Multiphase theory of diffuse interfaces

Richard Saurel
University Institute of France
SMASH Project, UMR CNRS 6595-IUSTI- INRIA

Outline

(i) Two-phase model for interfaces of simple contact

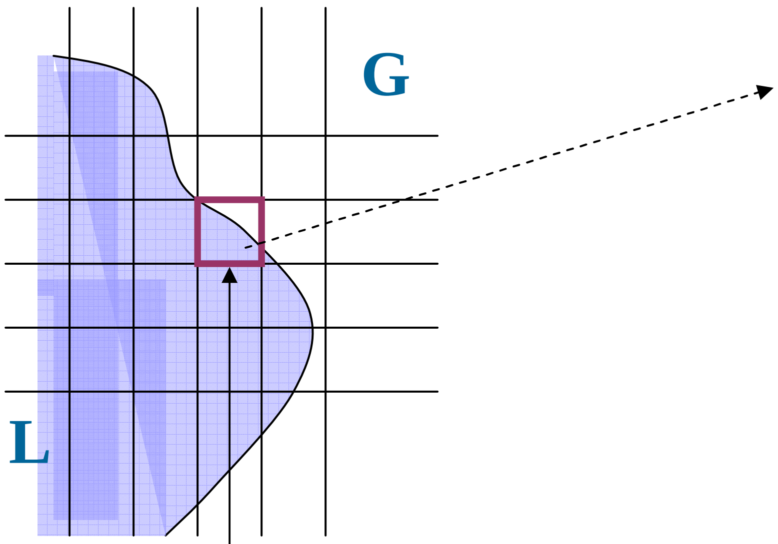
(ii) Associated shock relations

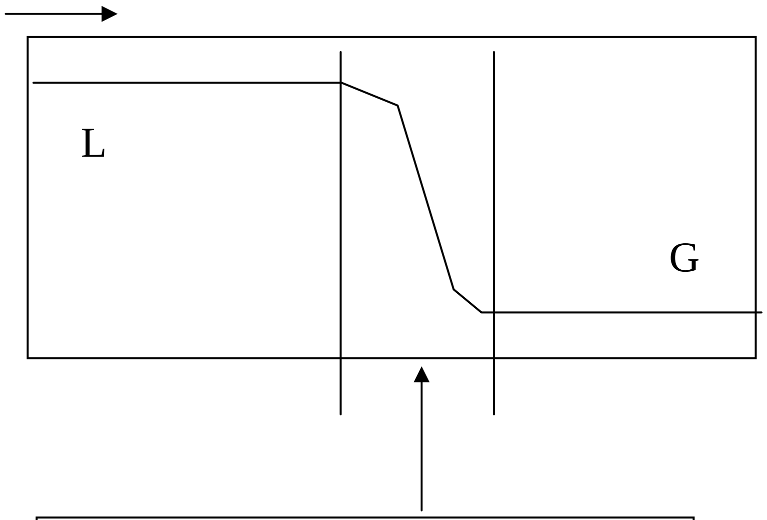
(iii) Capillary effects modeling

(iv) Heat and mass transfer modeling: Phase transition – Evaporation fronts

(v) Numerical method: The relaxation projection method for non-conservative hyperbolic systems

Diffuse interfaces appear as a consequence of numerical diffusion





How to compute the pressure in this artificial zone ?

The EOS are discontinuous with a restricted domain of validity.

- Mixture cell

Starting point: The seven equations model

$$\frac{\partial \alpha_1}{\partial t} + \bar{u}_i \frac{\partial \alpha_1}{\partial x} = \mu(p_1 - p_2)$$

$$\frac{\partial \alpha_1 \rho_1}{\partial t} + \frac{\partial \alpha_1 \rho_1 u_1}{\partial x} = 0$$

Each phase evolves in its own volume with its own velocity, energy and pressure.

