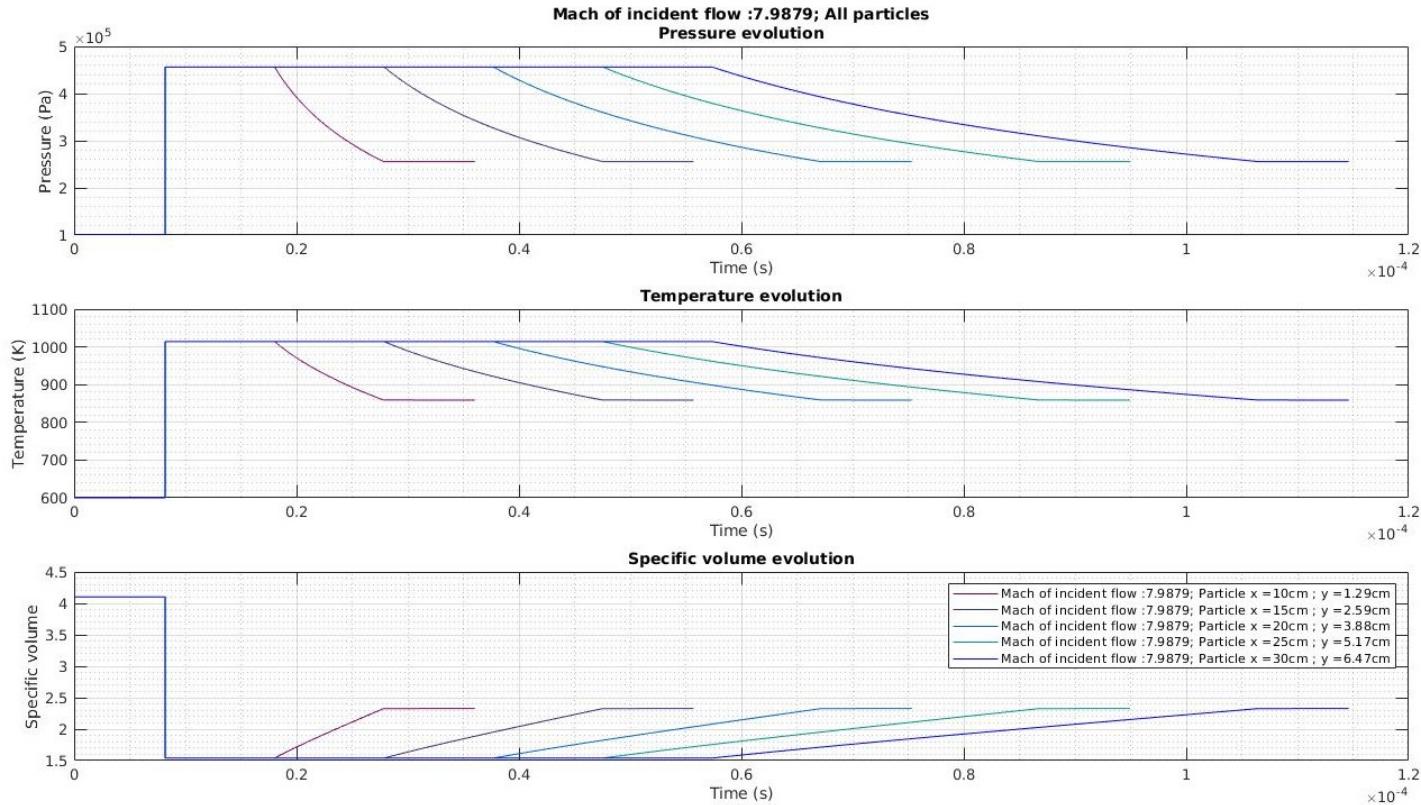
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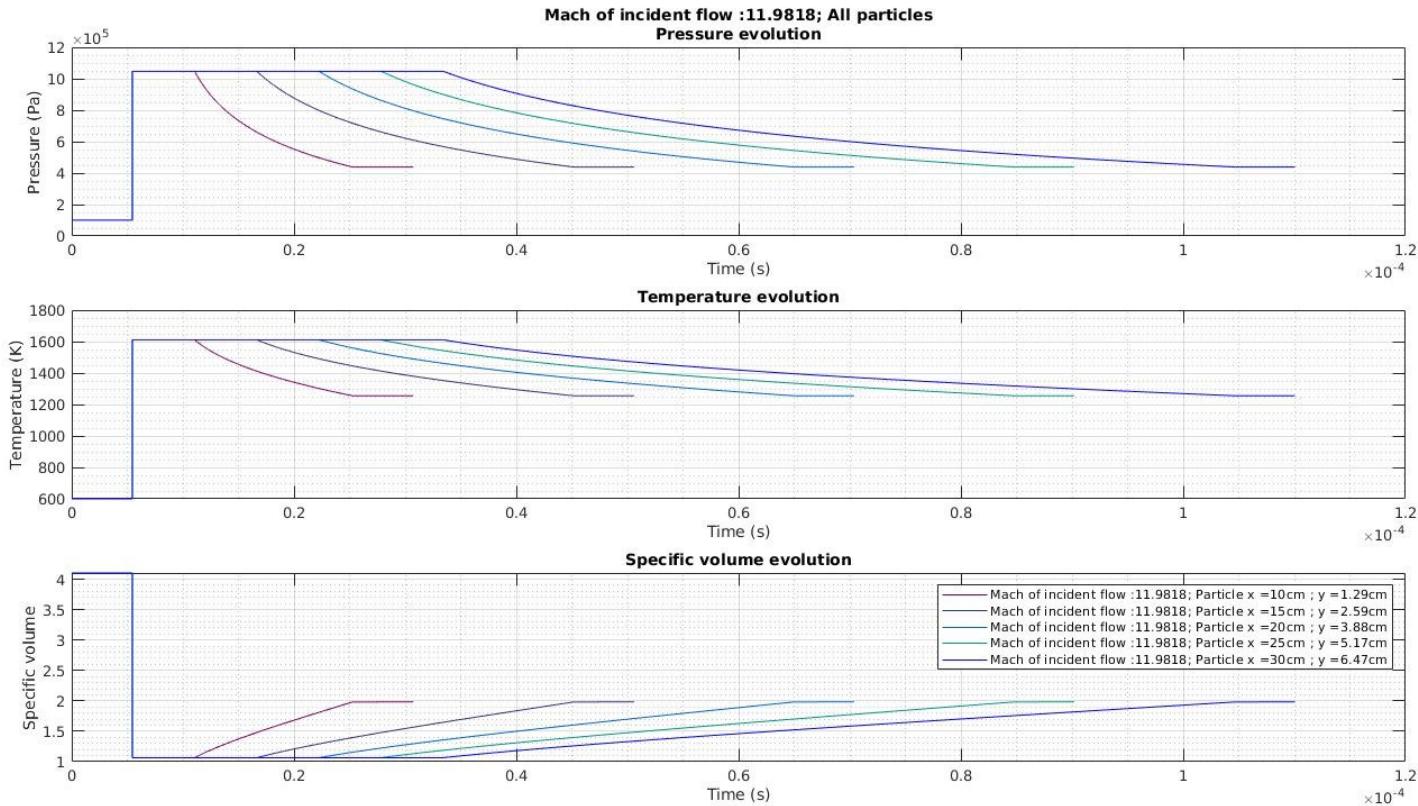
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Evolution depends on position of the particle...

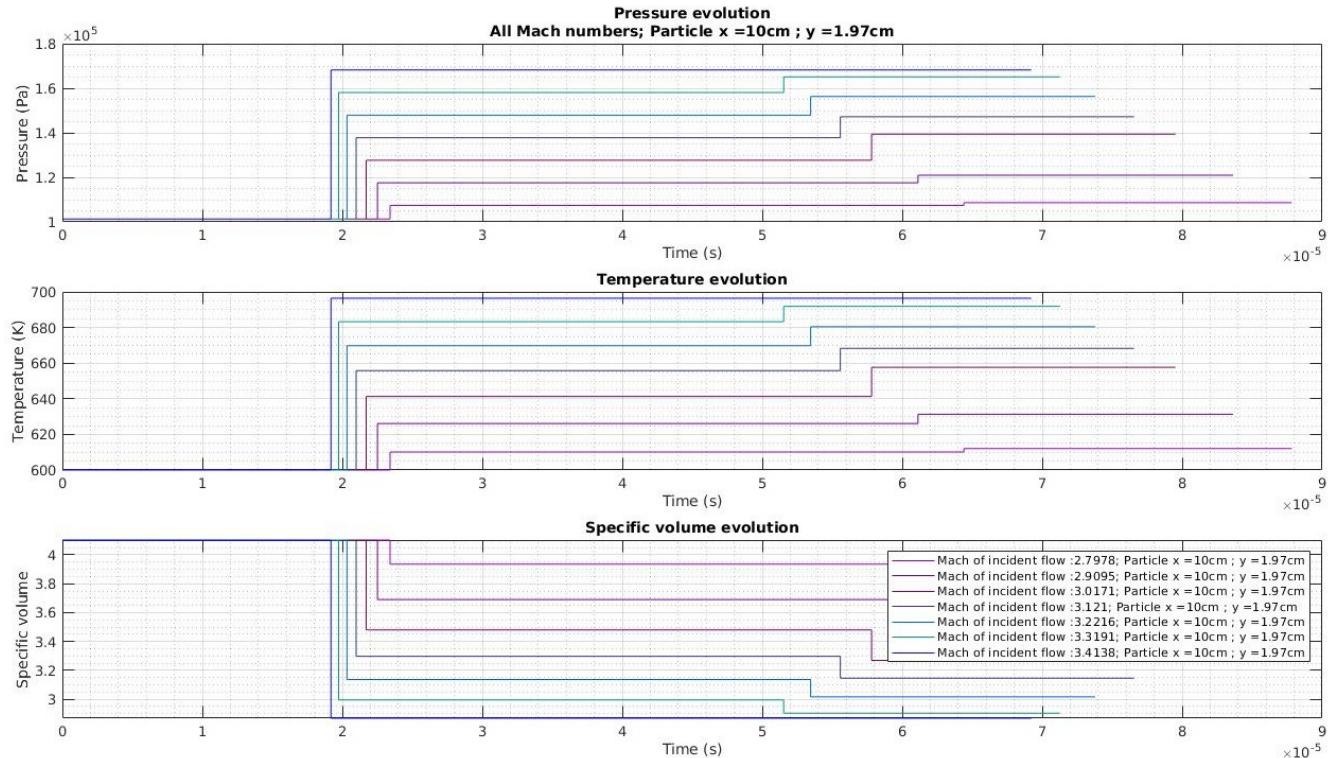


# RRE - Results given by the inert gas dynamics theory

Evolution depends on position of the particle...



