

Lagrangian particles evolution through RRE, RRR and BPR refraction structures

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Outline

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- 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
- 4 Transition between structures : polar diagrams and schemes
- 5 Bound Precursor Refraction and piston theory
 - BPR - Scheme and Notations
 - BPR - Theoretical resolution

Reminder of the different refraction structures

From Henderson 1976 and 1978

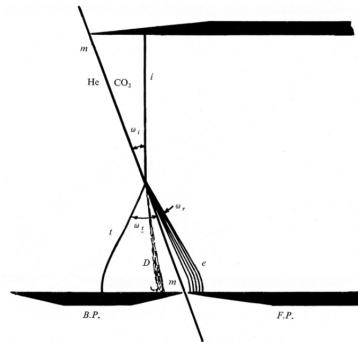
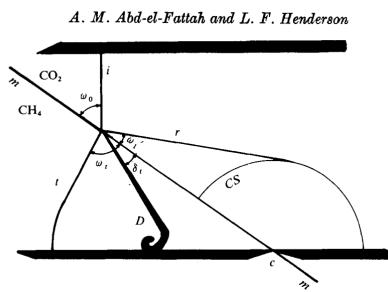


FIGURE 9. Regular refraction of a plane shock at a contaminated carbon dioxide-helium interface. For symbols see caption to figure 3.

(a) RRE struture



(b) RRR struture

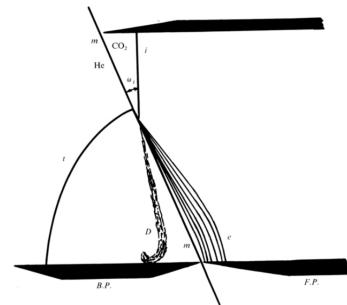


FIGURE 13. Bound-precursor irregular refraction of a plane shock at a contaminated carbon dioxide-helium interface. For symbols see captions to figures 3 and 10.

(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

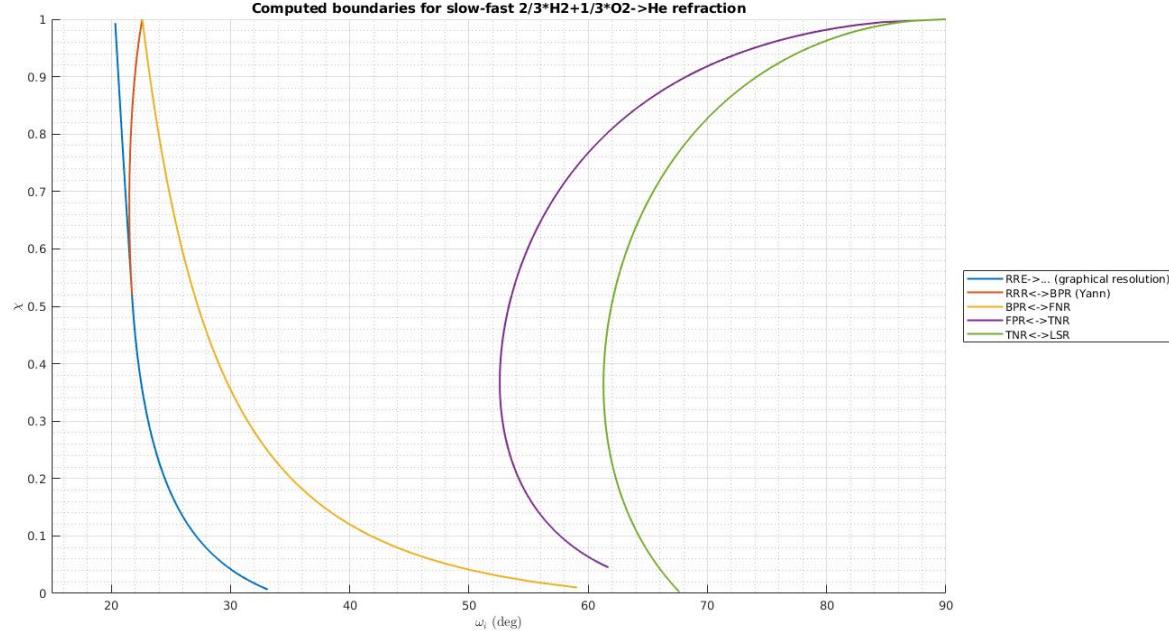


Figure 2: Boundaries of the different structures in the $\chi - \omega$ plane, for a $H_2 - O_2 // He$ system

Strength of the shock χ is related to Mach number of the shock M_{sh} .

Regular Refraction with reflected Expansion (RRE)

Relation between strength χ and Mach number M_{sh}

$$\chi = 1/\xi_i$$

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

where γ_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 :

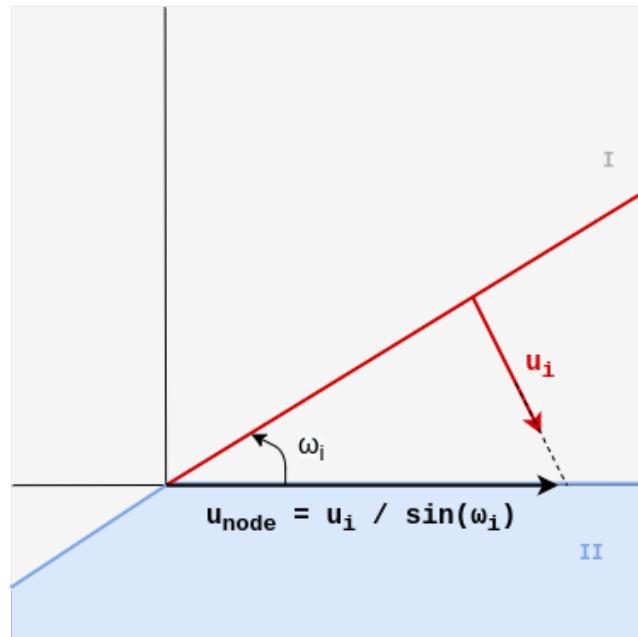
$$M_{sh} = \frac{M_1}{\sin(\omega_i)}$$

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

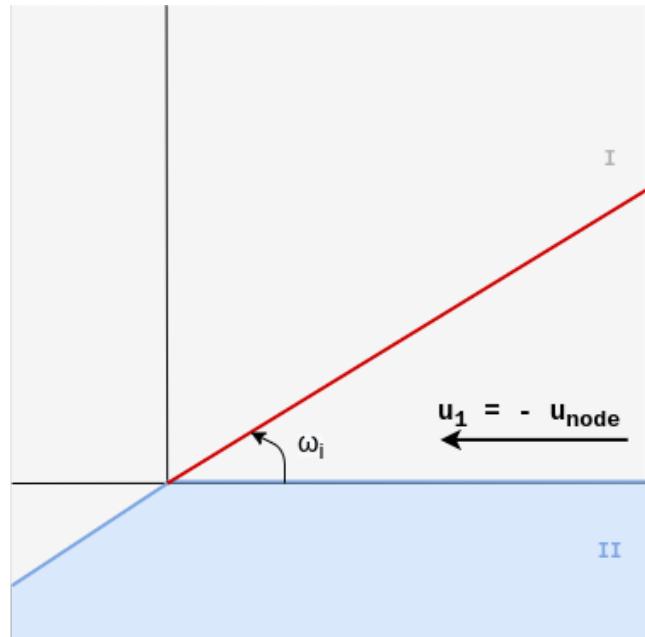
$$\chi \in [0.01; 1] \iff M_{sh} \in [1; 2.95] \iff M_1 \in [4; 11.78] \quad (1)$$

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

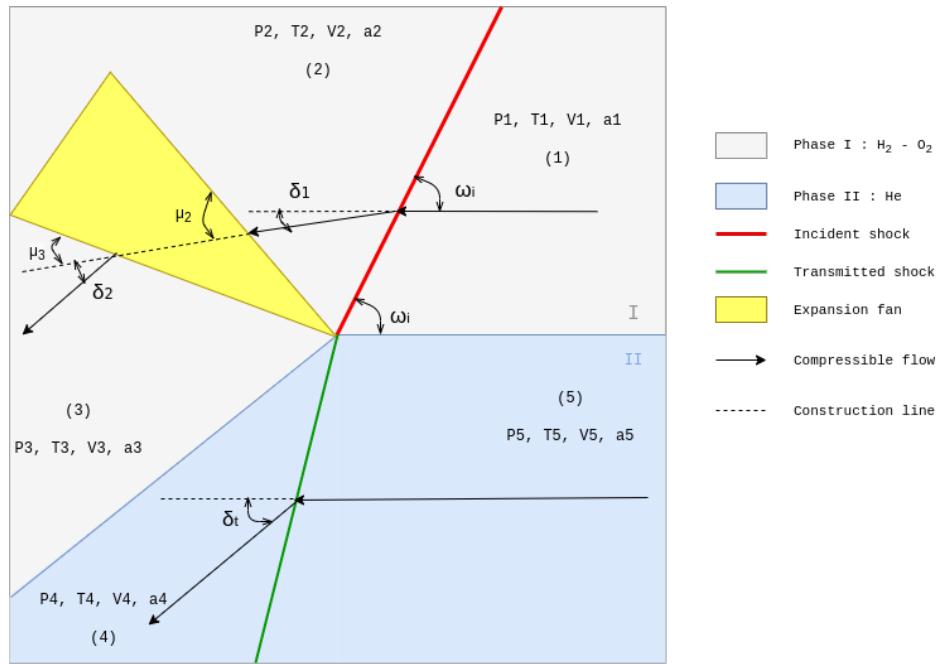


Figure 4: Symbols, zones and angles for computation

RRE - Theory and equations : gas dynamics

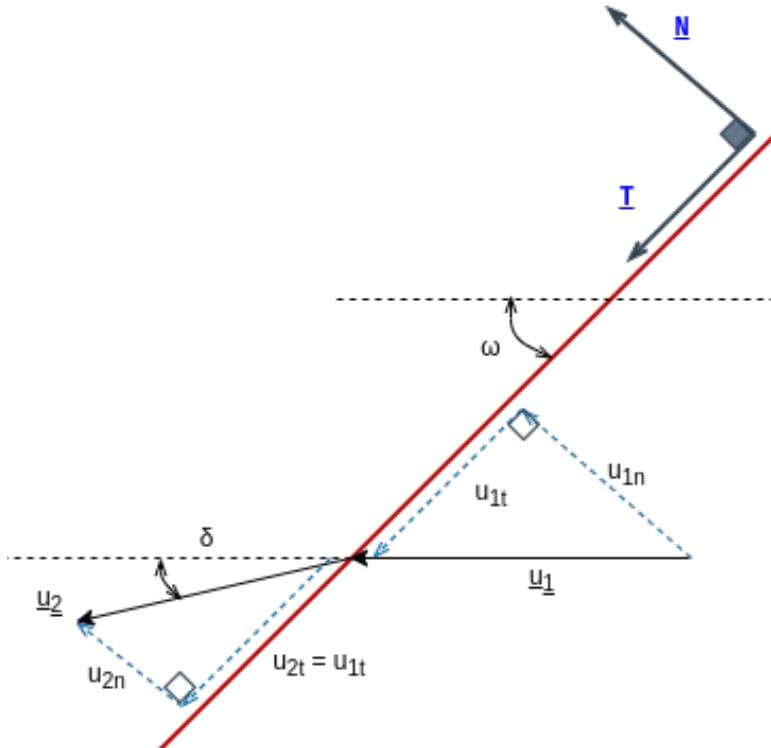
Initial conditions in zone (1)

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)	ω_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



$$\begin{aligned} M1_n &= \frac{u_{1n}}{a_1} \\ &= \frac{u_1 \sin(\omega_i)}{a_1} \\ &= M1 \sin(\omega_i) \end{aligned}$$

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

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 δ_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

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

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

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

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

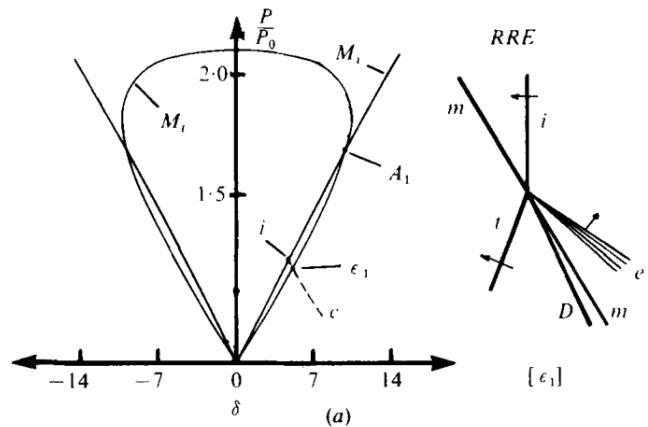
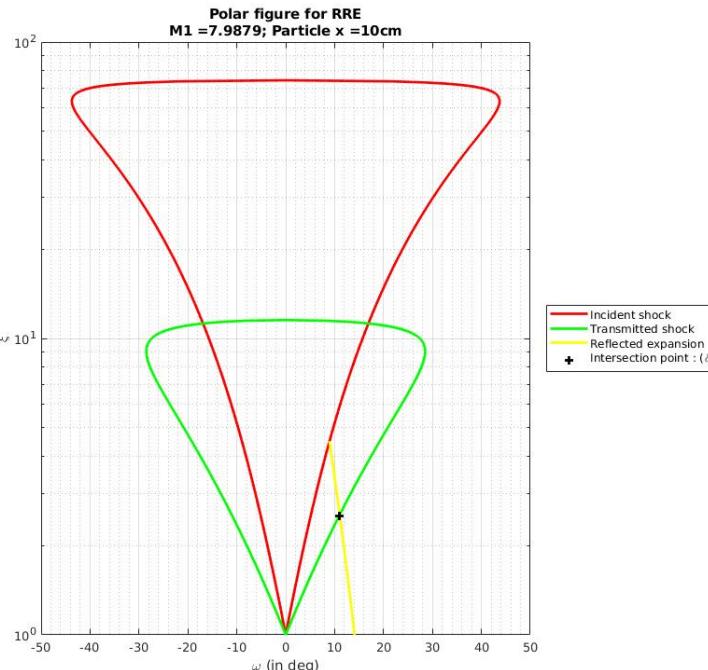
$$M4 = \frac{M4_n}{\sin(\omega_t - \delta_t)}$$

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

where δ_t is the angle of deflection behind the transmitted shock.
Unfortunately, ω_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, δ_t and ξ_t can be determined (intersection of expansion and transmitted shock polar). $P4$ thus $P3$ are known and so $M3$ thanks to Prandtl-Meyer relations. ν is the Prandtl-Meyer function, depending on the heat ratio of the gas at stake.