The pressure equilibrium condition is replaced by a differential equation → Hyperbolicity is preserved as well as the correct waves propagation

$$\frac{\partial \alpha_1 \rho_1 u_1}{\partial t} + \frac{\partial (\alpha_1 \rho_1 u_1{}^2 + \alpha_1 p_1)}{\partial x} = \bar{p}_i \frac{\partial \alpha_1}{\partial x} + \lambda(u_2 - u_1)$$

$$\frac{\partial \alpha_1 \rho_1 E_1}{\partial t} + \frac{\partial u_1(\alpha_1 \rho_1 E_1 + \alpha_1 p_1)}{\partial x} = \bar{p}_i \bar{u}_i \frac{\partial \alpha_k}{\partial x} - \mu \bar{p}_i'(p_1 - p_2) + \lambda \bar{u}_i{}'(u_2 - u_1)$$

3 symmetric equations are used for phase 2.

Closure relations: Interface pressure and velocity

$\overline{u}_i = u_2$ and $\overline{p}_i = p_1$

Baer and Nunziato (1986)

$$\overline{p}_I = \frac{Z_1 p_2 + Z_2 p_1}{Z_1 + Z_2} + \mathrm{sgn}\left(\frac{\partial \alpha_1}{\partial x}\right) \frac{Z_1 Z_2 (u_2 - u_1)}{Z_1 + Z_2}$$

$$\overline{u}_i = \frac{Z_1 u_1 + Z_2 u_2}{Z_1 + Z_2} + \mathrm{sgn}\left(\frac{\partial \alpha_1}{\partial x}\right) \frac{p_2 - p_1}{Z_1 + Z_2}$$

Symmetric closure relations and relaxation parameters: Abgrall and Saurel, JCP (2003), Saurel et. al., JFM (2003)

$$\mu = \frac{A_I}{Z_1 + Z_2} = \frac{\text{specific int erfacial area}}{\text{sum of acoustic impedance}}$$

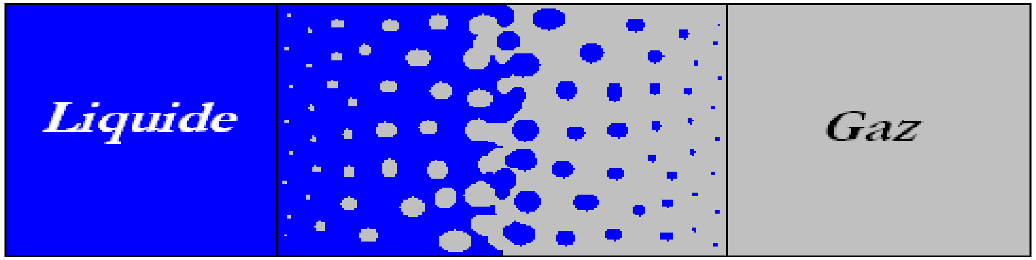
Pressure relaxation coefficient

$$\lambda = Z_1 Z_2 \mu$$

Velocity relaxation coefficient

Interface conditions in mixture cells

Interface conditions = equal normal velocities and pressures



$$\varepsilon < \alpha_k < 1 - \varepsilon$$

'Bubbles' growth in the mixture cells forces the pressure equilibrium

$$\frac{\partial \alpha_1}{\partial t} + \bar{u}_i \frac{\partial \alpha_1}{\partial x} = \mu (p_1 - p_2) \qquad \text{where } \mu \text{ tends to infinity}$$

The same relaxation method is used to guarantee velocities equality at the interface.

Central idea of Saurel and Abgrall, JCP, 1999

Limit model solved by such relaxation method: A mechanical equilibrium model (out of thermal equilibrium)

Interesting in order to:

•Facilitate numerical resolution (reduce the number of equations)

•Facilitate the extension to extra physics: surface tension, phase transition

The Chapman-Enskog method is employed:

$\lambda, \mu = 1/\varepsilon \to +\infty$ The relaxation coefficients tend to infinity

$f = f^{o} + \varepsilon f^{1}$ Each flow variable evolves with small perturbations around the initial mechanical equilibrium state

Consequence

The pressure relaxation term becomes a differential one:

$$\frac{\partial \alpha_1}{\partial t} + \bar{u}_i \frac{\partial \alpha_1}{\partial x} = \mu(p_1 - p_2)$$

$$\mu(p_1 - p_2) \to \frac{\left(\rho_2 c_2^{\,2} - \rho_1 c_1^{\,2}\right)}{\left(\dfrac{\rho_1 c_1^2}{\alpha_1} + \dfrac{\rho_2 c_2^2}{\alpha_2}\right)} \frac{\partial u}{\partial x}$$