# RRE - Results given by the inert gas dynamics theory ... and on Mach number of the shock



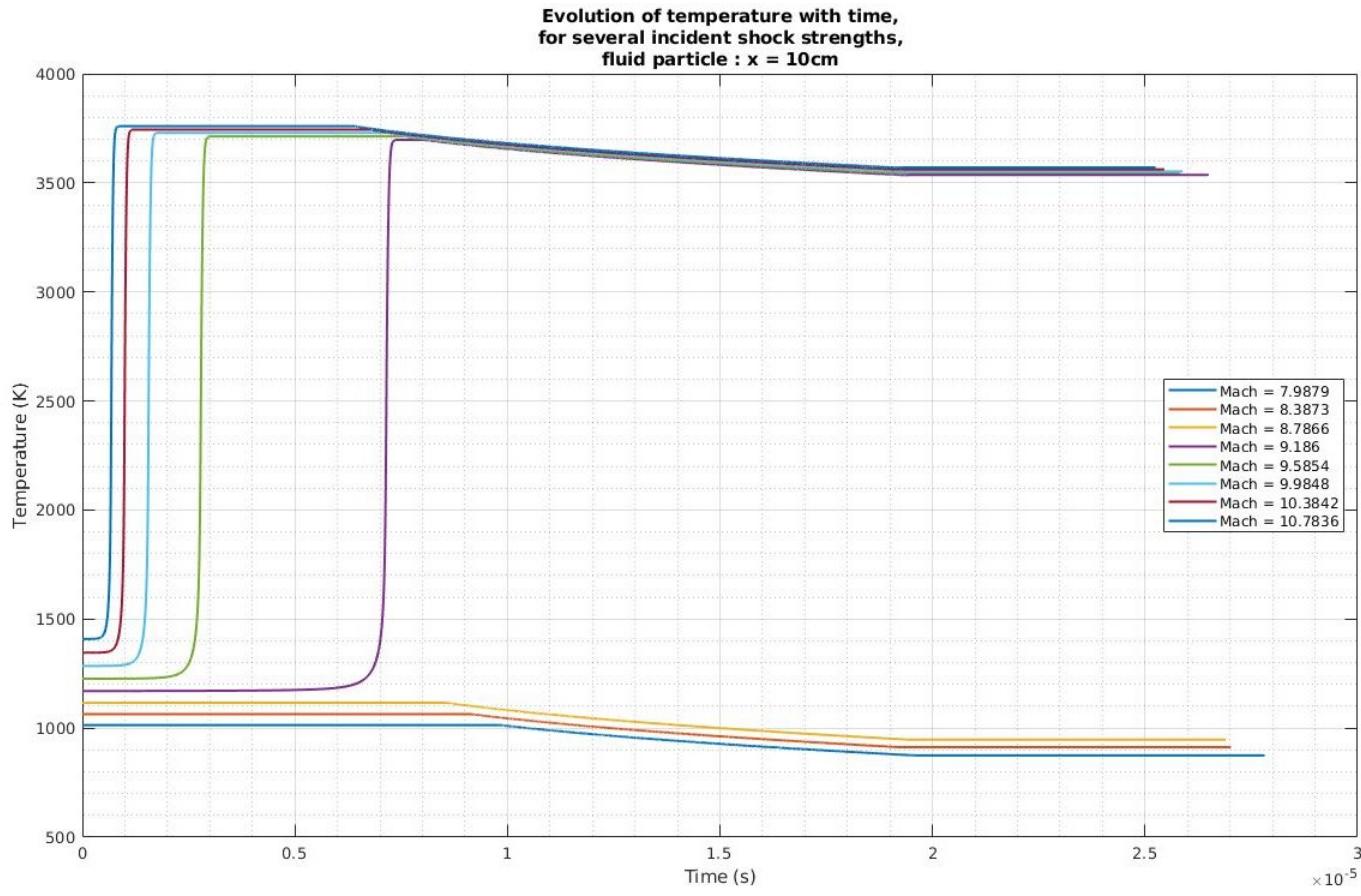
For a single particle, increasing  $M_{sh}$  leads to a rise in temperature and pressure : don't forget that  $H_2 - O_2$  is a reactive phase. Is an ignition possible under certain conditions?

# RRE - Main steps for chemistry calculus

- Calculate evolution of specific volume of different Lagrangian particles, for  $\omega_i = 14.5^\circ$ , for different Mach numbers (see slide 29).
- Use of CHEMKIN II to calculate chemical reactions in the reactive phase
- Outputs of CHEMKIN II : evolution of pressure, temperature and ratios of chemical species
- Temperature jump in CHEMKIN II output = detonation

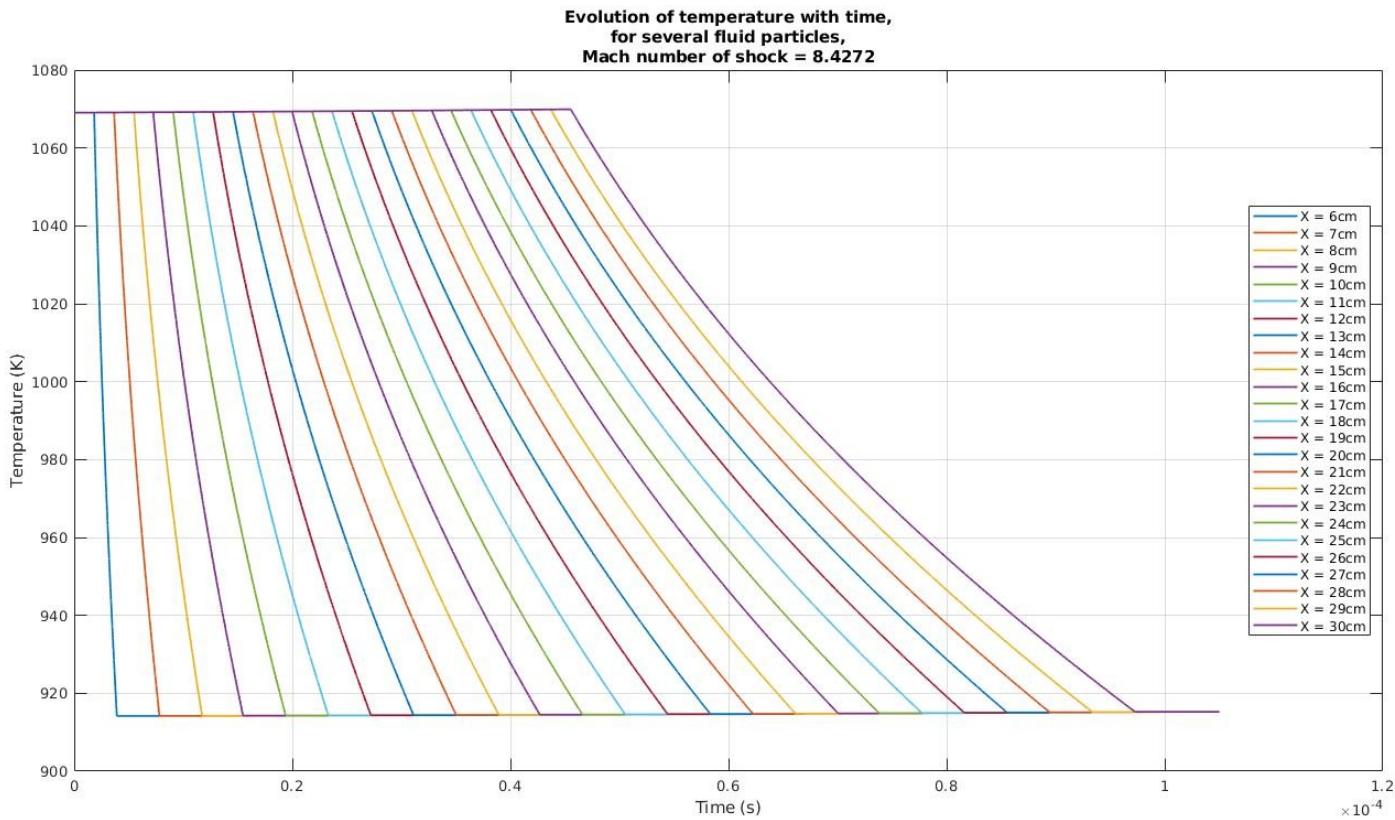
# RRE - Results of the chemical calculus