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

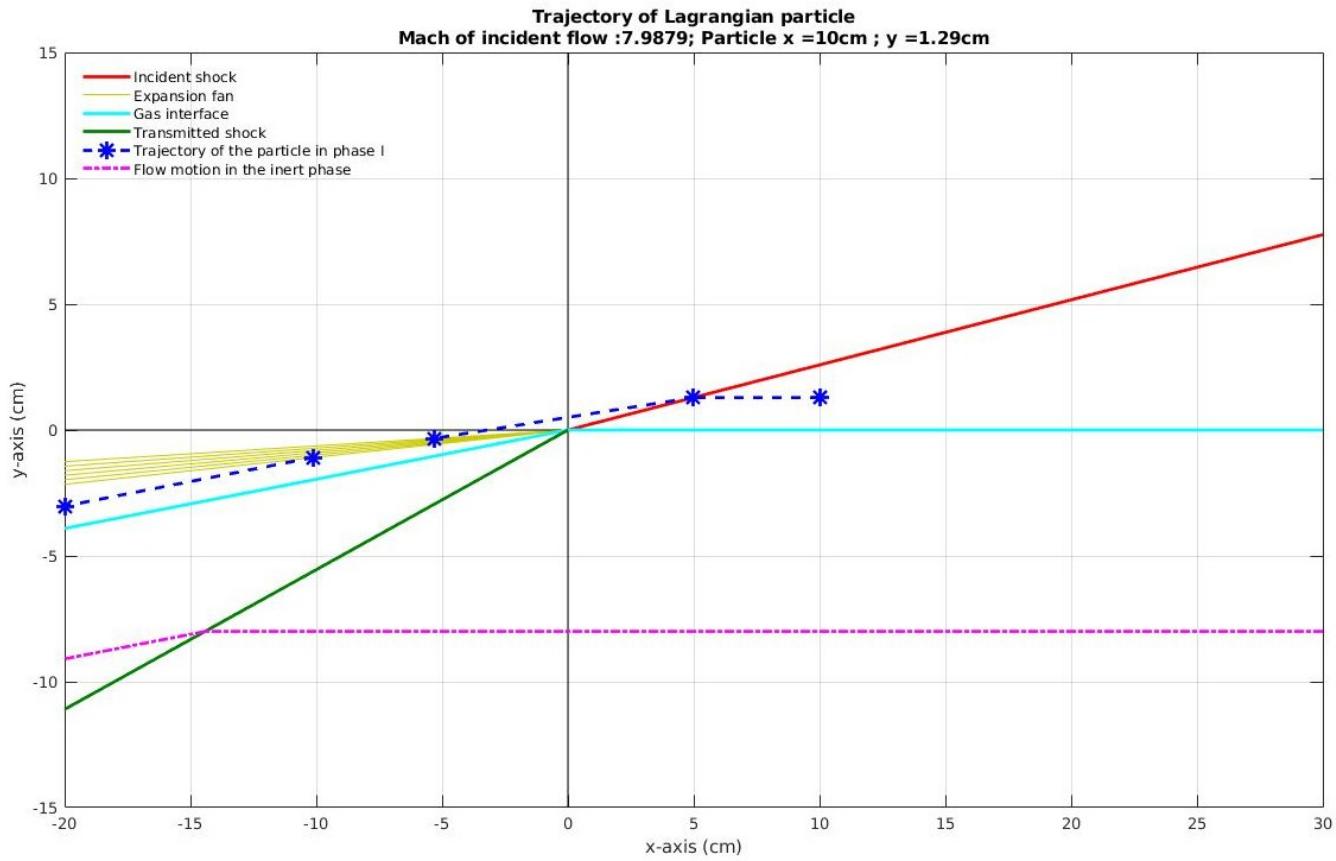
$$P3 = P4 = P5 \times \xi_t$$

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

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

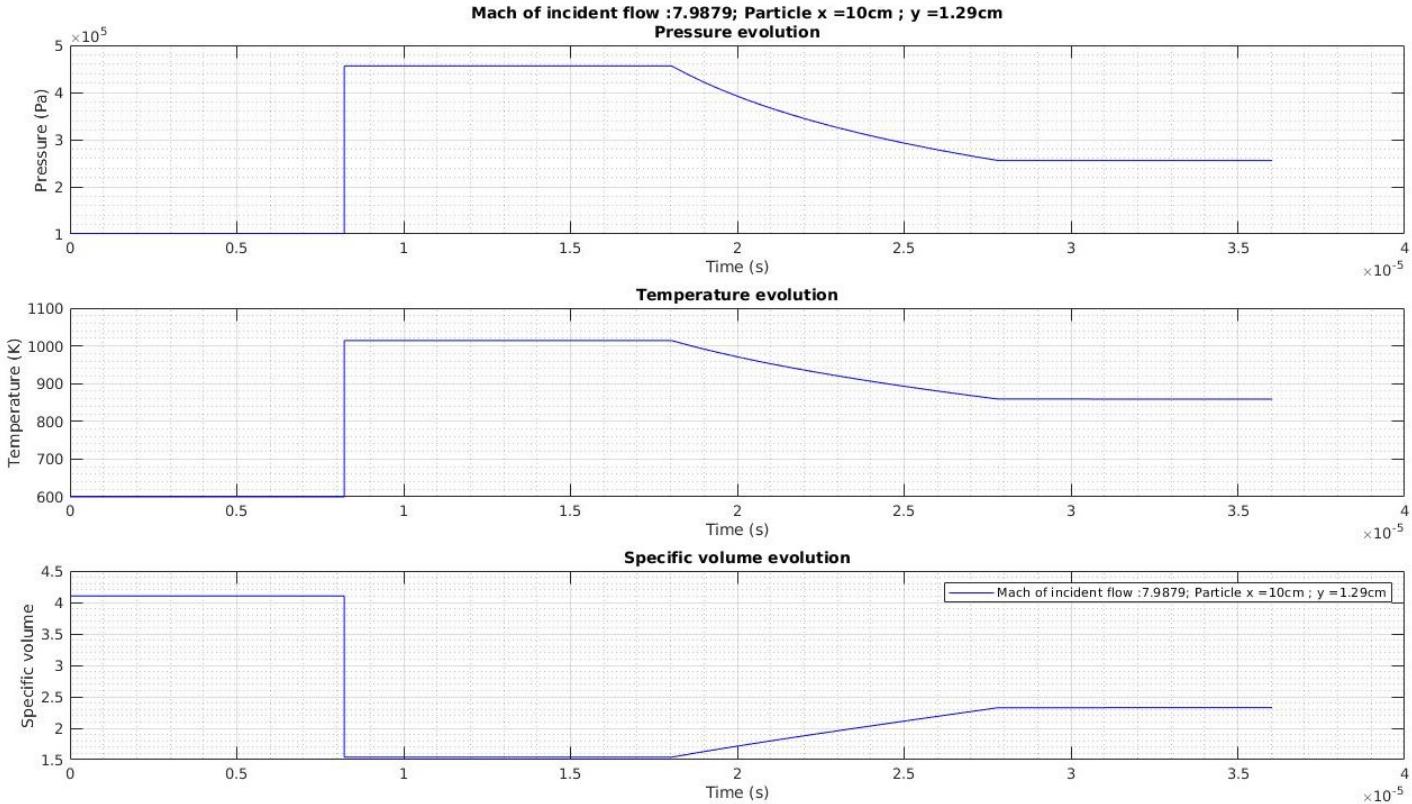
RRE - Results given by the inert gas dynamics theory

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



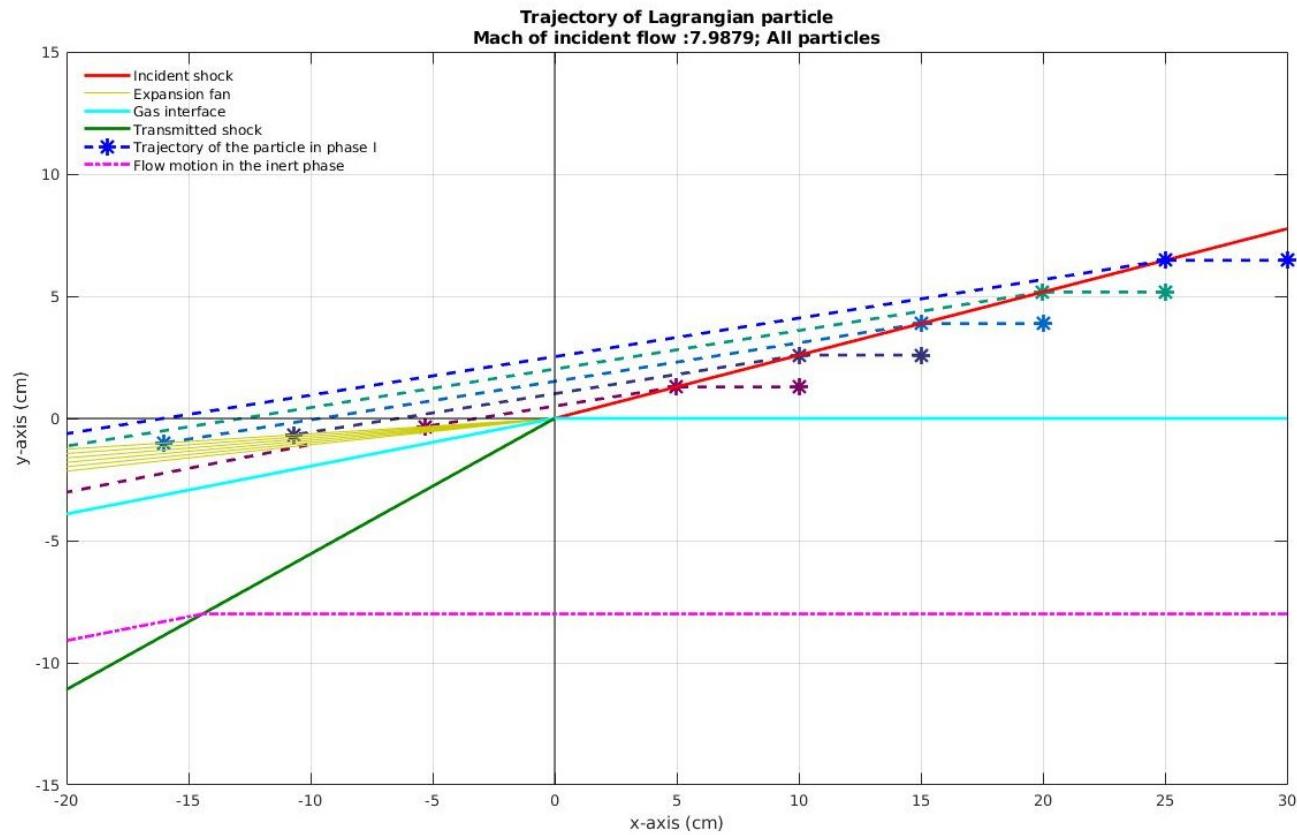
RRE - Results given by the inert gas dynamics theory

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



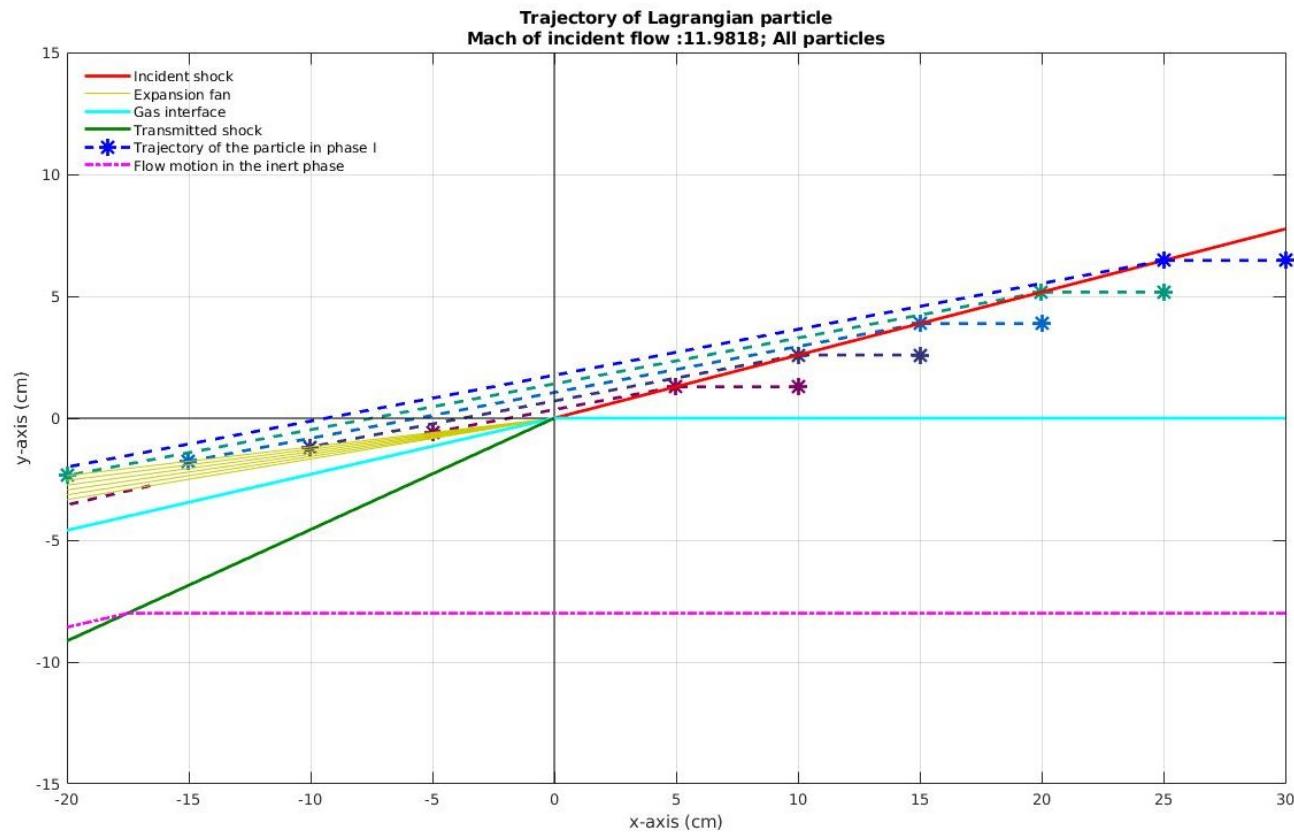
RRE - Results given by the inert gas dynamics theory

Evolution depends on position of the particle...



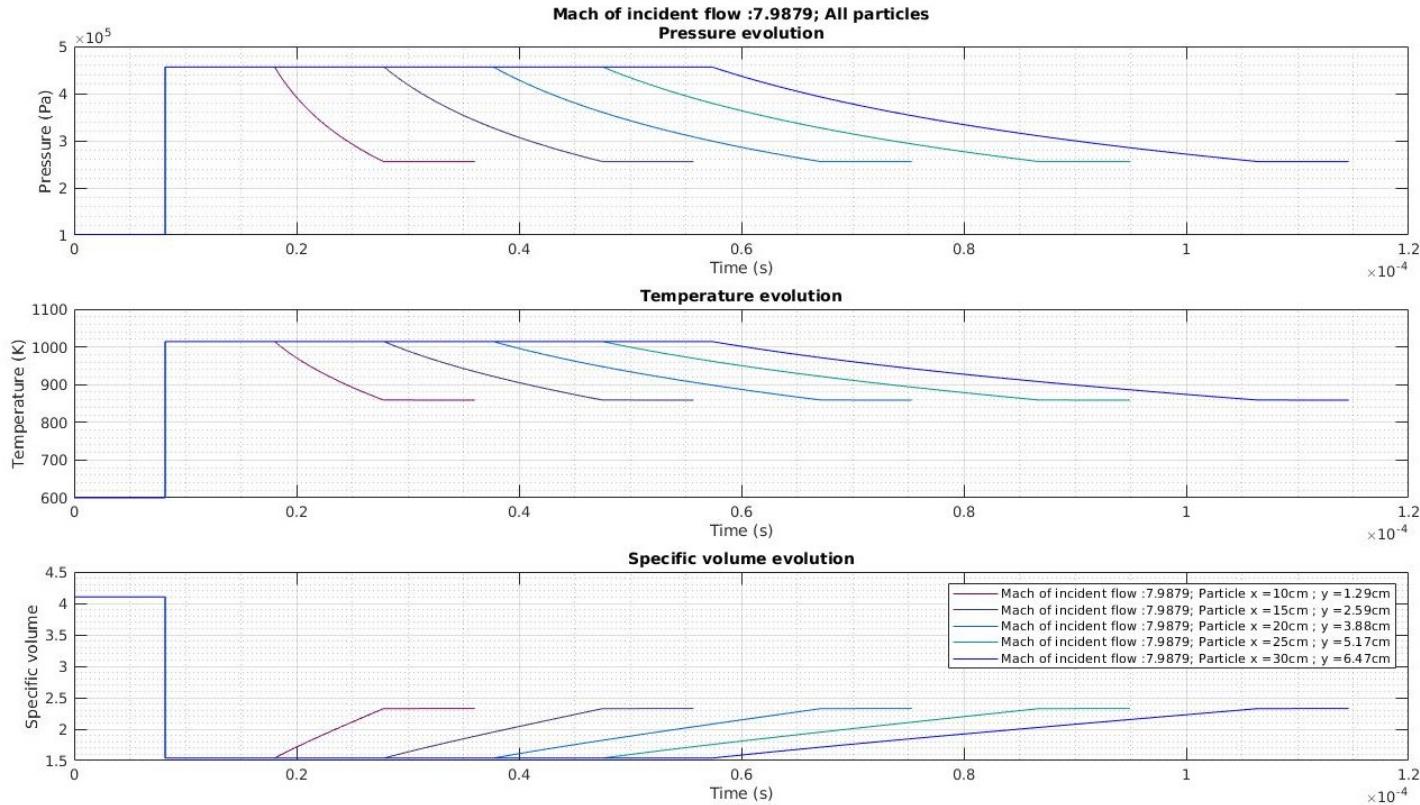
RRE - Results given by the inert gas dynamics theory

Evolution depends on position of the particle...