The reduced model (Kapila et al., Phys. Fluids, 2001)

$$\frac{\partial \alpha_1}{\partial t} + u\,\frac{\partial \alpha_1}{\partial x} = \frac{(\rho_2 c_2^2 - \rho_1 c_1^2)}{\dfrac{\rho_1 c_1^2}{\alpha_1} + \dfrac{\rho_2 c_2^2}{\alpha_2}}\frac{\partial u}{\partial x}$$

$$\frac{\partial \alpha_1 \rho_1}{\partial t} + \frac{\partial \alpha_1 \rho_1 u}{\partial x} = 0$$

$$\frac{\partial \alpha_2 \rho_2}{\partial t} + \frac{\partial \alpha_2 \rho_2 u}{\partial x} = 0$$

$$\frac{\partial \rho u}{\partial t} + \frac{\partial (\rho u^2 + p)}{\partial x} = 0$$

$$\frac{\partial \rho E}{\partial t} + \frac{\partial u(\rho E + p)}{\partial x} = 0$$

A mixture EOS is derived from the energy definition and pressure equilibrium:

$$p = p(\rho, e, \alpha_1) = \frac{\rho e - \left(\dfrac{\alpha_1 \gamma_1 p_{\infty 1}}{\gamma_1 - 1} + \dfrac{\alpha_2 \gamma_2 p_{\infty 2}}{\gamma_2 - 1}\right)}{\dfrac{\alpha_1}{\gamma_1 - 1} + \dfrac{\alpha_2}{\gamma_2 - 1}}$$

$$\rho = \alpha_1 \rho_1 + \alpha_2 \rho_2$$

Difficulty: This model is not closed in the presence of shocks: The first equation is not conservative.

Rankine Hugoniot system

- Shock conditions = 7 unknowns : α_1, Y_1, ρ, u, P, e, σ
- 4 conservation laws :

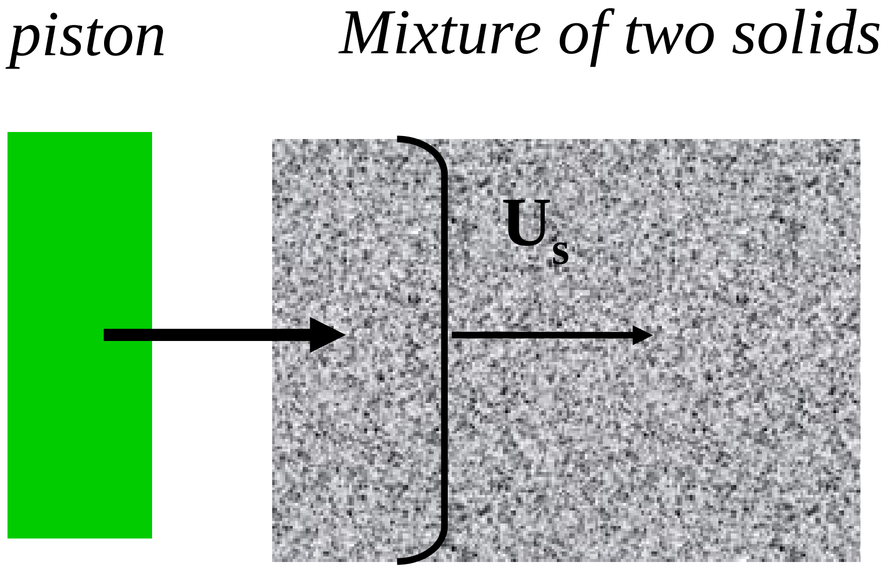
$$\begin{cases} Y_1 = cte \\ m = \rho(u-\sigma) = cte \\ P - P_0 - m^2(v - v_0) = 0 \\ e - e_0 + \dfrac{P+P_0}{2}(v - v_0) = 0 \end{cases}$$

- Mixture EOS : $P = P(\rho, e, \alpha)$
- One of the variable behind the shock is given (often σ or P)

An extra relation is needed : Jump of volume fraction or any other thermodynamic variable (or relation between them)