Existence of a threshold : Mach number of ignition



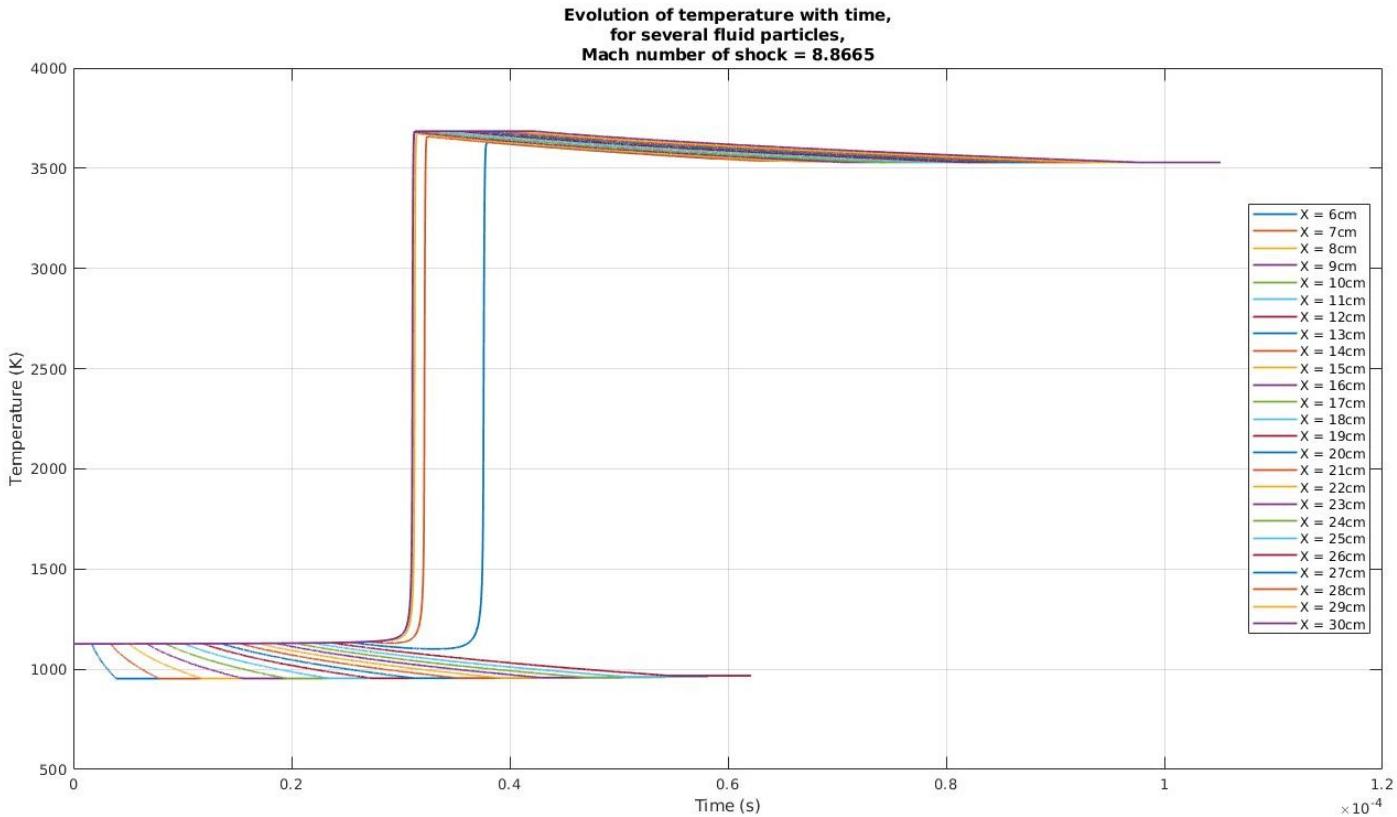
# RRE - Results of the chemical calculus

Each particle has its own  $M_{ignit}$



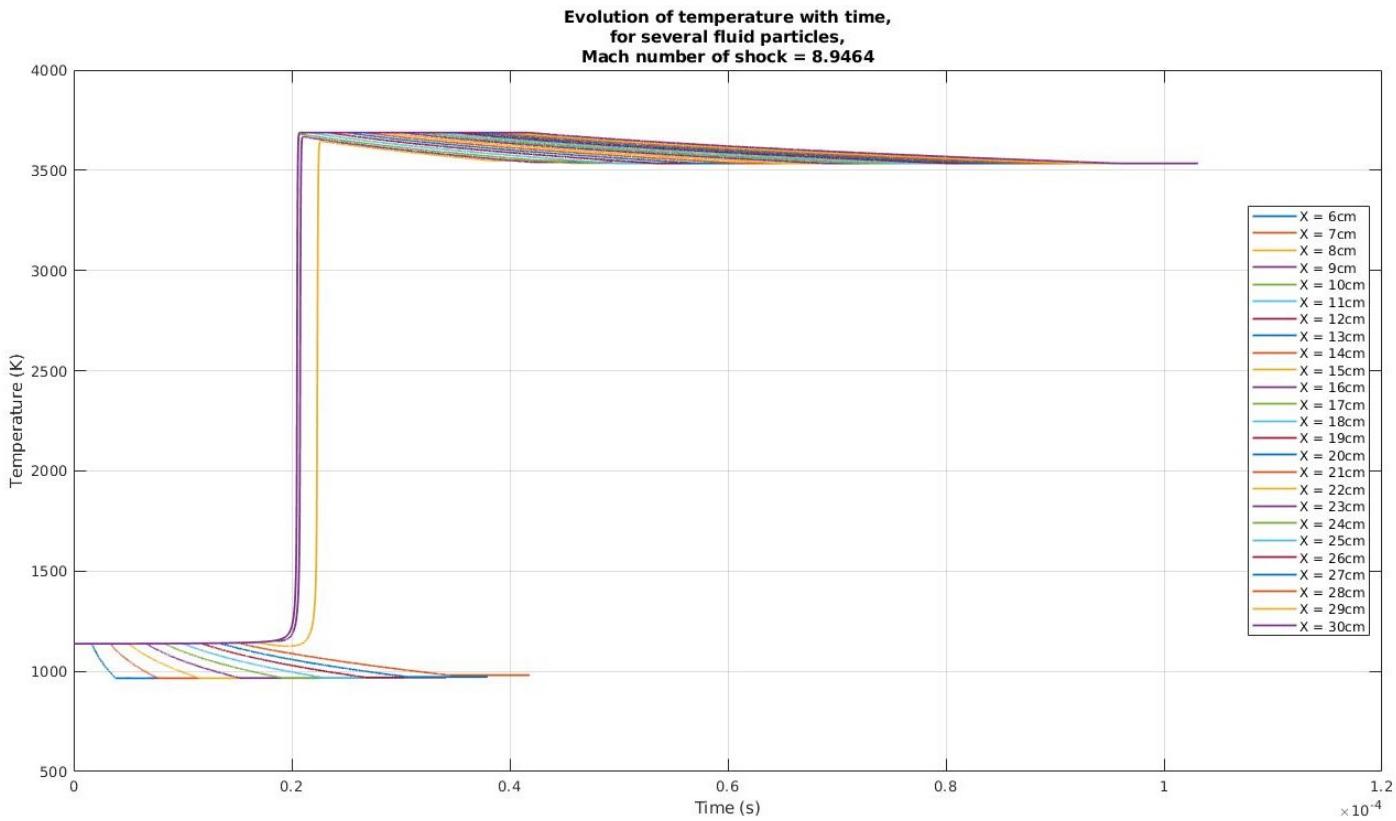
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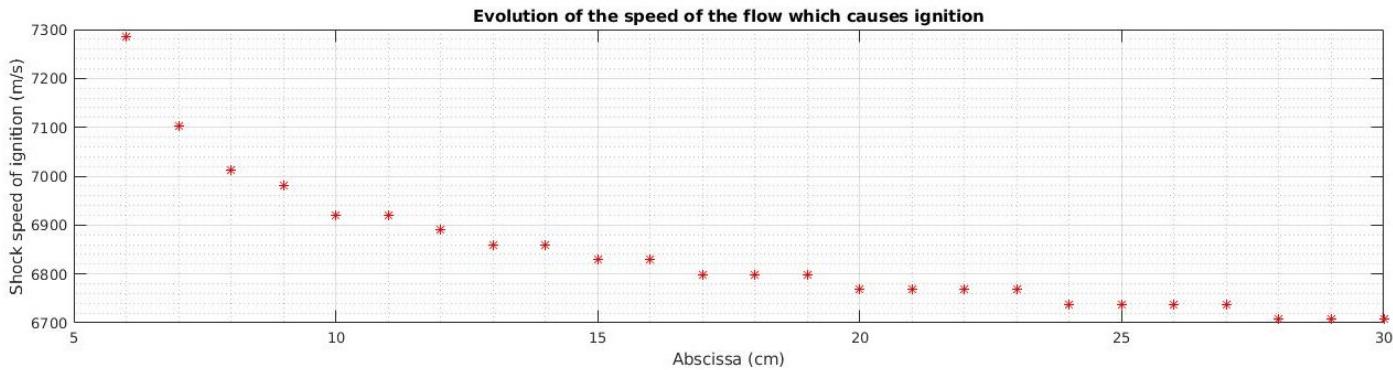
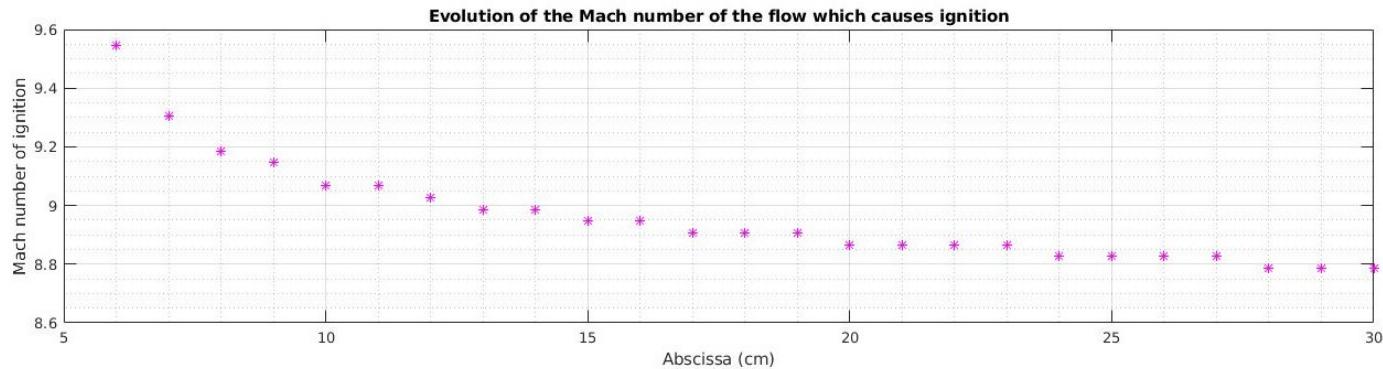
# RRE - Results of the chemical calculus