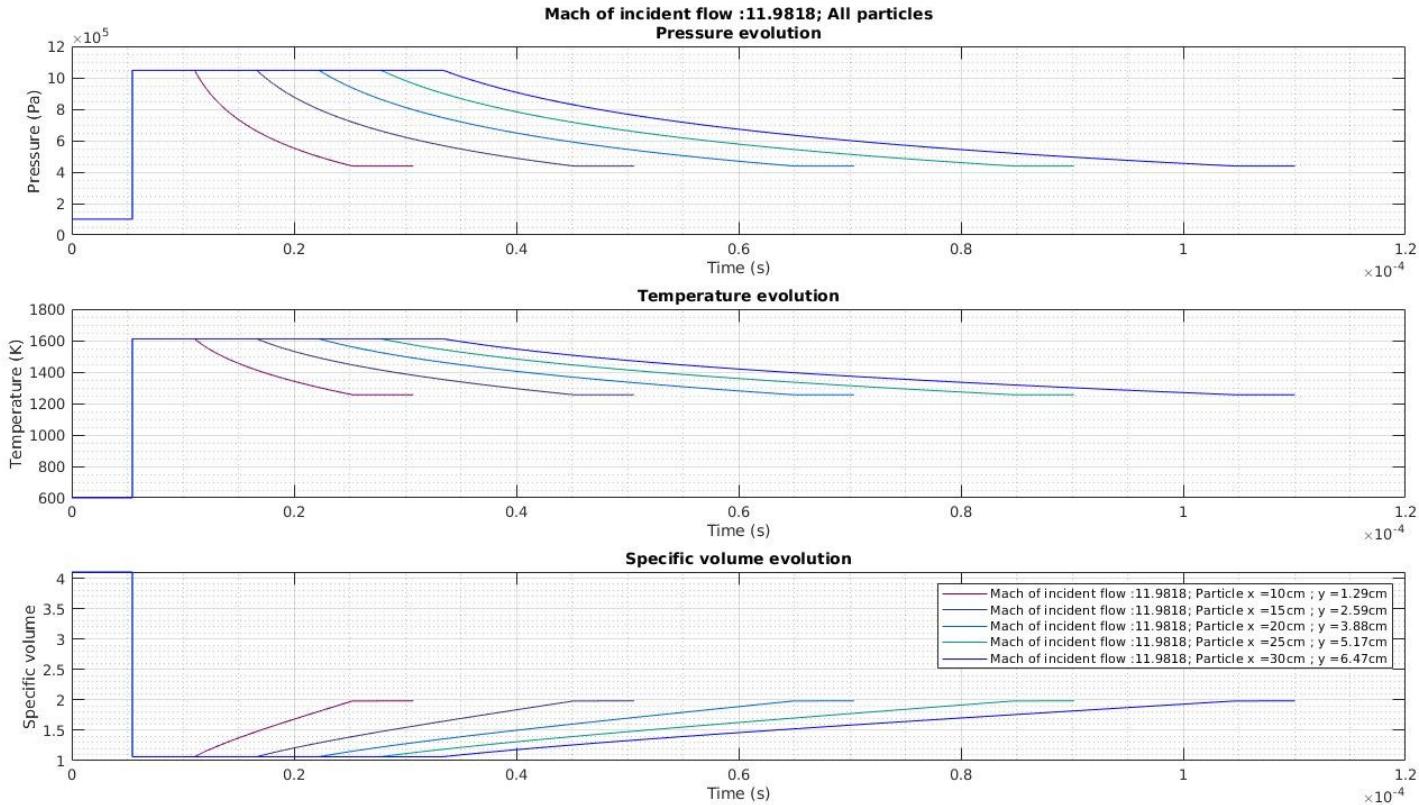
RRE - Results given by the inert gas dynamics theory

Evolution depends on position of the particle...

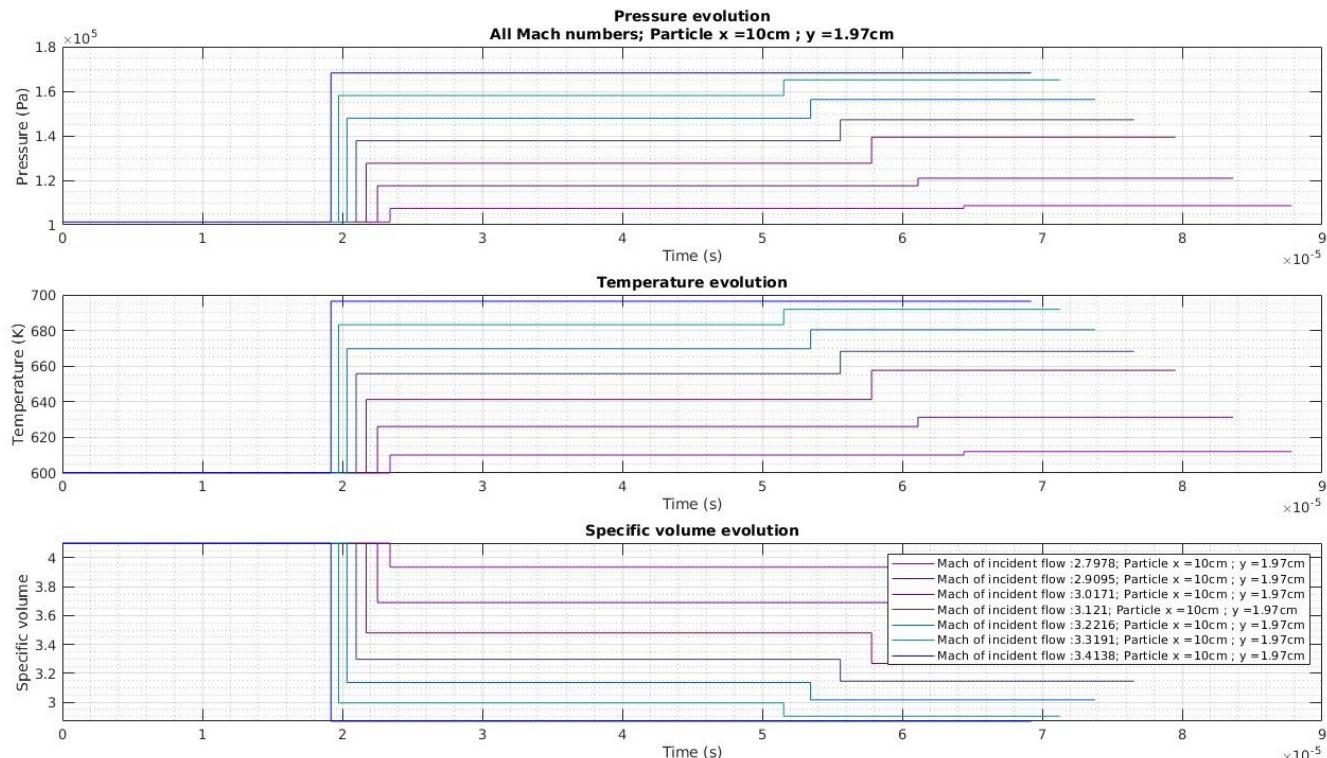


RRE - Results given by the inert gas dynamics theory

Evolution depends on position of the particle...



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



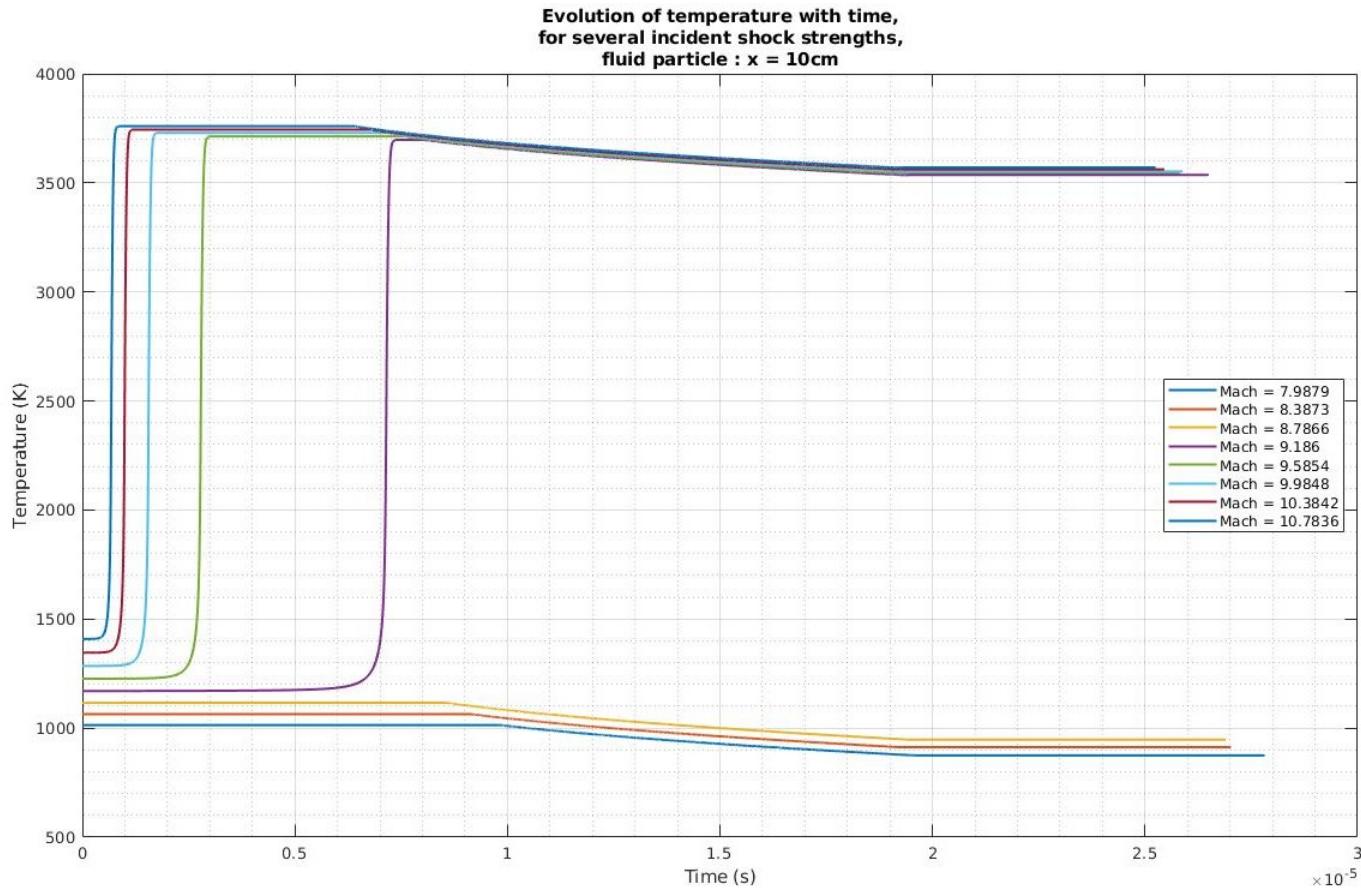
For a single particle, increasing M_{sh} leads to a rise in temperature and pressure : don't forget that $H_2 - O_2$ is a reactive phase. Is an ignition possible under certain conditions?