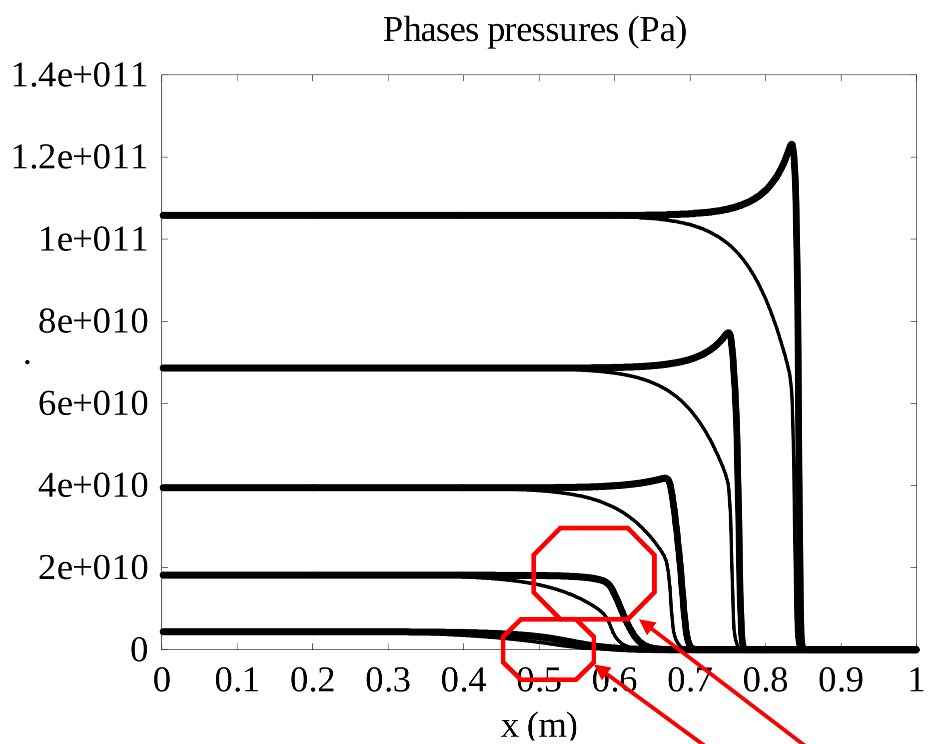
How to determine such kinetic relation ?