Each particle has its own  $M_{ignit}$



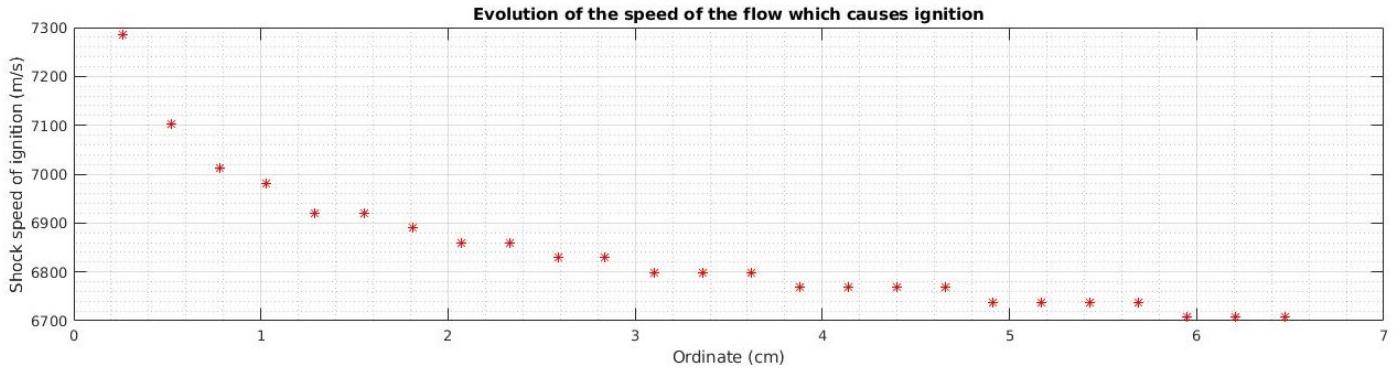
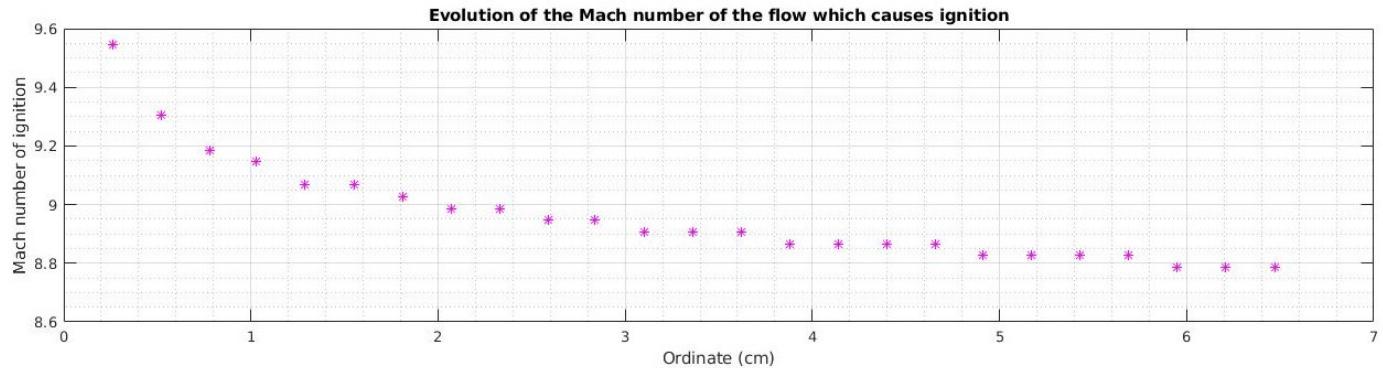
# RRE - Results of the chemical calculus

$M_{sh}$  plotted as a function of ordinate of the particle



# RRE - Results of the chemical calculus

$M_{sh}$  plotted as a function of ordinate of the particle



# Regular Refraction with Reflected Shock (RRR)

Strength  $\chi$  and Mach number  $M_{sh}$  domains

For this structure, an angle of incidence of  $\omega_i = 21.5^\circ$  has been chosen so as to explore the largest range of Mach numbers which finally leads to :

$$\chi \in [0.6; 1] \iff M_{sh} \in [1; 1.26] \iff M_1 \in [2.76; 3.41] \quad (2)$$

The method employed for this structure will be highly similar to the method used for the RRE structure, and even simpler because of the reflected wave : a shock instead of an expansion fan.

# RRR - Theory and equations : gas dynamics

## Change and rotation of frame of reference

The change and rotation of frame of reference keeps the same and the symbols used for this structure are very similar with the previous ones : here is a little reminder

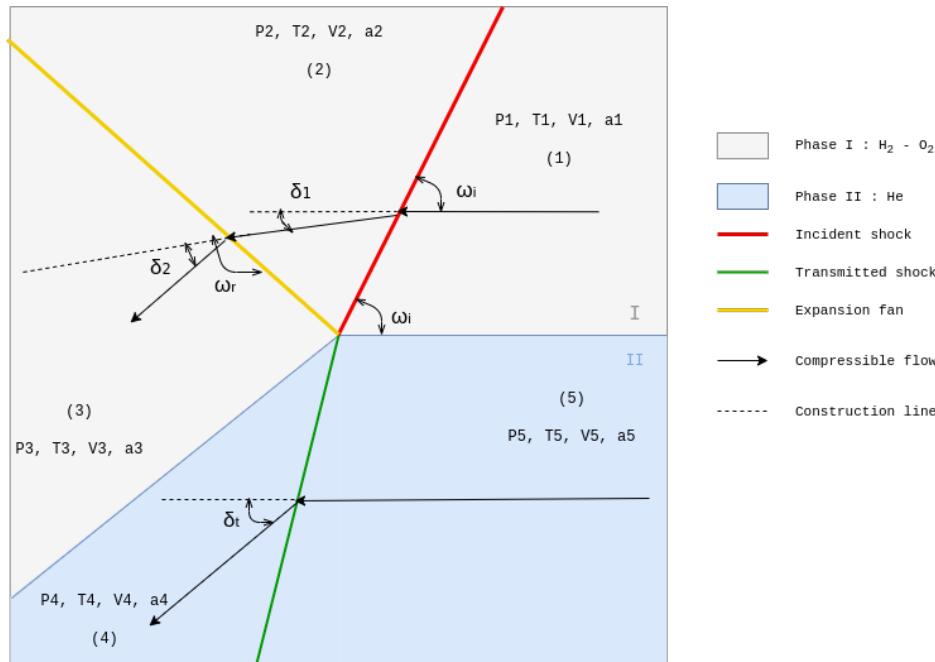


Figure 7: Symbols, zones and angles for computation

# RRR - Theory and equations : gas dynamics

## Initial conditions in zone (1)

Measure (unit)	Symbol	Value
Pressure (Pa)	$P_1$	101 325
Temperature (K)	$T_1$	600
Specific Volume	$V_1$	$V_1 = R_I * T_1 / P_1$
Mach number	$M_1$	6
Angle of incidence (deg)	$\omega_i$	21.5
Normal mach number	$M_{1n}$	$M_{1n} = M_1 \sin(\omega_i)$
Speed of sound (m/s)	$a_1$	$a_1 = \sqrt{\gamma_I R_I T_1}$

Table 2: Initial conditions

Definition of the normal Mach number  $M_{1n}$  is not changed.