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

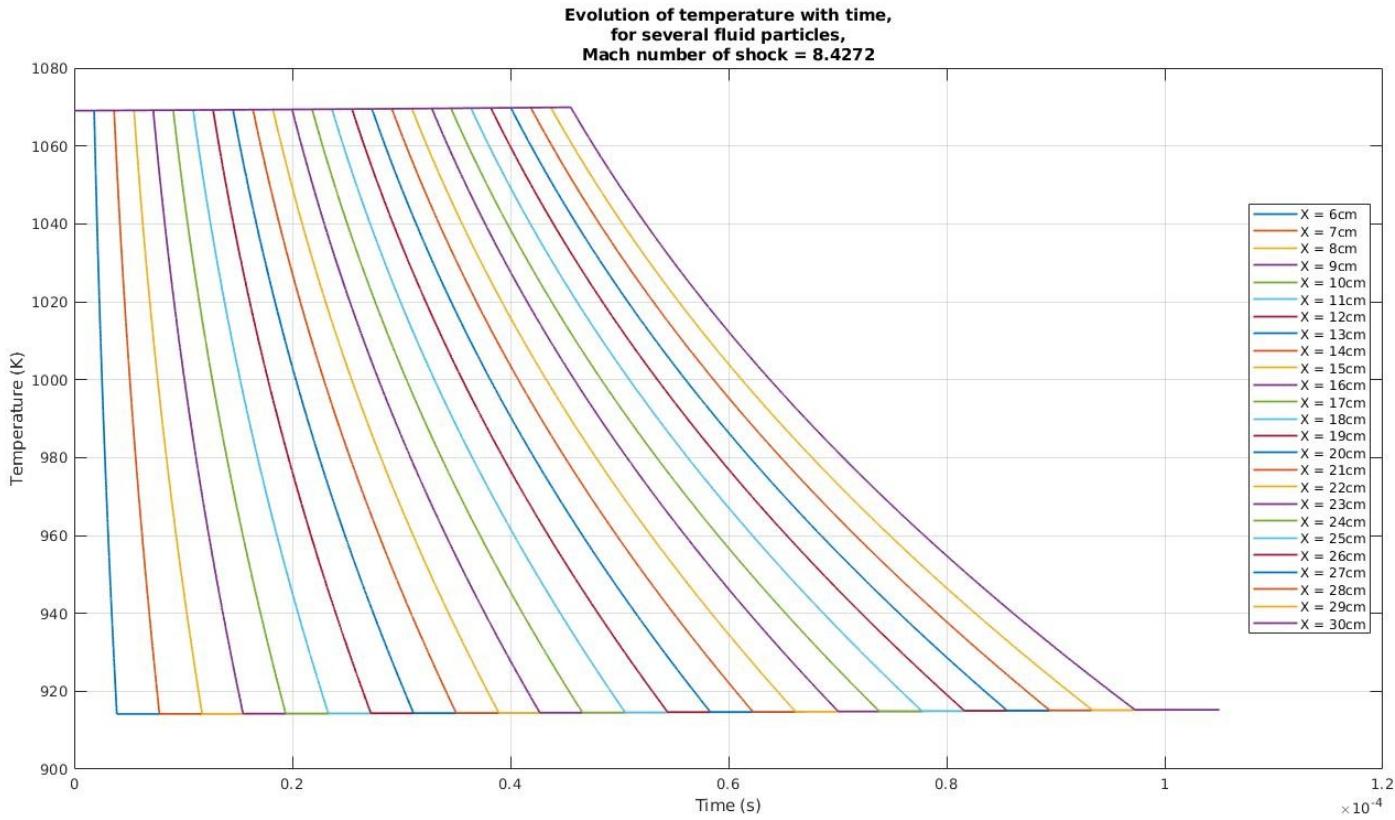
RRE - Results of the chemical calculus

Existence of a threshold : Mach number of ignition



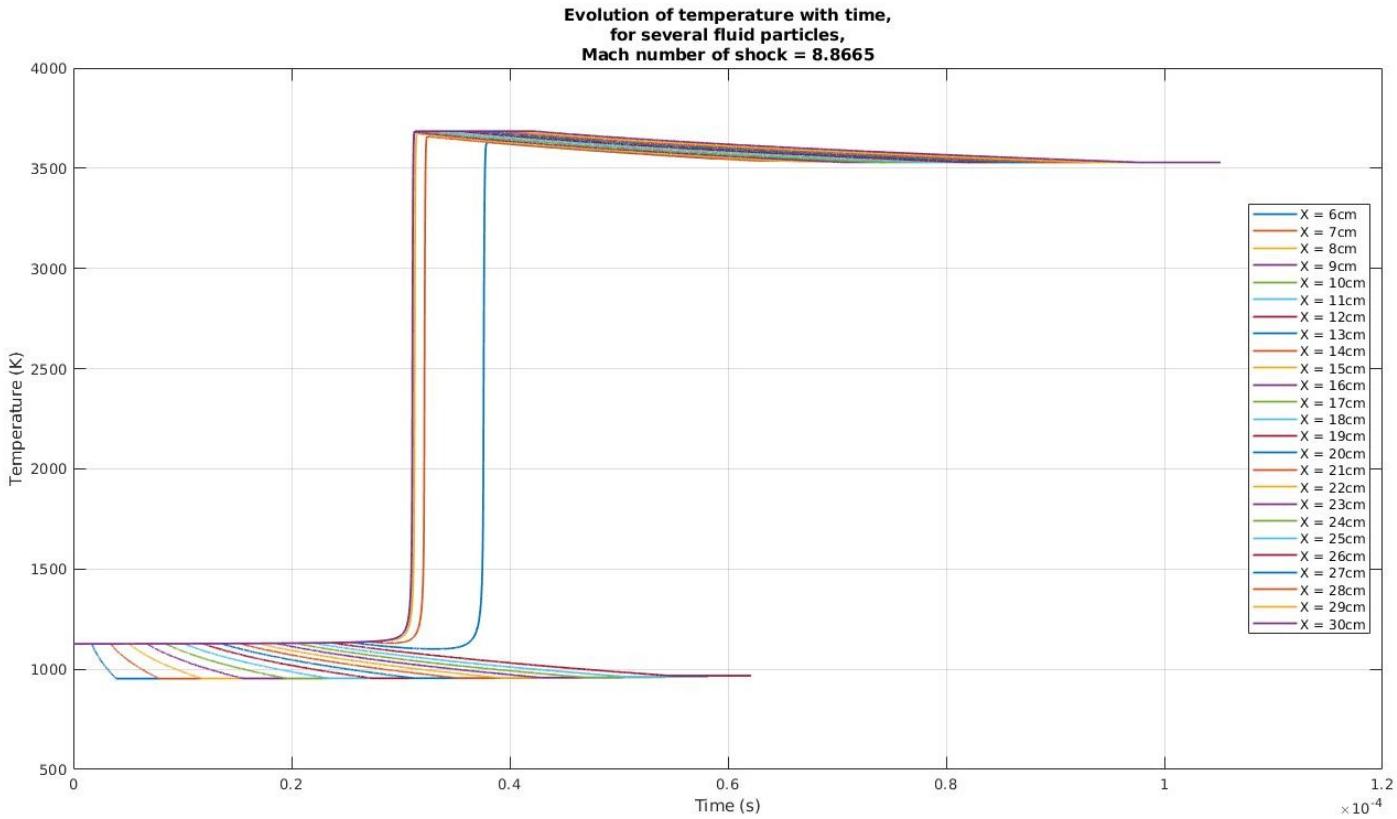
RRE - Results of the chemical calculus

Each particle has its own M_{ignit}



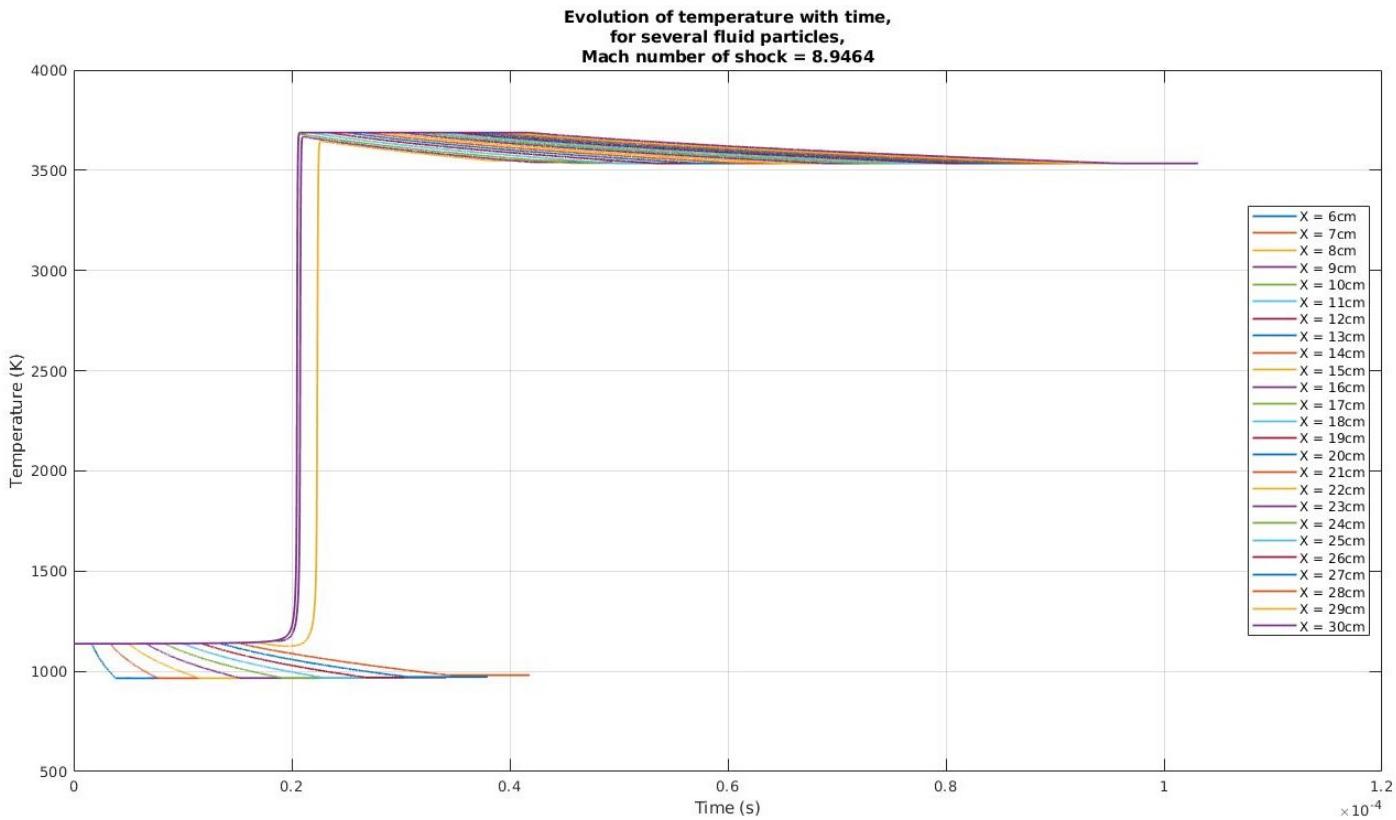
RRE - Results of the chemical calculus

Each particle has its own M_{ignit}



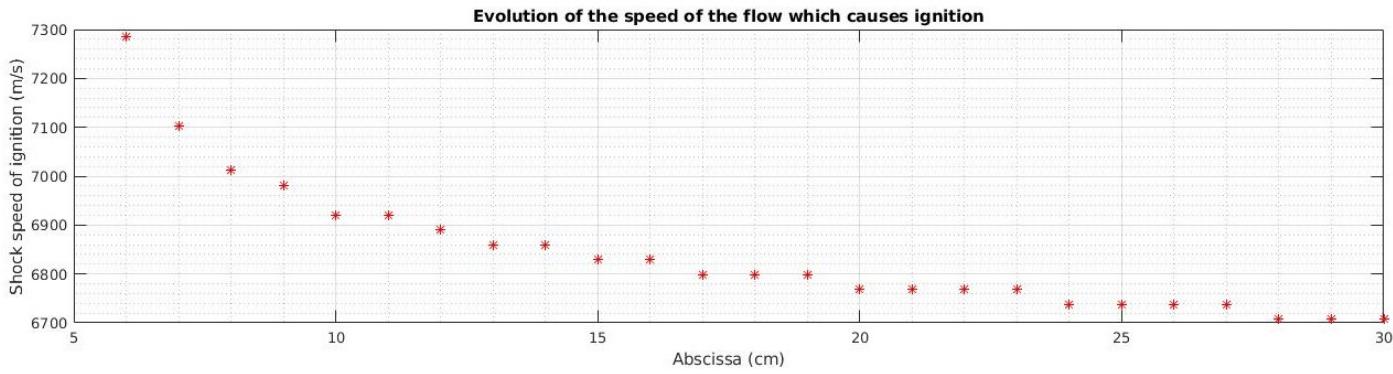
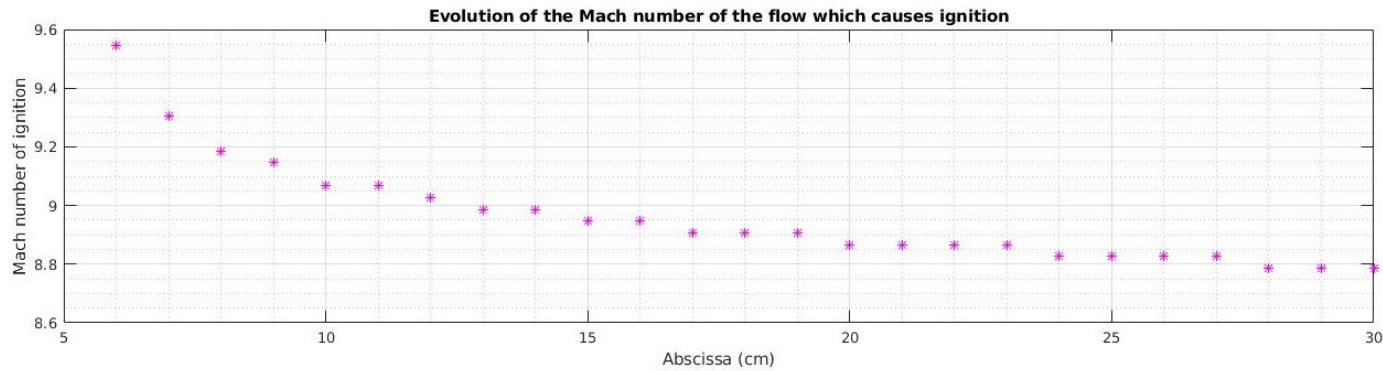
RRE - Results of the chemical calculus

Each particle has its own M_{ignit}



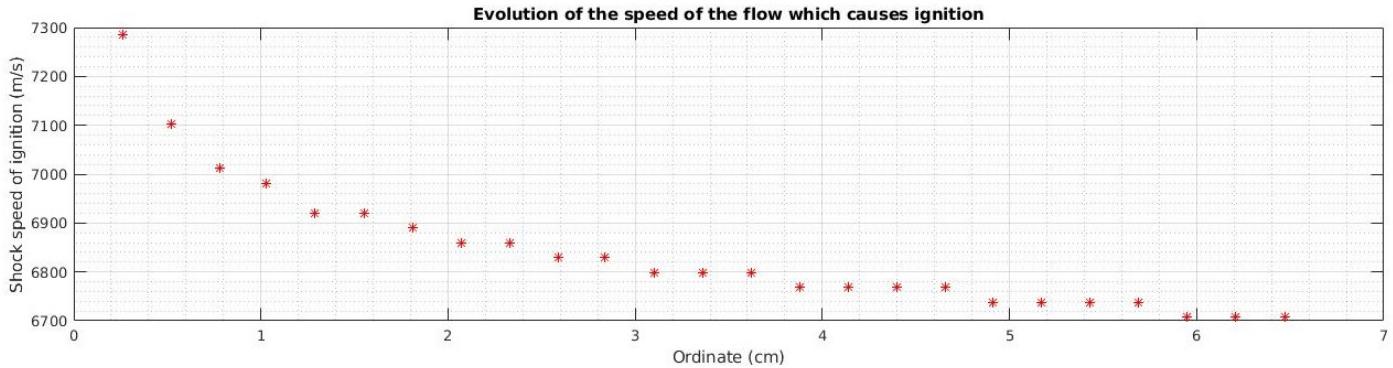
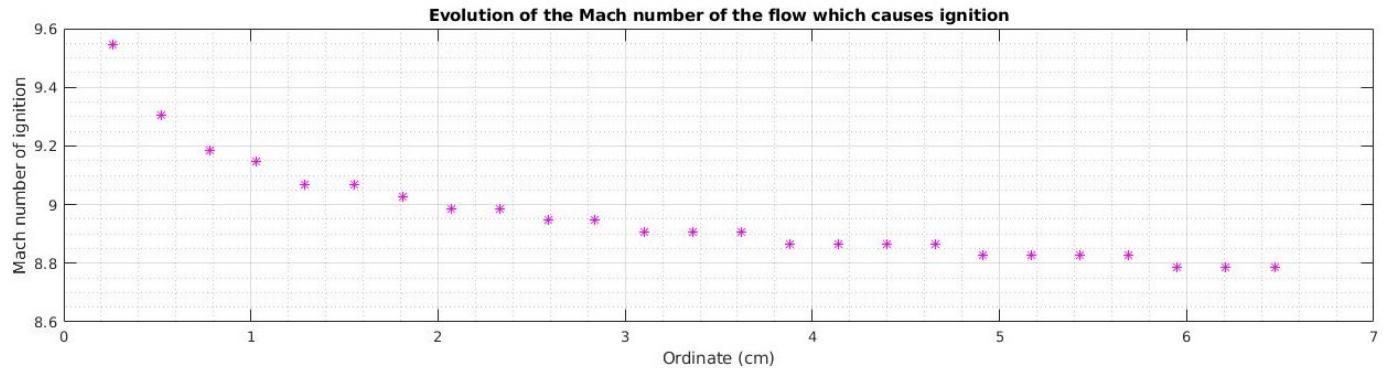
RRE - Results of the chemical calculus

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 χ 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

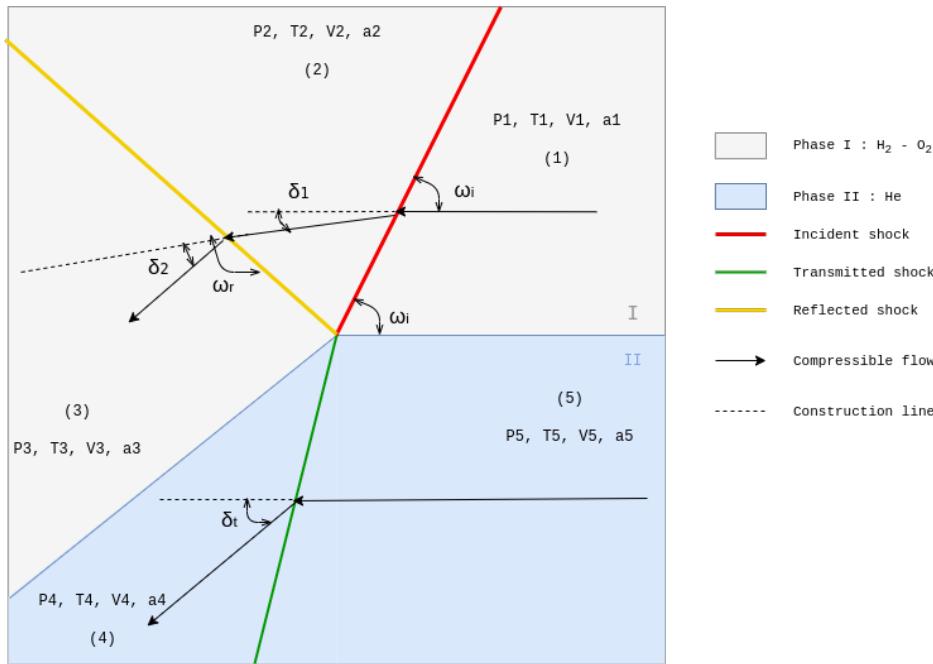


Figure 7: Symbols, zones and angles for computation

RRR - Theory and equations : gas dynamics

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

See slides 9, 10 and 11 : definitions and computations keep exactly the same.