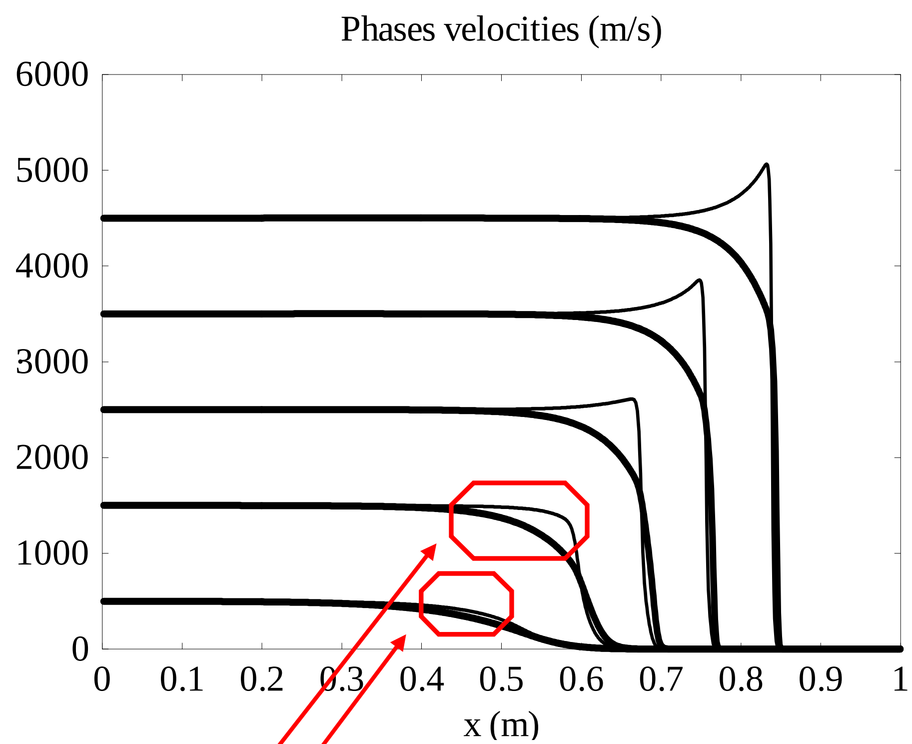
Information from the 7 equations model



For each piston velocity the shock relaxation zone is computed

Flow profiles for several piston velocities

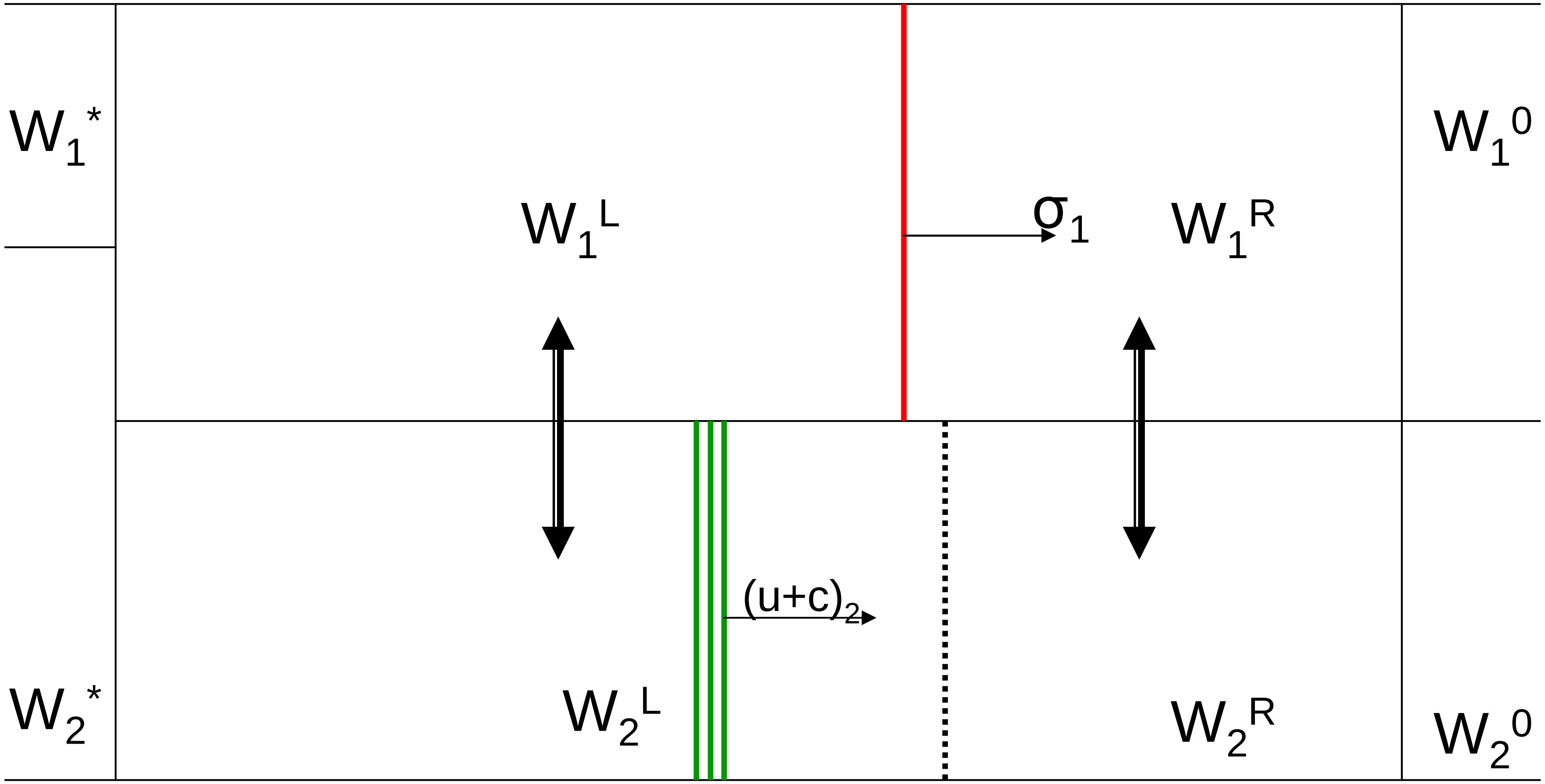




Fully dispersed waves

Why are the waves dispersed in the mixture ?