# RRR - Theory and equations : gas dynamics

From zone (1) to zone (2): oblique shock

$$M1_n = M1 \sin(\omega_i)$$

$$\frac{V2}{V1} = \frac{(\gamma_I + 1) M1_n^2}{2 + (\gamma_I - 1) M1_n^2}$$

$$M2_n^2 = \frac{1 + \frac{\gamma_I - 1}{2} M1_n^2}{\gamma_I M1_n^2 - \frac{\gamma_I - 1}{2}}$$

$$\frac{P2}{P1} = 1 + \frac{2\gamma_I}{\gamma_I + 1} (M1_n^2 - 1)$$

$$M2 = \frac{M2_n}{\sin(\omega_i - \delta_1)}$$

$$\frac{T2}{T1} = \frac{P2}{P1} \frac{V2}{V1}$$

where  $\delta_1$  is the angle of deflection behind the incident shock.

$$\tan(\delta_1) = 2 \cot(\omega_i) \frac{M1_n^2 - 1}{M1^2(\gamma_I + \cos 2\omega_i) + 2}$$

# RRR - Theory and equations : gas dynamics

From zone (5) to zone (4) : oblique shock of unknown angle

$$M5_n = M5 \sin(\omega_t)$$

$$\frac{V4}{V5} = \frac{(\gamma_{II}+1)M5_n^2}{2+(\gamma_{II}-1)M5_n^2}$$

$$M4_n^2 = \frac{1 + \frac{\gamma_{II}-1}{2} M5_n^2}{\gamma_{II} M5_n^2 - \frac{\gamma_{II}-1}{2}}$$

$$\frac{P4}{P5} = 1 + \frac{2\gamma_{II}}{\gamma_{II}+1} (M5_n^2 - 1)$$

$$M4 = \frac{M4_n}{\sin(\omega_t - \delta_t)}$$

$$\frac{T4}{T5} = \frac{P4}{P5} \frac{V4}{V5}$$

where  $\delta_t$  is the angle of deflection behind the transmitted shock.  
Unfortunately,  $\omega_t$ , the angle between the transmitted shock and the flow in zone (5), remains unknown.

# RRR - Theory and equations : gas dynamics

Membrane equilibrium between zone (4) and zone (3)

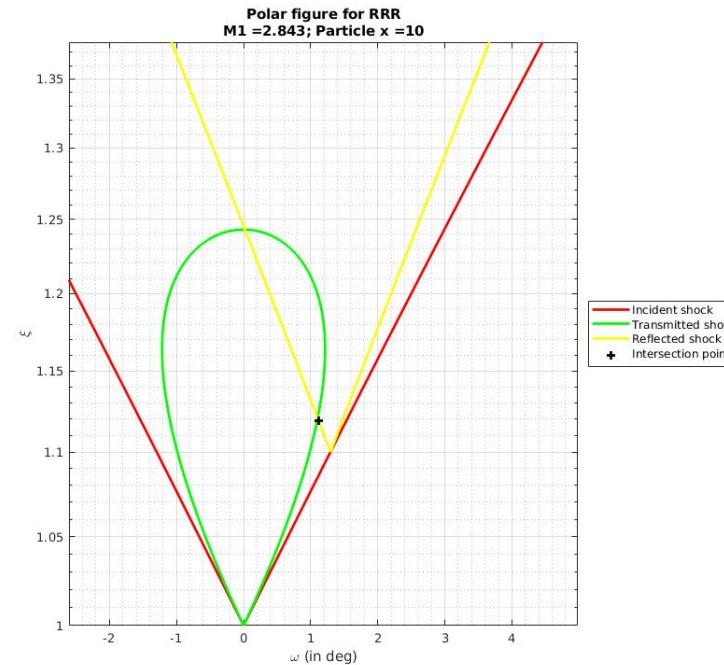
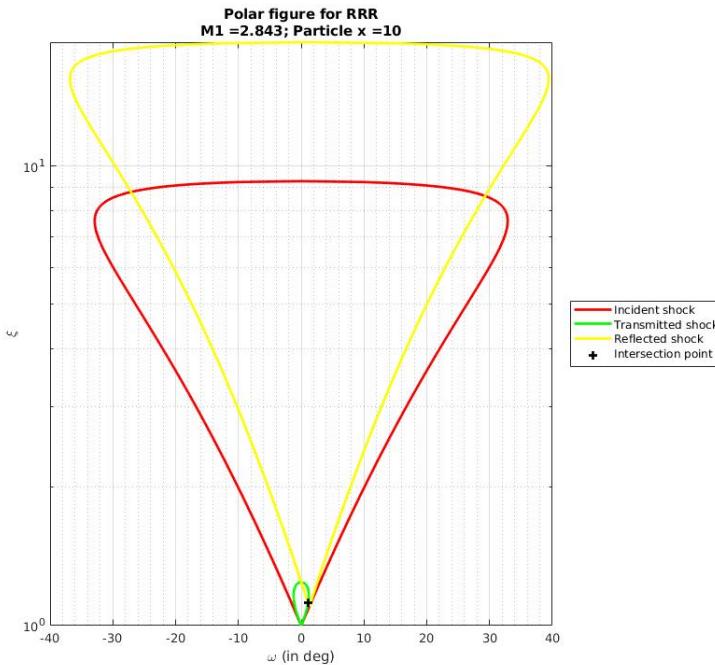
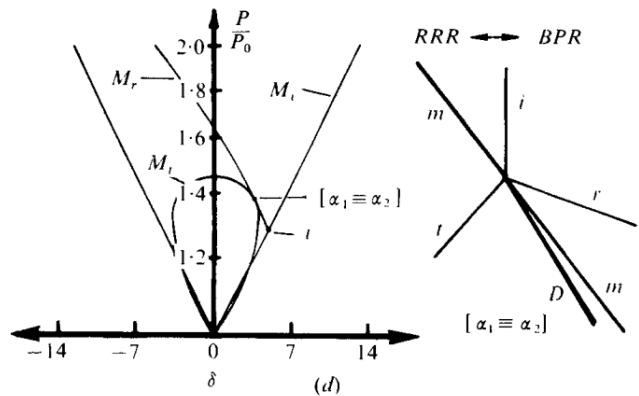
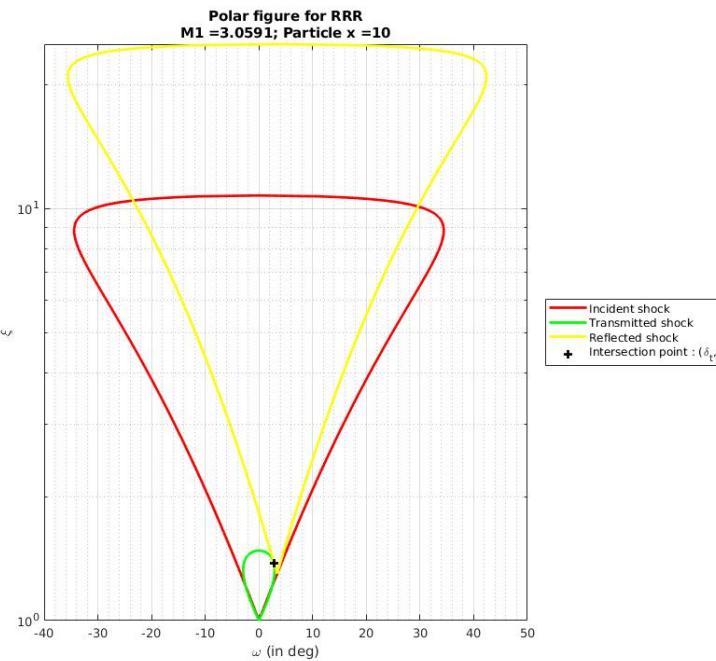


Figure 8: Polars for RRR structure, zoom on the intersection point on the right

# RRR - Theory and equations : gas dynamics

Membrane equilibrium between zone (4) and zone (3)



$$\delta_t = \delta_1 + \delta_2$$

$$P3 = P4$$

Figure 9: Polars for RRR structure, reference from Henderson et al. 1978 on the right