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 δ_t is the angle of deflection behind the transmitted shock.
Unfortunately, ω_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)

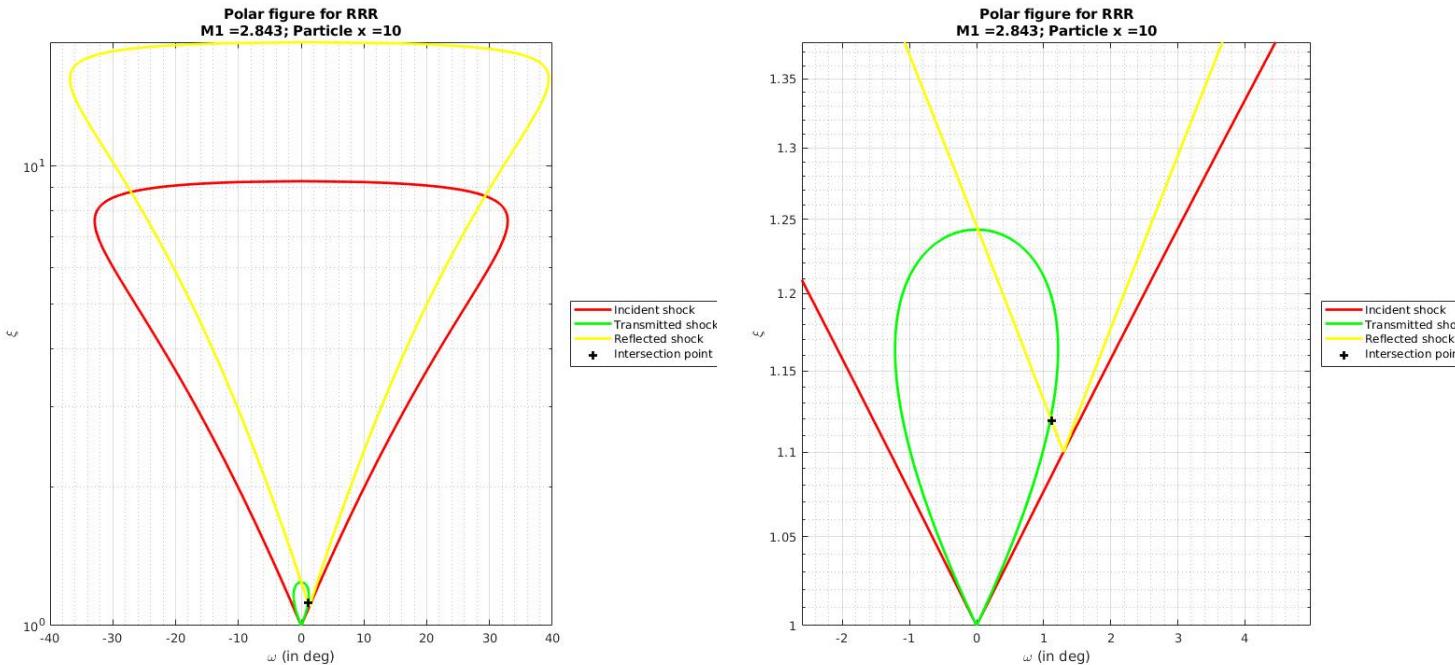
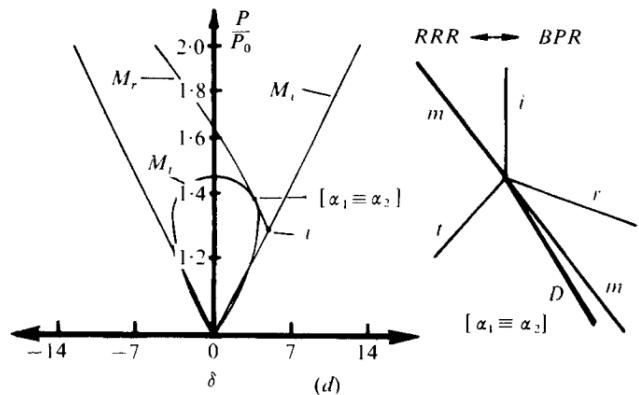
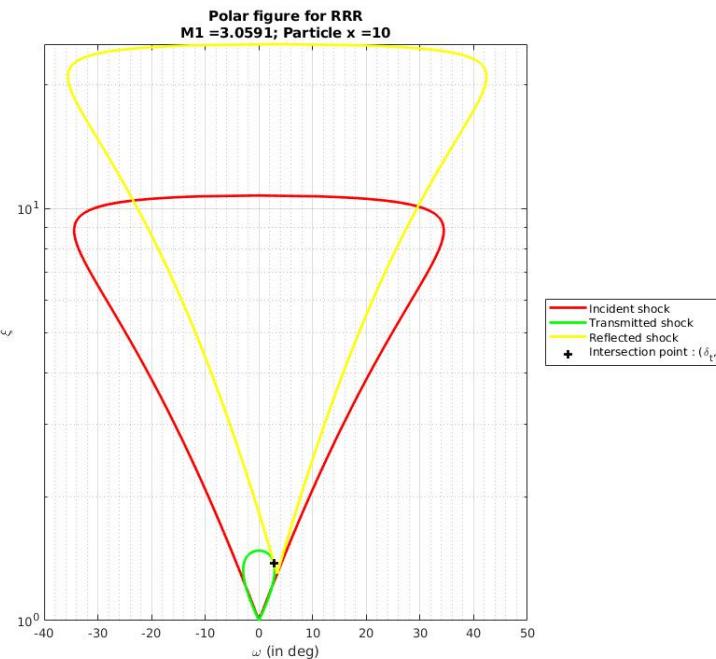


Figure 8: Polars for RRR structure, zoom on the intersection point on the right

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

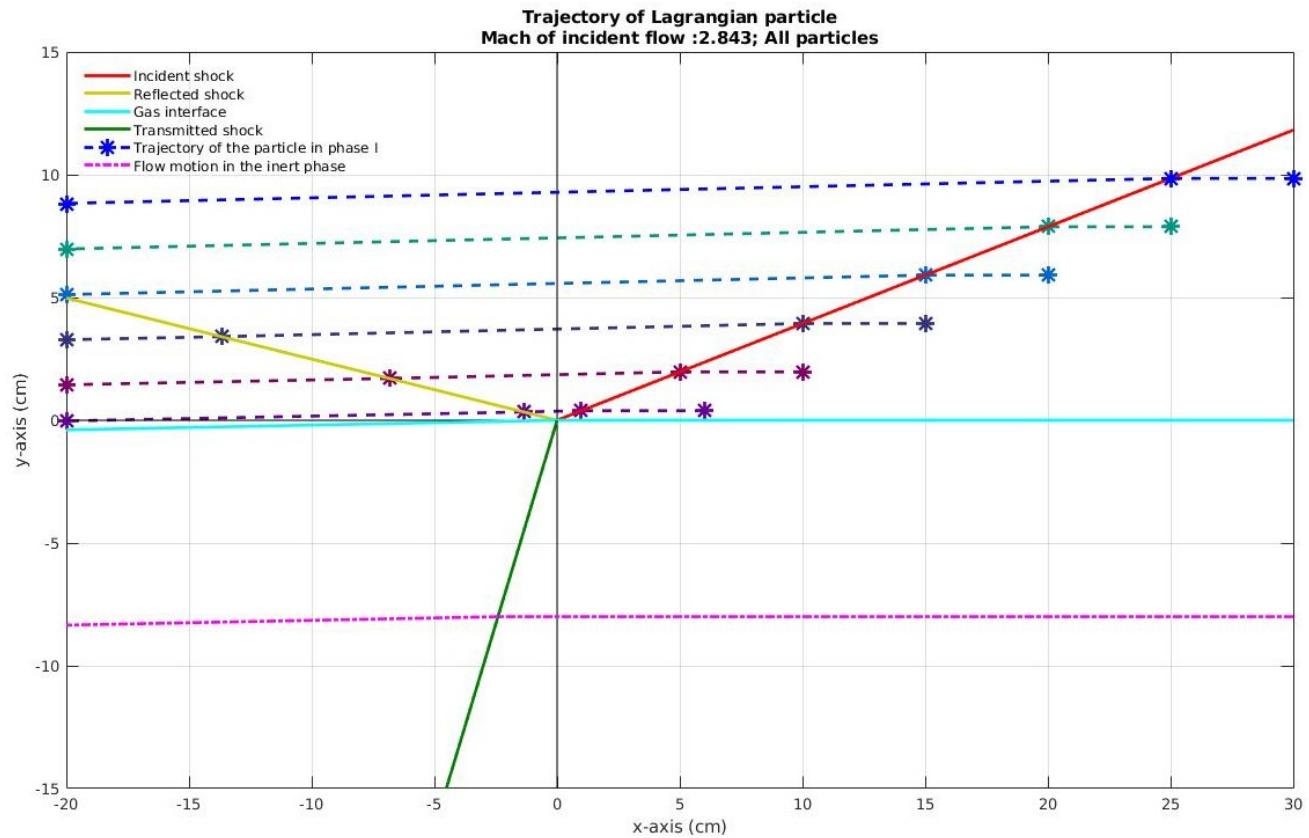
RRR - Theory and equations : gas dynamics

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

Thanks to the polars of the shock, δ_t and ξ_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.

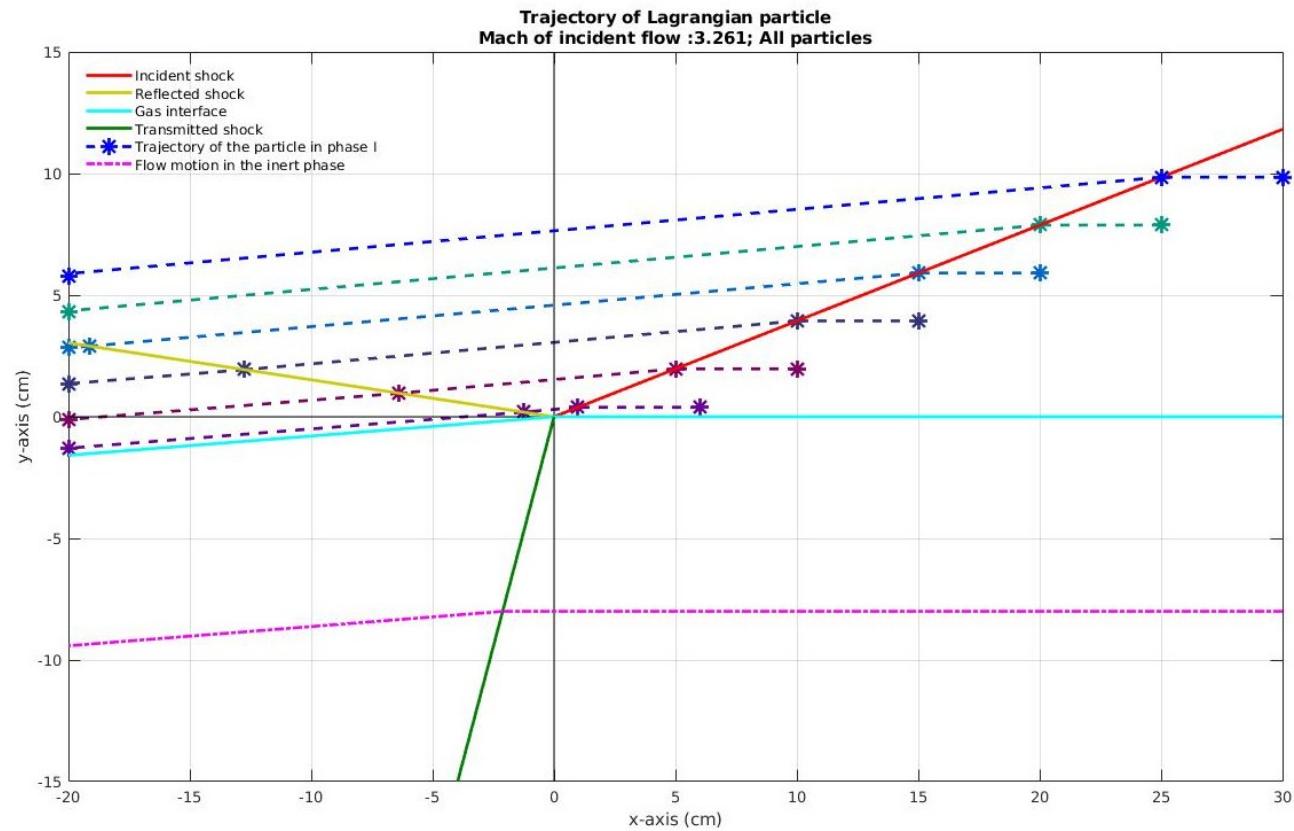
RRR - Results given by the inert gas dynamics theory

Evolution depends on position of the particle...



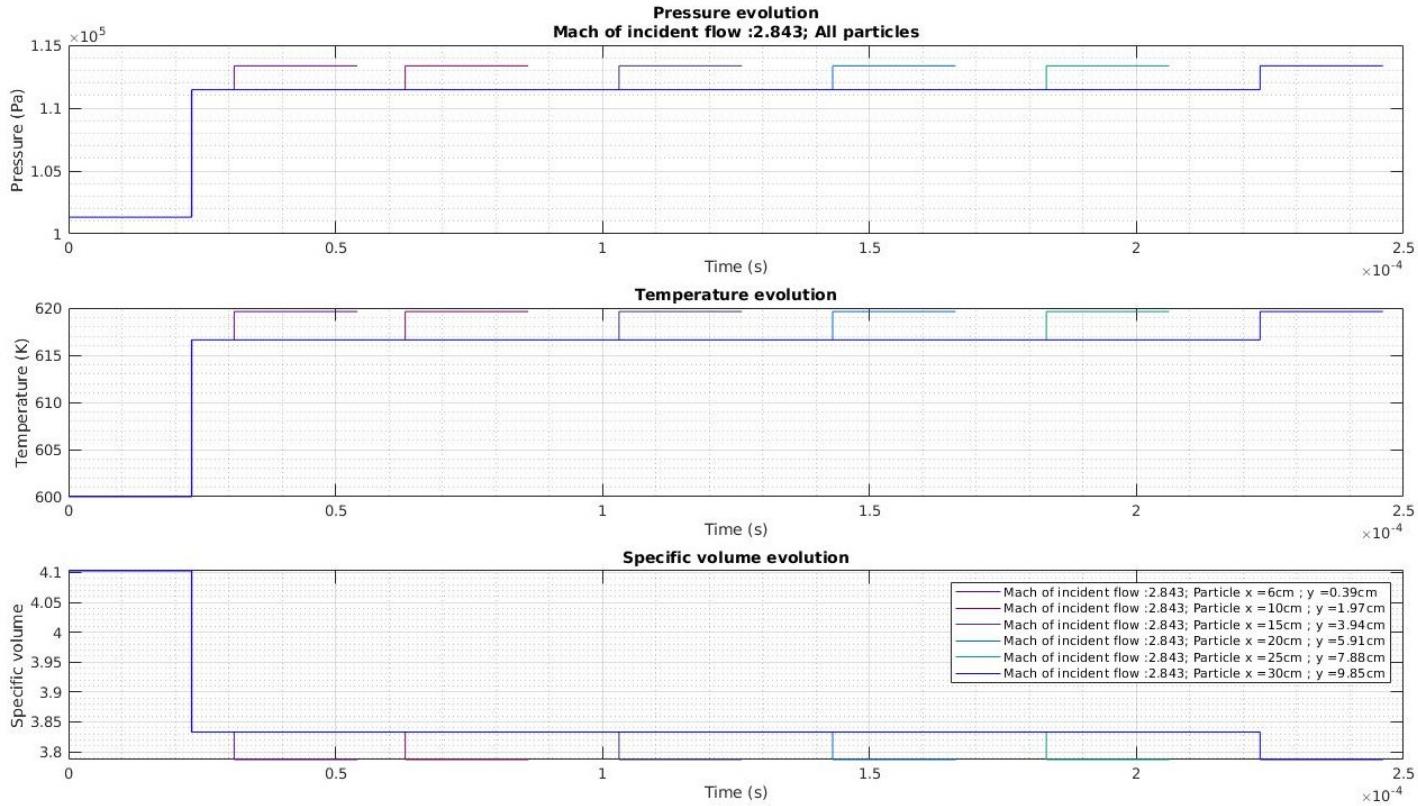
RRR - Results given by the inert gas dynamics theory

Evolution depends on position of the particle...



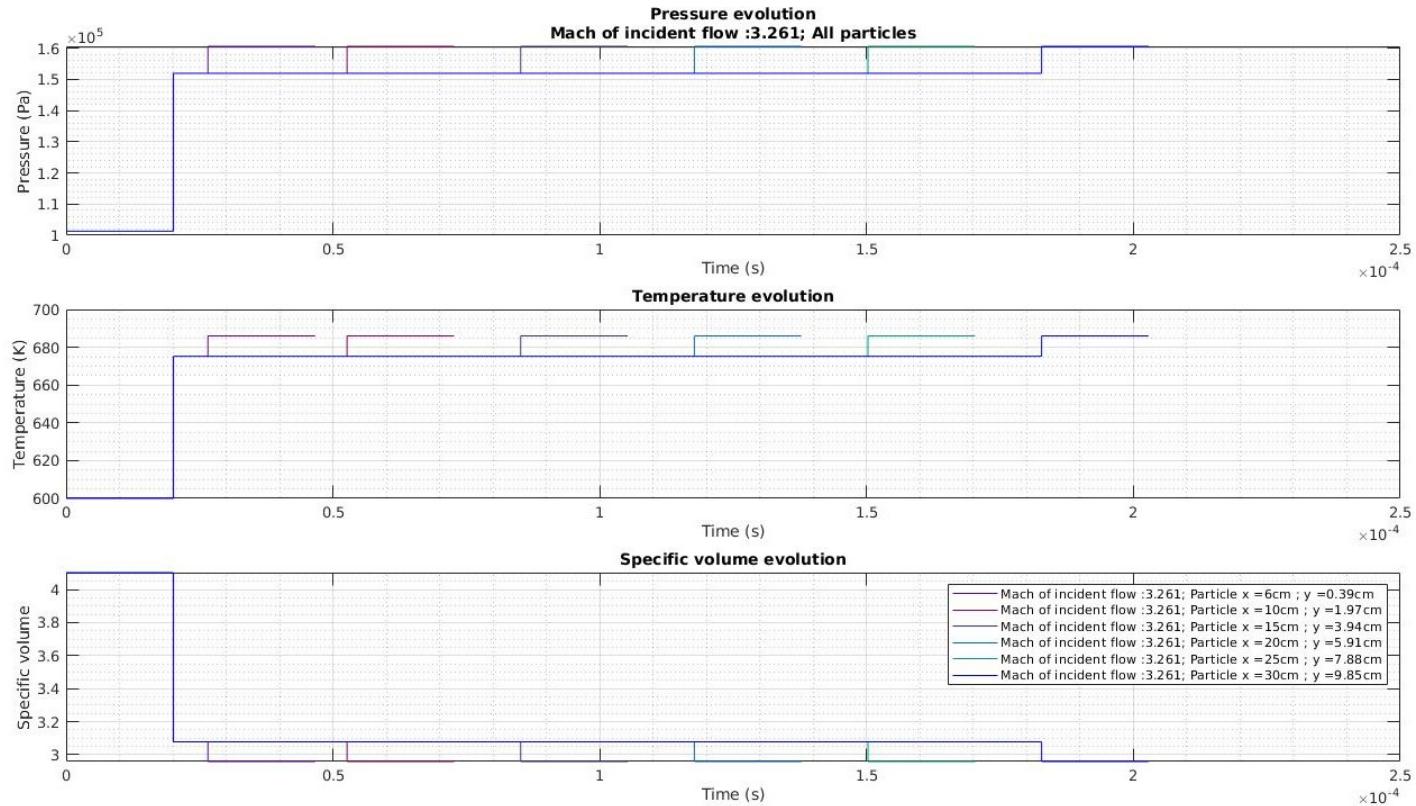
RRR - Results given by the inert gas dynamics theory

Evolution depends on position of the particle...



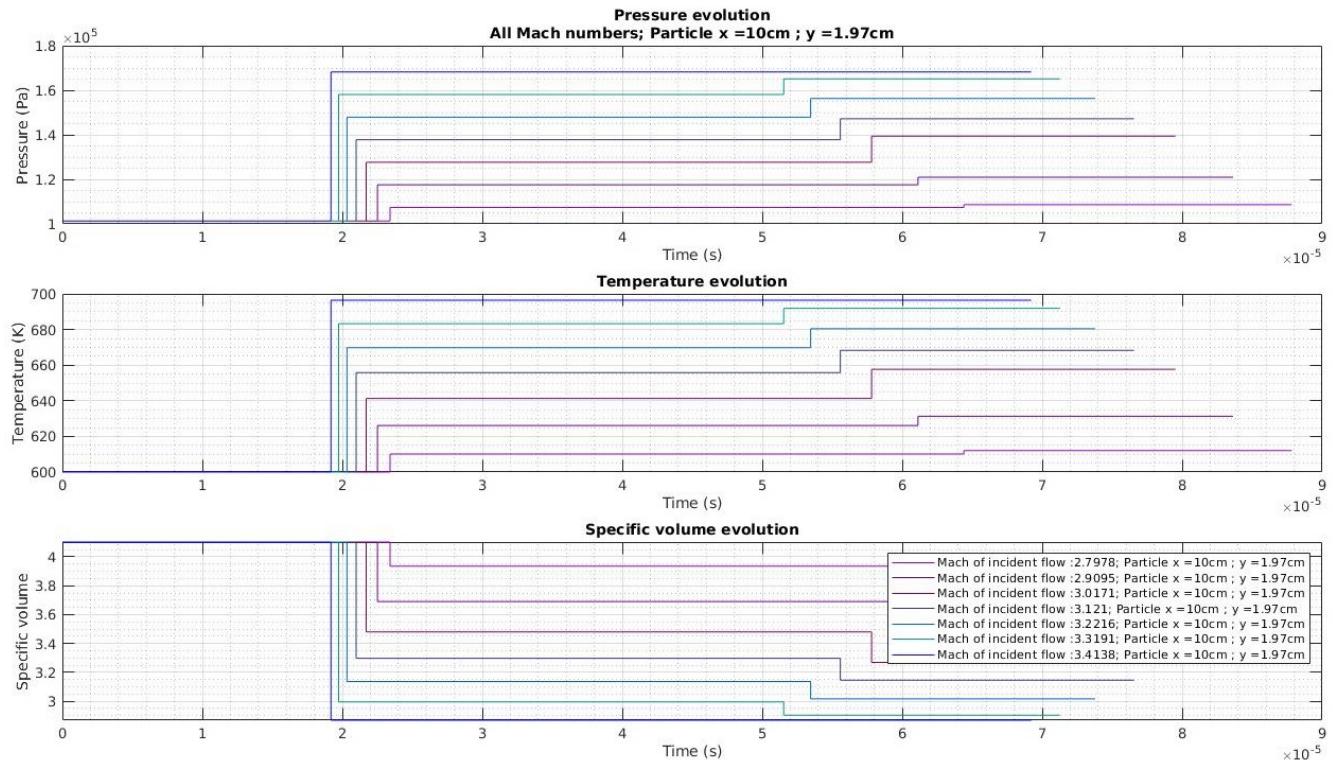
RRR - Results given by the inert gas dynamics theory

Evolution depends on position of the particle...



Results given by the inert gas dynamics theory

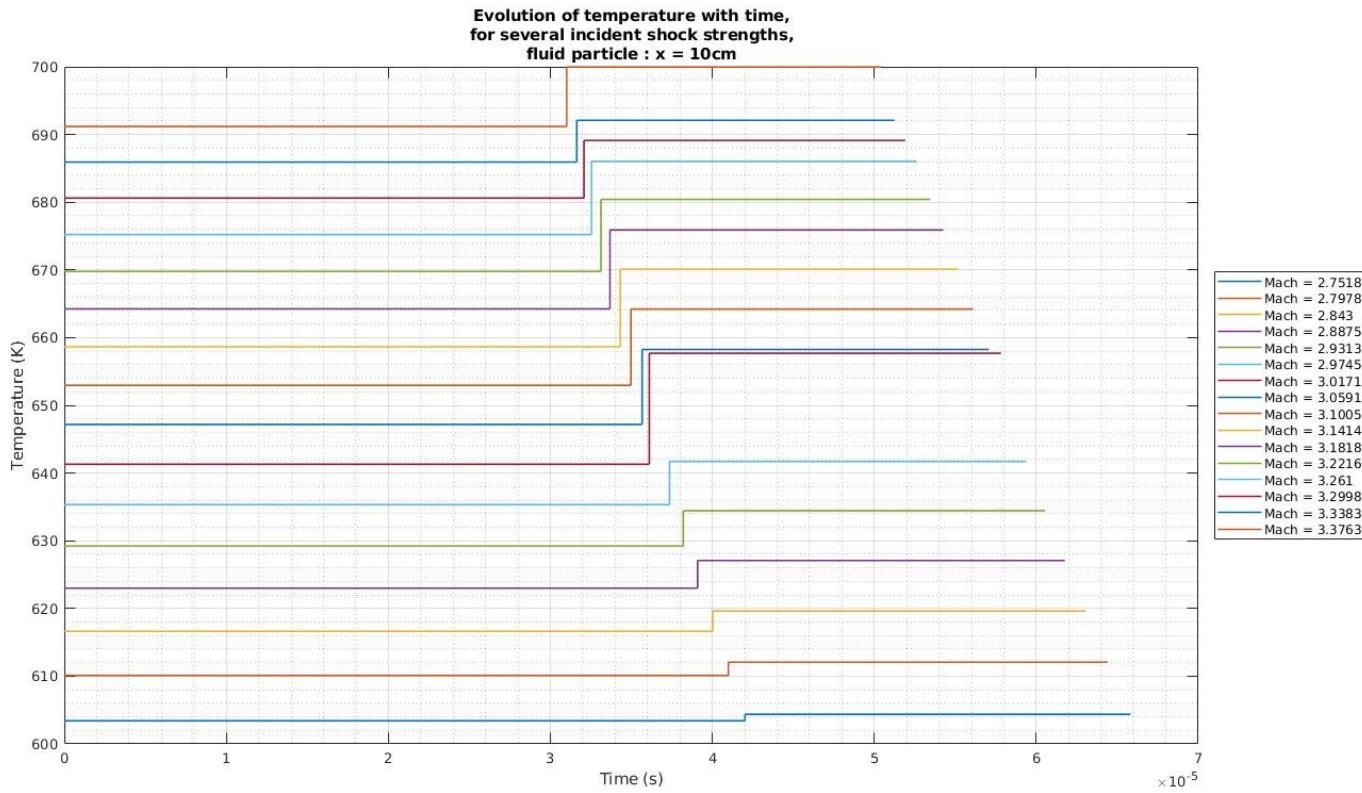
... and on Mach number of the shock



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?