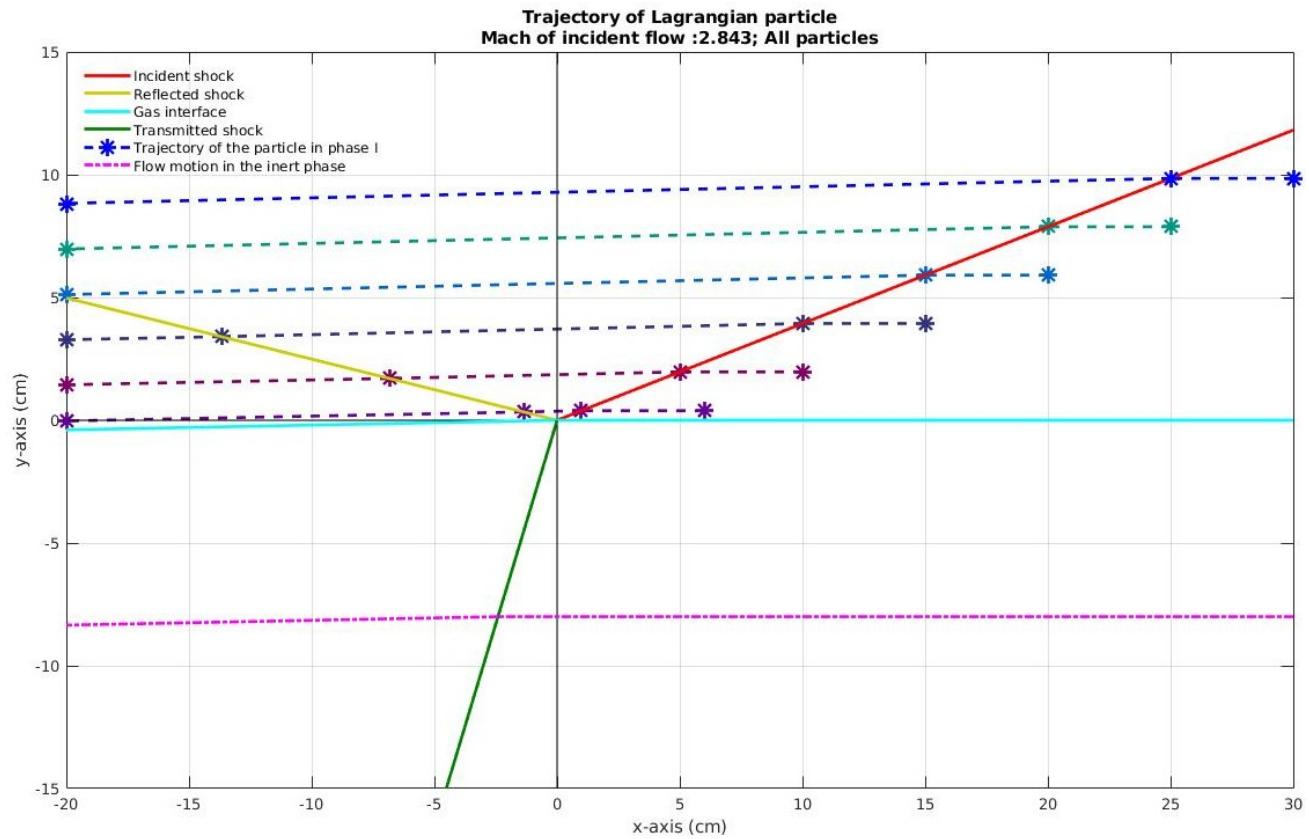
# RRR - Theory and equations : gas dynamics

From zone (2) to zone (3) : oblique shock of unknown angle

Thanks to the polars of the shock,  $\delta_t$  and  $\xi_t$  can be determined (intersection of expansion and transmitted shock polar) :  $P4$  thus  $P3$  are known. Then  $\xi_r = \frac{P3}{P2}$  can be computed and all quantities in zone (3) can be easily deduced.

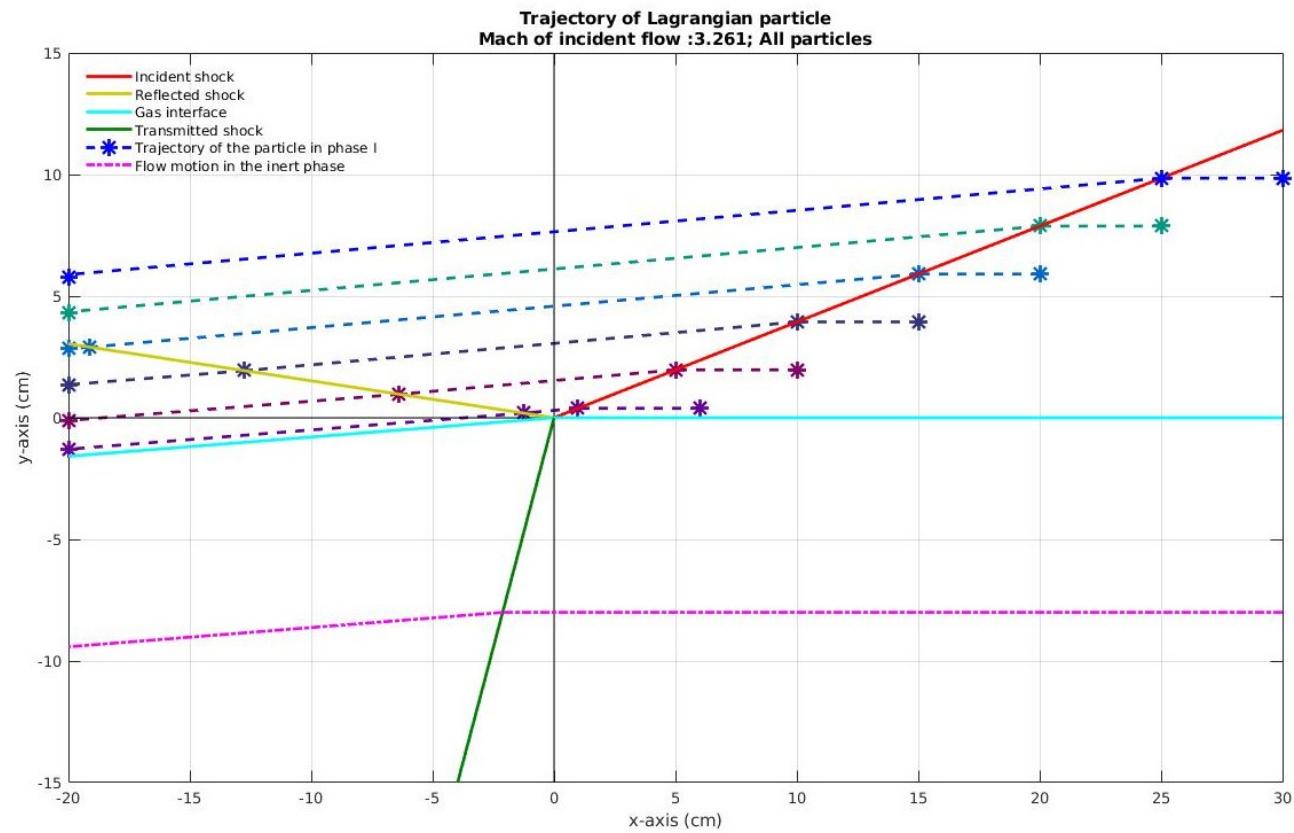
# RRR - Results given by the inert gas dynamics theory

Evolution depends on position of the particle...



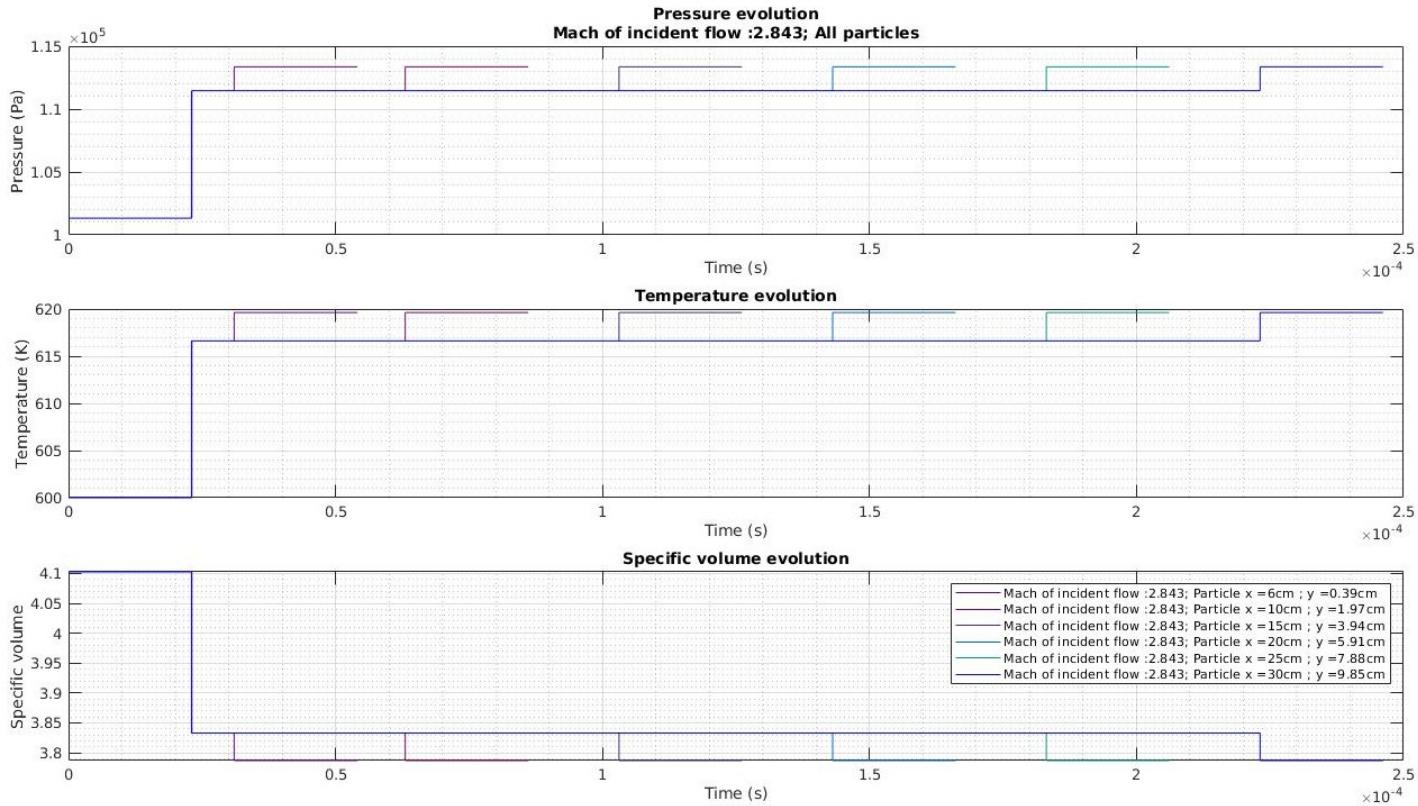
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Evolution depends on position of the particle...



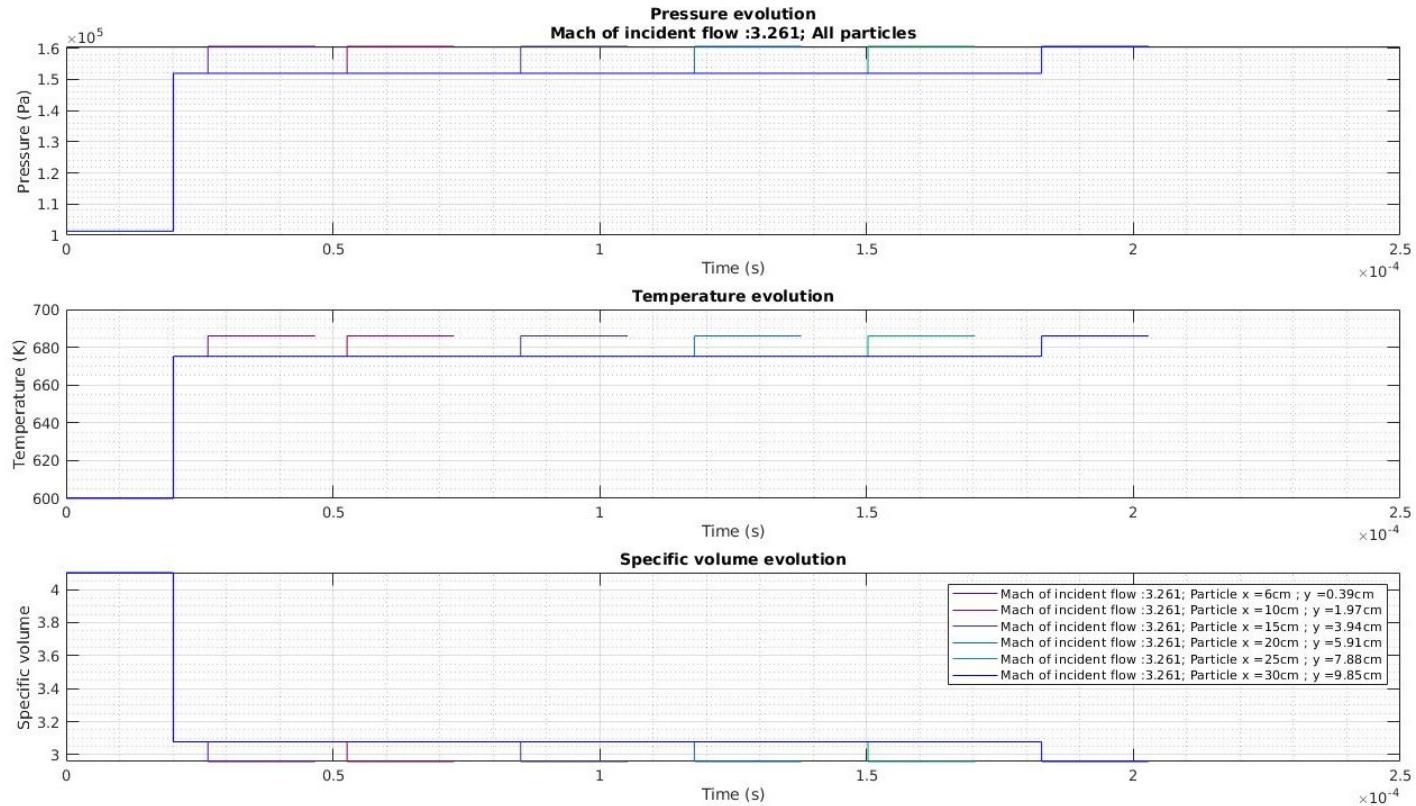
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Evolution depends on position of the particle...



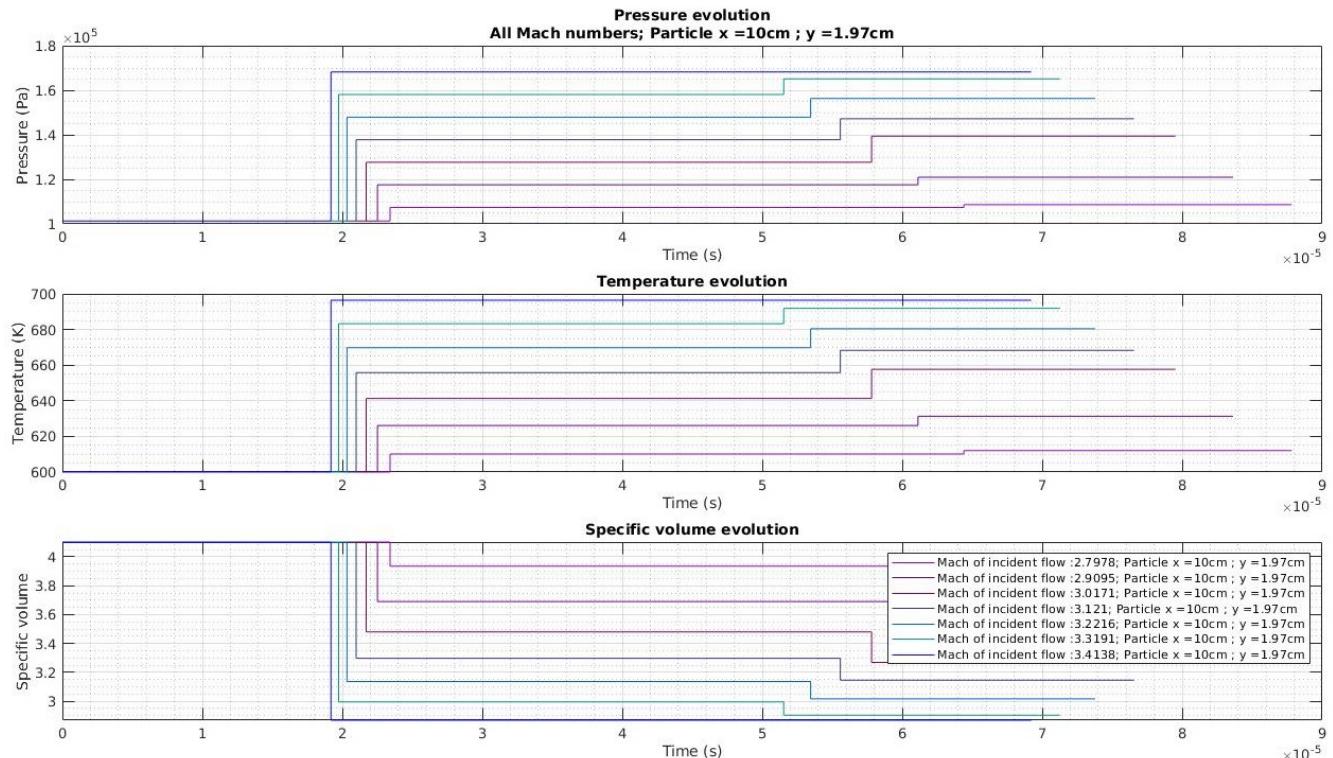
# RRR - Results given by the inert gas dynamics theory

Evolution depends on position of the particle...