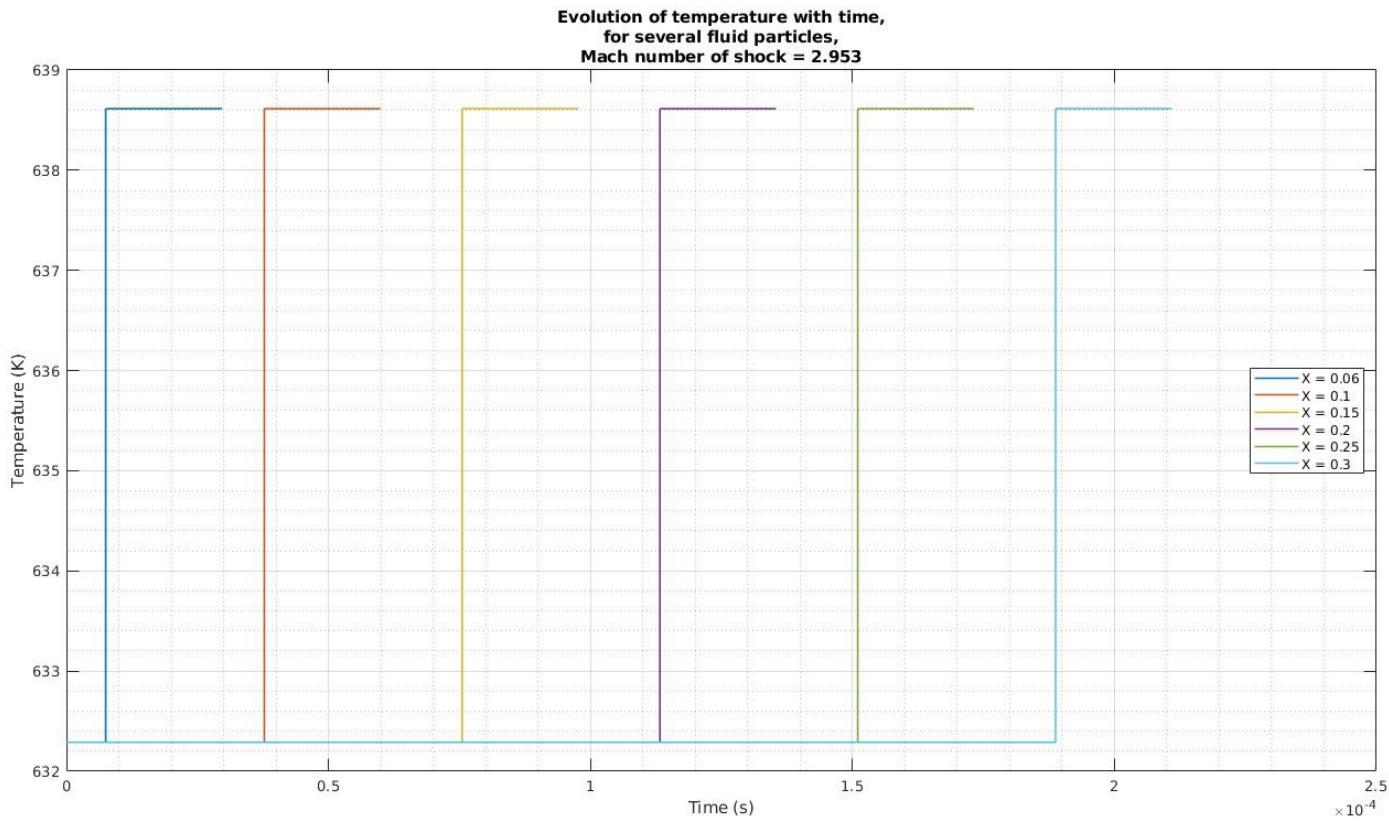
RRR - Results of the chemical calculus

Ignition doesn't occur for such low Mach numbers



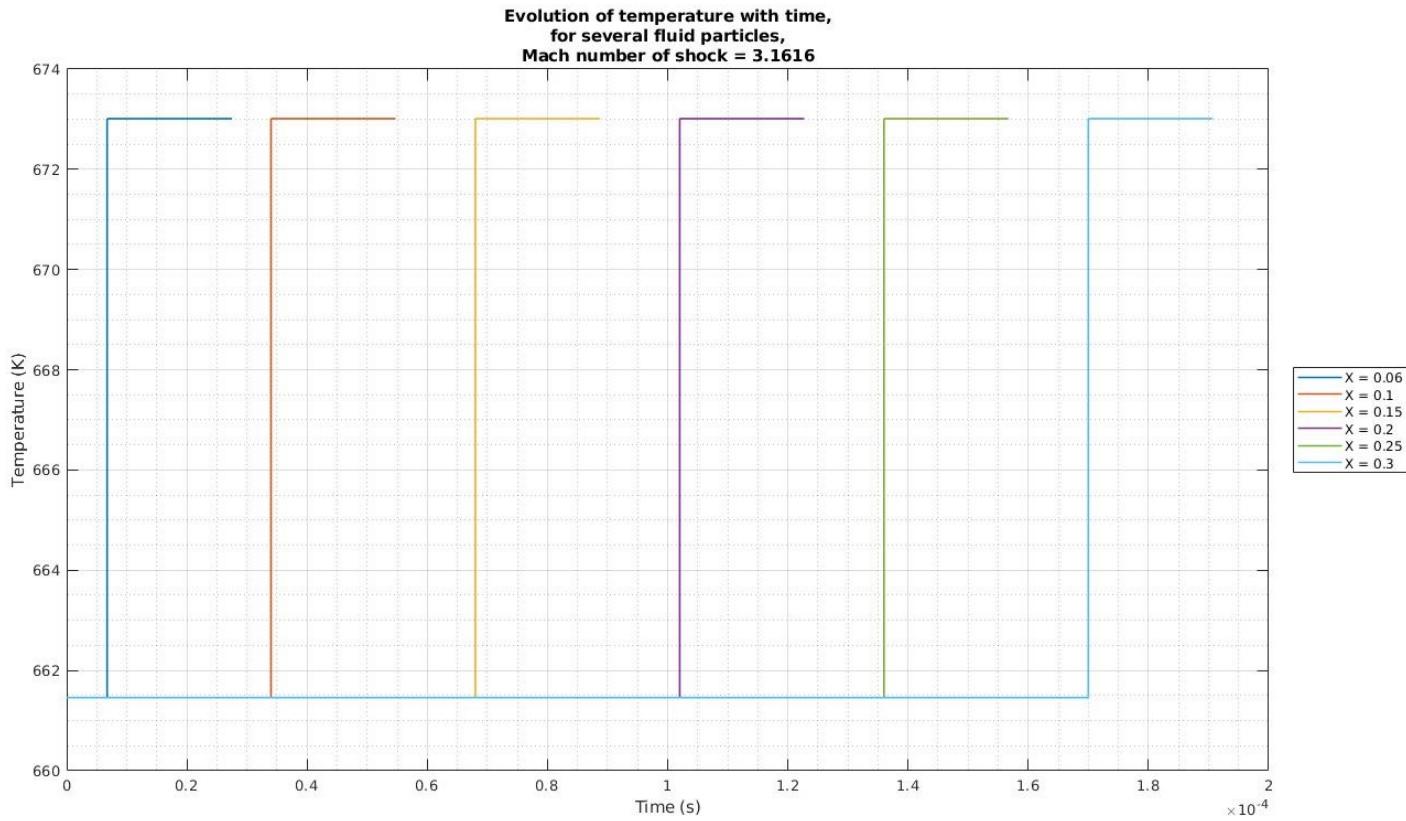
RRR - Results of the chemical calculus

Ignition doesn't occur for such low Mach numbers



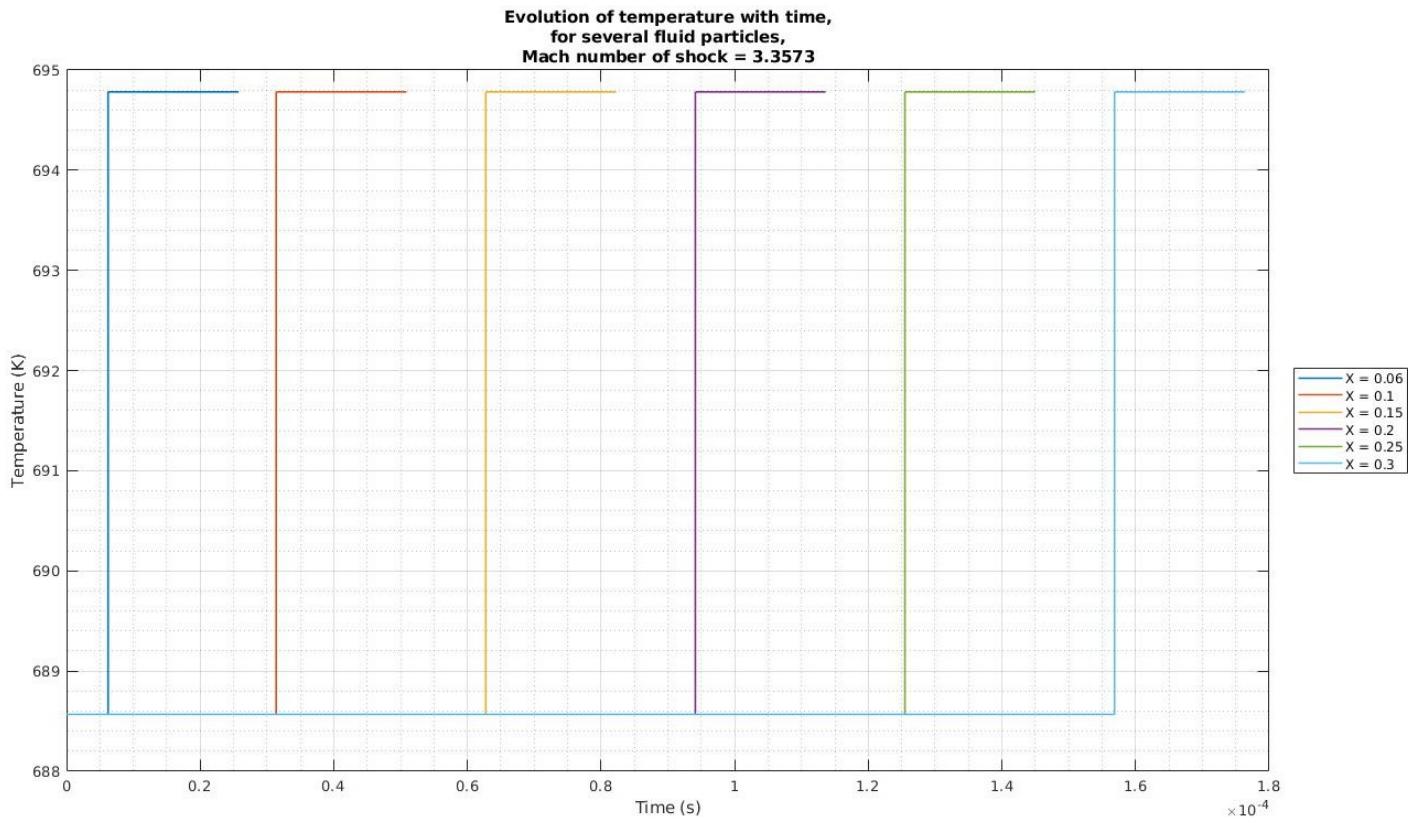
RRR - Results of the chemical calculus

Ignition doesn't occur for such low Mach numbers



RRR - Results of the chemical calculus

Ignition doesn't occur for such low Mach numbers



Transition between structures : focus on low angles of incidence

Boundaries between structures

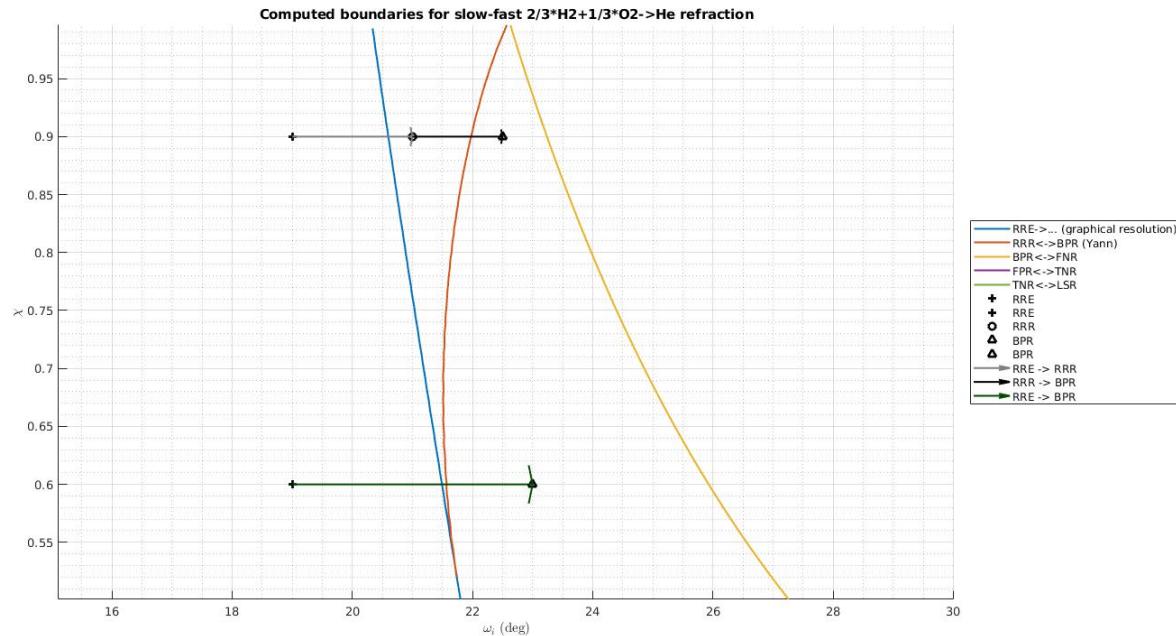


Figure 10: Boundaries of the different structures at stake here in the $\chi - \omega$ plane, for a $H_2 - O_2 // He$ system

Regular Refraction with reflected Expansion RRE

Polar diagram

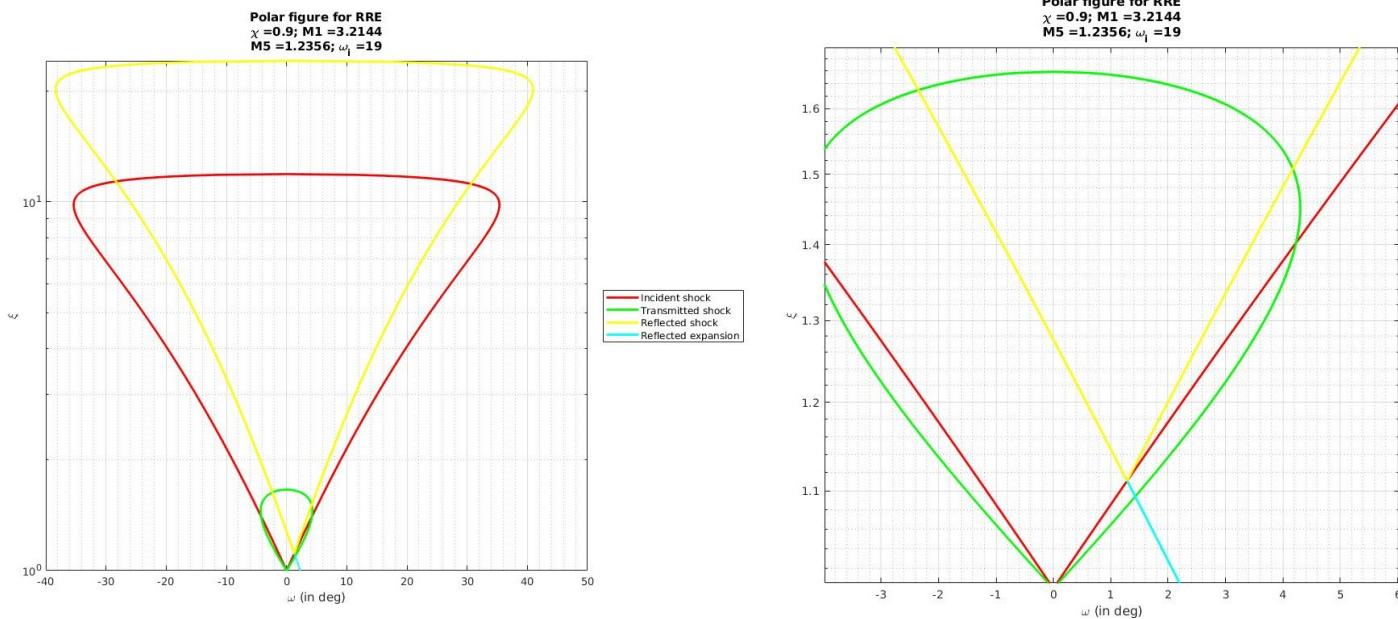


Figure 11: Polar diagram for RRE structure, zoom on the intersection point on the right