# Results given by the inert gas dynamics theory

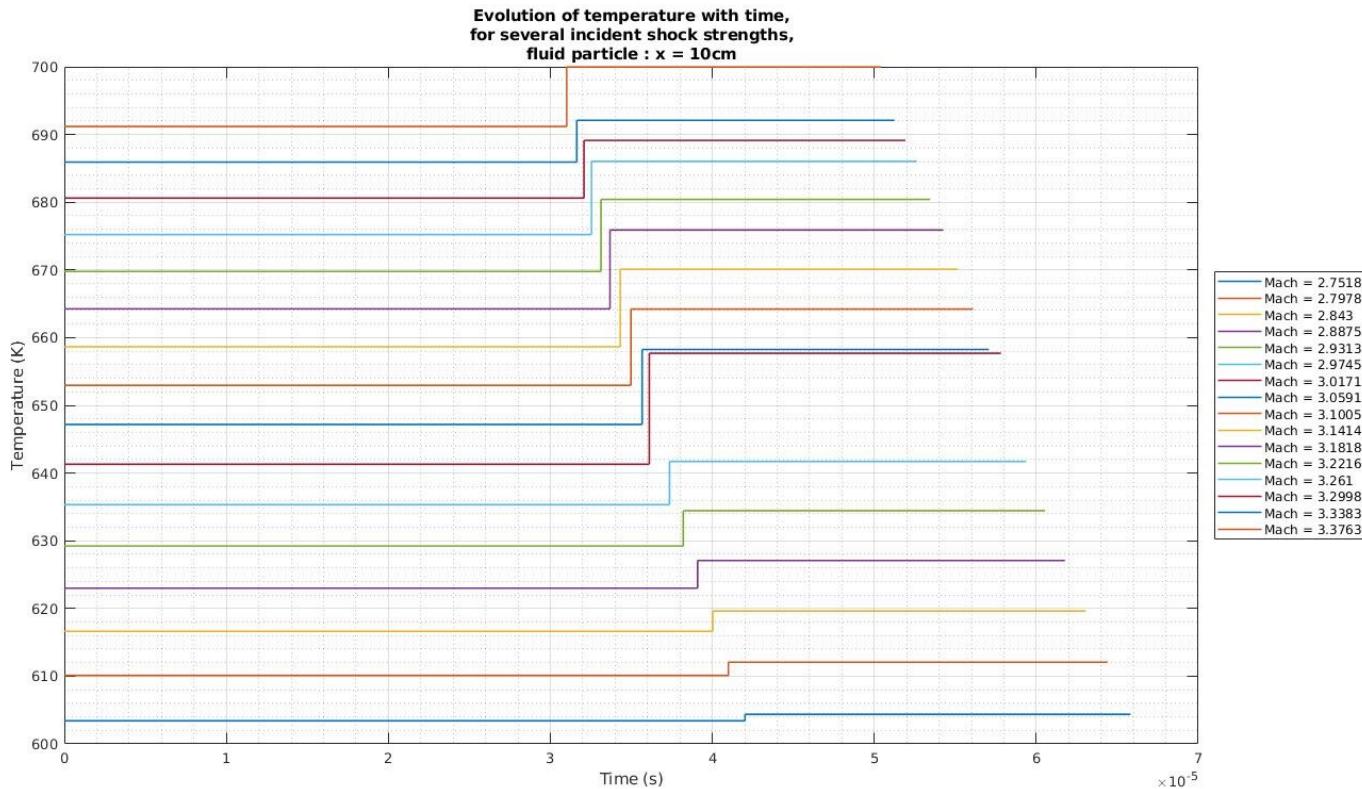
... and on Mach number of the shock



For a single particle, increasing  $M_{sh}$  leads to a rise in temperature and pressure : don't forget that  $H_2 - O_2$  is a reactive phase. Is an ignition possible under certain conditions?

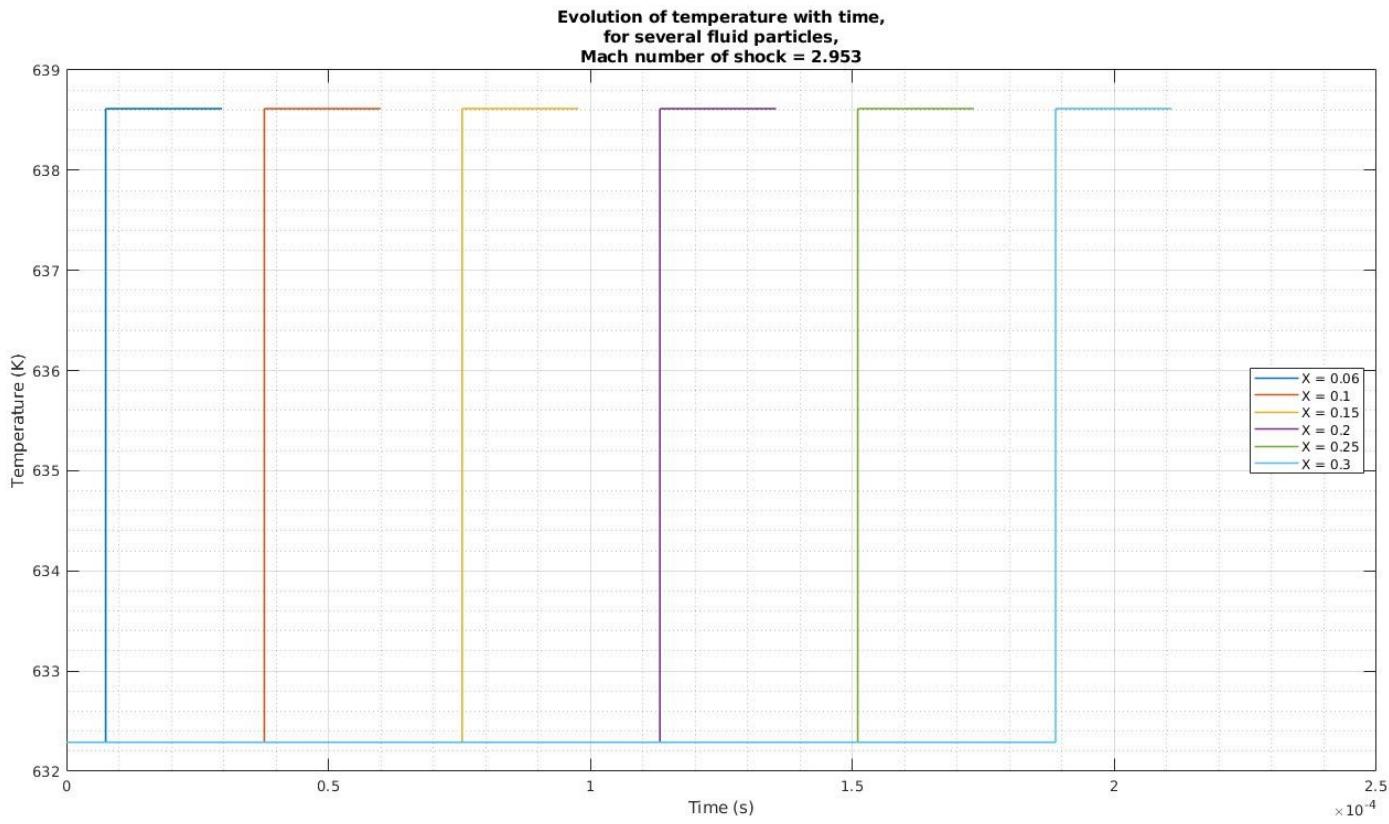
# RRR - Results of the chemical calculus

Ignition doesn't occur for such low Mach numbers



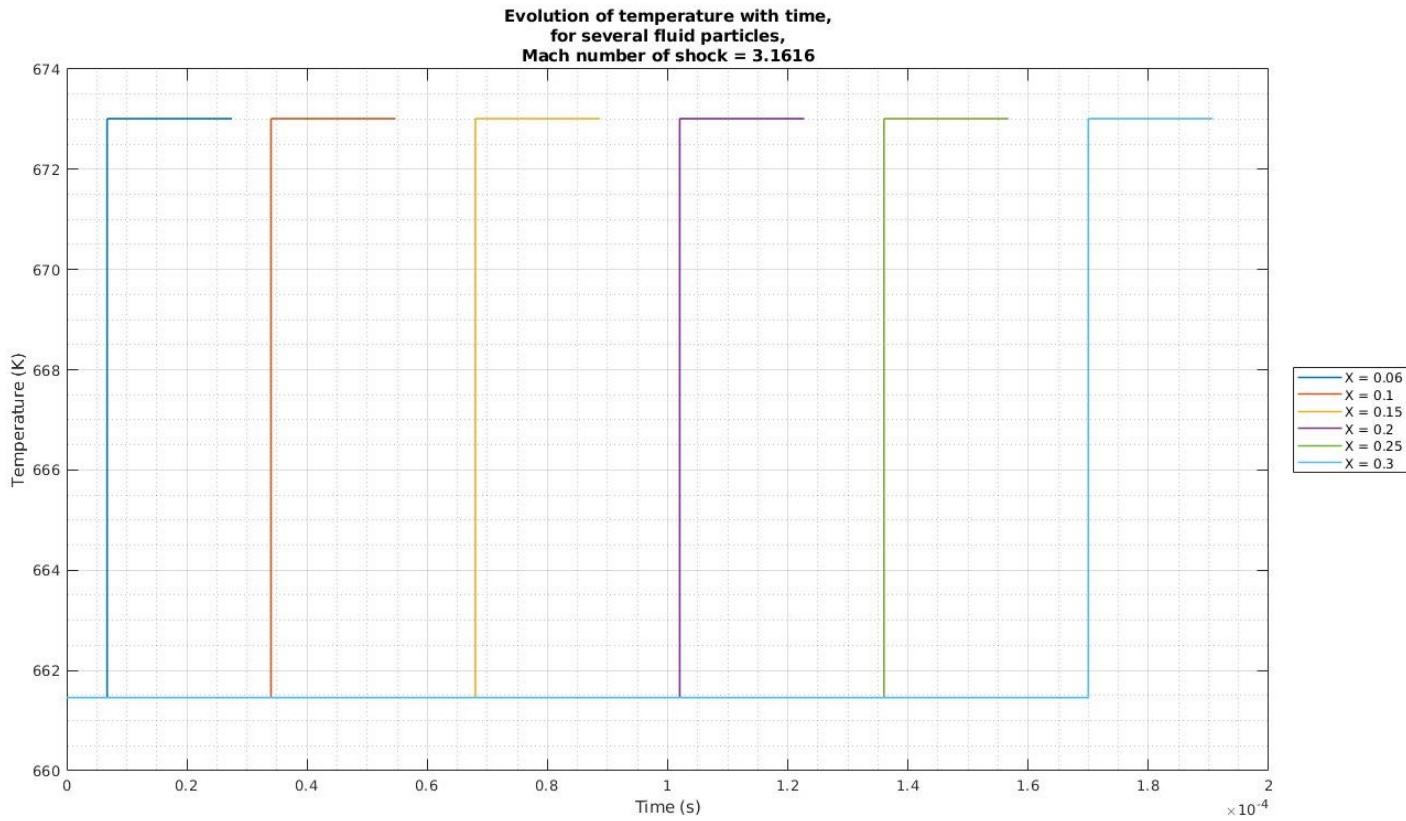
# RRR - Results of the chemical calculus

Ignition doesn't occur for such low Mach numbers



# RRR - Results of the chemical calculus

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