Regular Refraction with Reflected shock RRR

Polar diagram

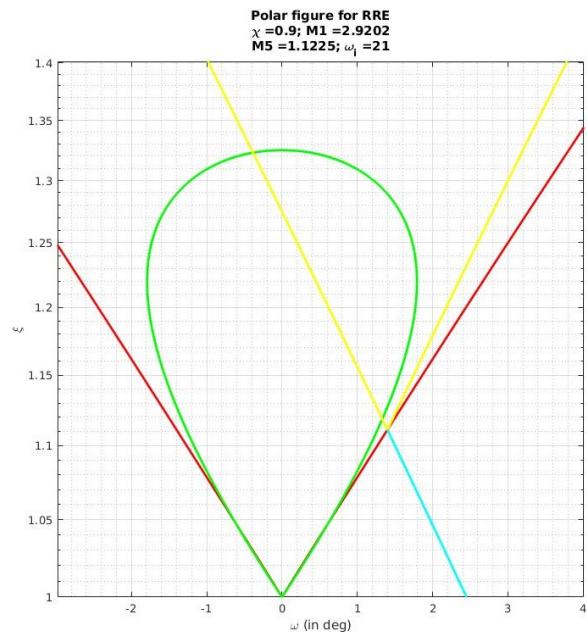
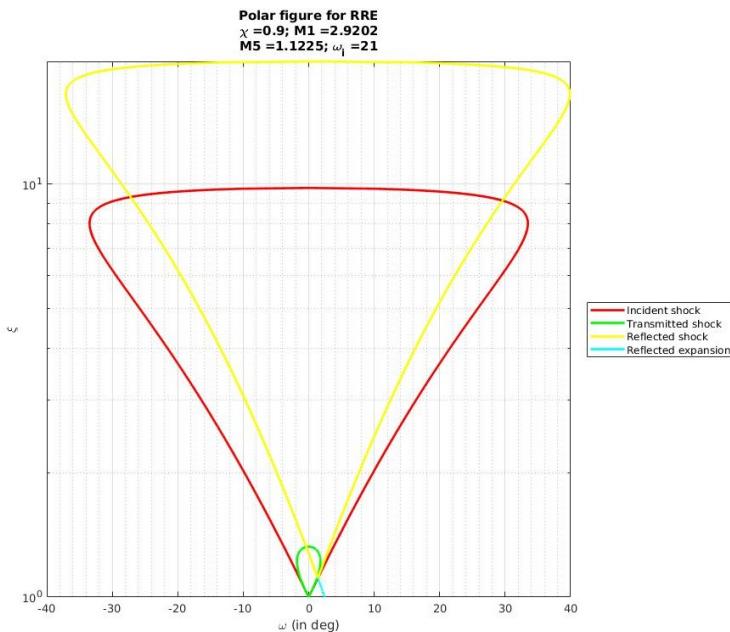


Figure 12: Polar diagram for RRR structure, zoom on the intersection point on the right

Bound Precursor Refraction BPR

Polar diagram

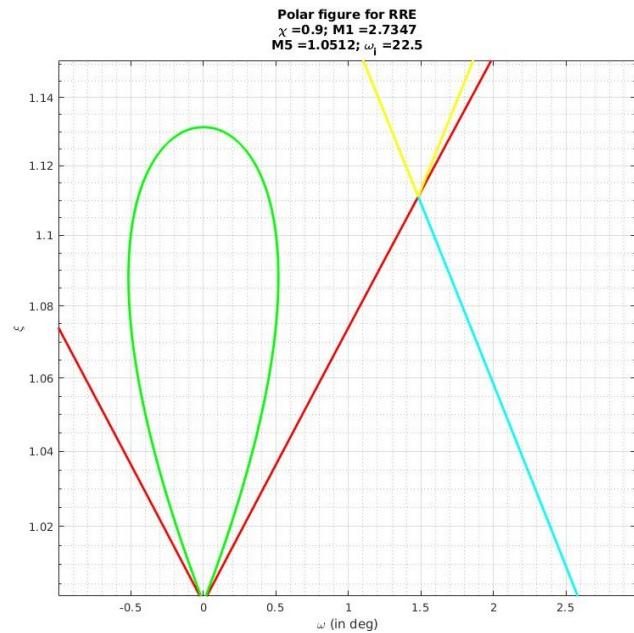
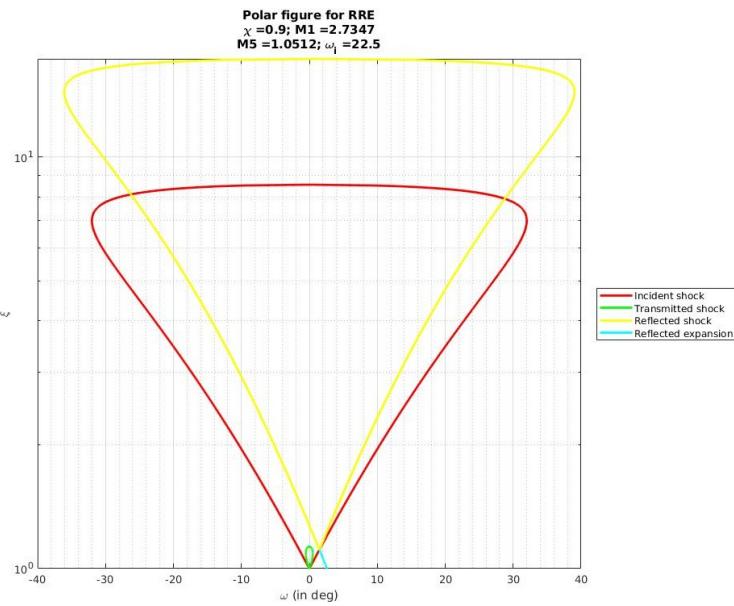


Figure 13: Polar diagram for BPR structure, zoom on the intersection point on the right

Strong RRE : two intersection points

Polar diagram and Scheme

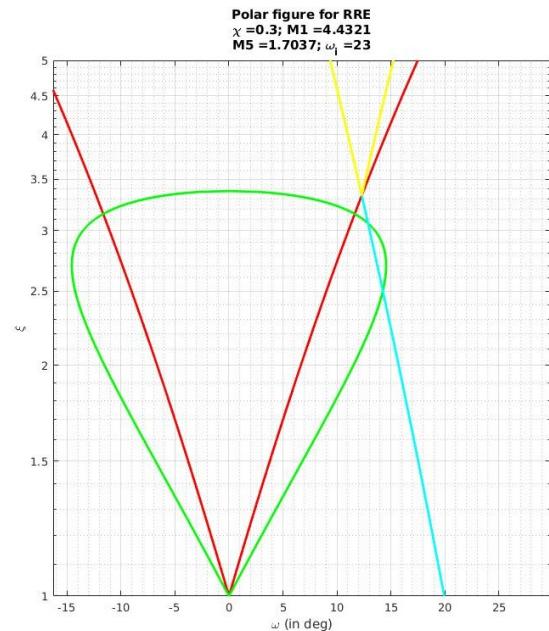
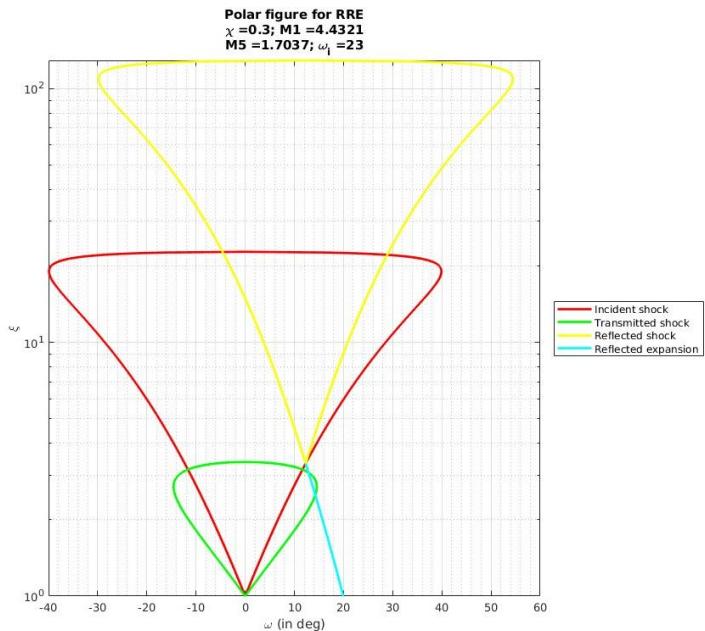


Figure 14: Polar diagram for RRE structure with high shock strength, zoom on the intersection point on the right

Strong BPR structure

Polar diagram

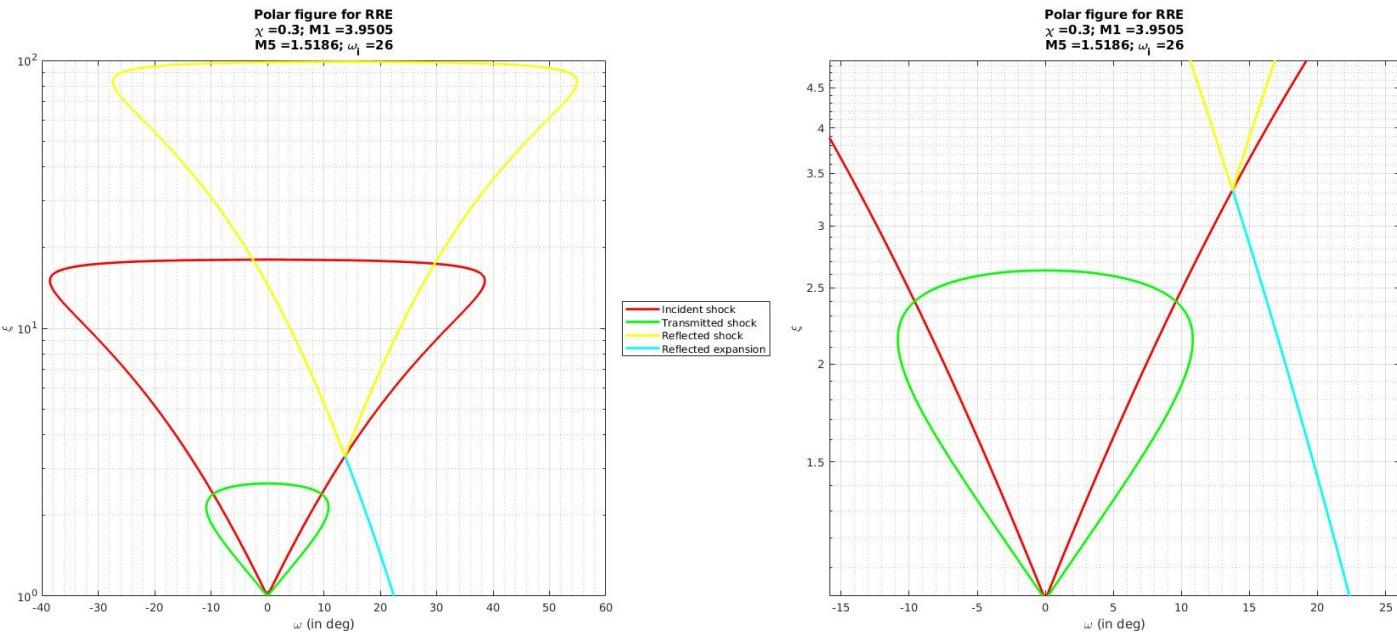


Figure 15: Polar diagram for BPR structure with high shock strength, zoom on the intersection point on the right

BPR - Scheme and Notations

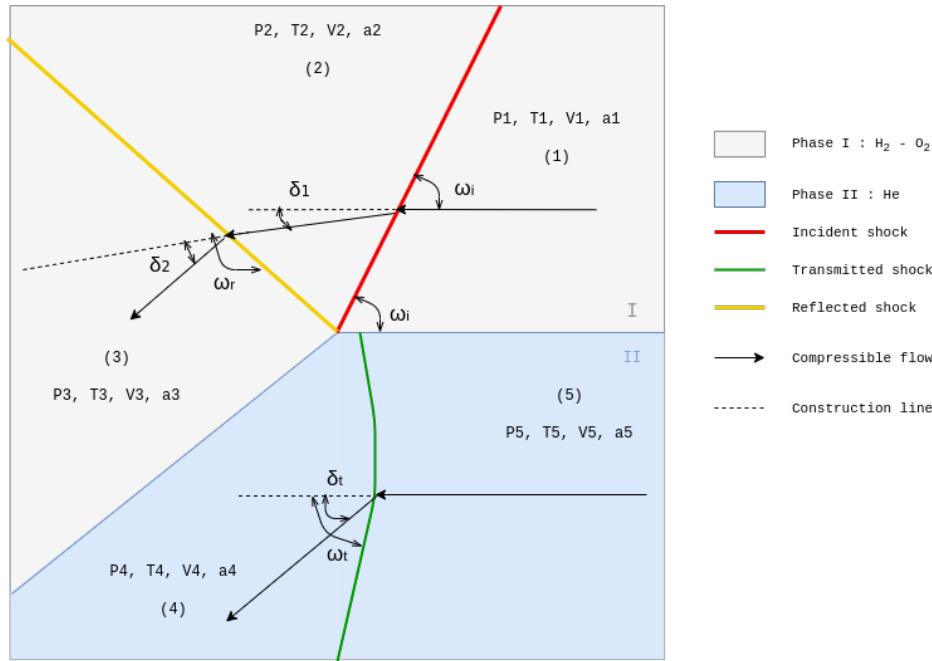


Figure 16: Symbols, zones and angles for computation

Notice that the transmitted shock is softly cylindrical and a bit ahead of the intersection point between the incident shock, the reflected wave and the interface : it is called a bound precursor.

BPR - Theoretical resolution

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

See slides 9, 10 and 11 : definitions and computations keep exactly the same.

BPR - Theoretical resolution

From zone (2) to zone (3) : unknown structure

As long as we are not studying a regular refraction anymore, it is difficult to know whether the reflected wave is a shock or an expansion.

- Does it depend on the situation before transition (RRE or RRR)?
- Does it depend on the shape of the transmitted wave?

BPR - Theoretical resolution

From zone (5) to zone (4) : piston theory

- Developed by Abd-el-Fattah, Henderson and Lozzi (1976) [2]
- Allows to calculate the velocity of a shock by assuming it is related to velocity of a fictive piston.



Figure 17: Scheme for the piston theory : in red the considered shock with velocity V_w , in white, the fictive driving piston with velocity V_p . $a_{1,2}$ is for the speed of sound resp. in the undisturbed and disturbed gases

If γ is the specific heat ratio of the gas at stake, then those two velocities are related with the following equation :

$$V_p = \frac{2}{\gamma + 1} \frac{V_w^2 - a_1^2}{V_w}$$

BPR - Theoretical resolution

From zone (5) to zone (4) : piston theory

Henderson et al. [2] have experimentally shown that, whatever the refraction structure, the incident shock and the transmitted shock can be approximated with the same piston velocity V_p . Thus, the following equality is obtained :

$$V_p = \frac{2}{\gamma_I + 1} \frac{V_i^2 - a_1^2}{V_i} = \frac{2}{\gamma_{II} + 1} \frac{V_t^2 - a_5^2}{V_t}$$

because the transmitted shock is travelling in phase II and the undisturbed zone is (5).

Note that V_i and V_t are the *normal* velocities of resp. the incident and the transmitted shock.

BPR - Theoretical resolution

From zone (5) to zone (4) : piston theory

After some calculation, Henderson et al. [2] finally got a formula for the velocity of the transmitted shock V_t , independent from ω_i the angle of incidence of the incident shock.

$$V_t = \frac{1}{2} \left(b + \sqrt{b^2 + 4a_5^2} \right)$$

$$\text{where } b = \frac{\gamma_{II}+1}{\gamma_I+1} \frac{V_i^2 - a_1^2}{V_i}$$

In the particular case of a bound precursor, the transmitted shock moves ahead of the incident shock but not faster. It is thus possible to assume that the speeds are equal on either side of the interface (some kind of Snell's law):

$$\frac{V_t}{\sin(\omega_t)} = \frac{V_i}{\sin(\omega_i)}$$

BPR - Theoretical resolution

From zone (5) to zone (4) : piston theory

Finally, the expression of ω_t is given and the normal Mach number in zone (5) can be deduced from V_t : this is all we need to compute the evolution of the flow between zones (4) and (5).

Thanks to the membrane equilibrium we already used for RRE and RRR, it is possible to determine the state of the gas in zone (3).

Maybe this information can be a discriminating criterion to determine whether the reflected wave is a shock or not.

If $P_3 > P_2$ then a reflected shock is observed, if $P_3 < P_2$ then a reflected expansion occurs.

BPR - Some more remarks

In 1991, Henderson, Colella and Puckett tempted to give a full description of BPR structure for the first time [6].

- Probable existence of a 4th wave, in phase II
- Existence of a BPR when $\omega_t > \pi/2$
- No idea of what the reflected wave can be

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