Dispersion mechanism: consider a two-layers mixture



A ‘circular process’ combining pressure and velocity relaxation and acoustic propagation results in a ‘smooth’ two-phase shock.

Dispersed shocks

- The two-phase shock is smooth
- shock = succession of mechanical equilibrium states
- We can use the 7 equations model in the limit $\lambda \to +\infty$ and $\mu \to +\infty$

that is easier to integrate between pre- and post-shock states.

- In that case, the energy equations reduce to :

$$\alpha_k\left(\rho_k \frac{de_k}{dt} + p\frac{\partial u}{\partial x}\right) = -p\frac{d\alpha_k}{dt} \quad \text{or} \quad \frac{de_k}{dt} + P\frac{dv_k}{dt} = 0 \quad \text{or} \quad \frac{ds_k}{dt} = 0$$

It is interesting to note that the drag work is absent while the pressure work $\left(-p\frac{d\alpha_k}{dt}\right)$ is still present in this limit. Pressure work is thus the dominant interaction effect.

Integration of the energy equations between pre- and post- shock states

$$\int_{-\infty}^{+\infty} \frac{de_k(x)}{dx}dx + \int_{-\infty}^{+\infty} p(x)\frac{dv_k(x)}{dx}dx = 0$$

$$e_k^* - e_k^0 + \hat{p}_k \int_{-\infty}^{+\infty} \frac{dv_k(x)}{dx}dx = 0 \quad \text{with} \quad \hat{p}_k = \frac{\int_{-\infty}^{+\infty} p(x)\frac{dv_k(x)}{dx}dx}{\int_{-\infty}^{+\infty} \frac{dv_k(x)}{dx}dx} = \frac{\int_{-\infty}^{+\infty} p(x)\frac{dv_k(x)}{dx}dx}{v_k^* - v_k^0}$$

The closure necessitates a link between the pressure averages $\hat{p}_1$ and $\hat{p}_2$

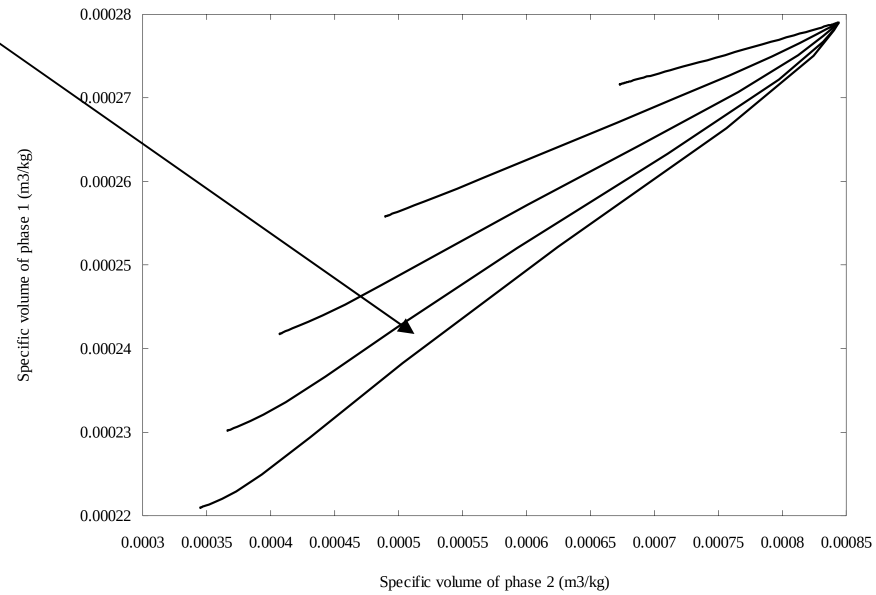
The ratio $\frac{dv_1}{dv_2}$ is assumed constant in the shock layer for a given shock speed:

$$\frac{dv_1}{dv_2} = \frac{v_1^* - v_1^0}{v_2^* - v_2^0}$$ necessarily valid for weak shocks.

It imply: $$\hat{p}_1 = \frac{\int_{-\infty}^{+\infty} p(x)\frac{dv_1}{dv_2}\frac{dv_2(x)}{dx}dx}{v_1^* - v_1^0} = \frac{\int_{-\infty}^{+\infty} p(x)\frac{dv_2(x)}{dx}dx}{v_2^* - v_2^0} = \hat{p}_2$$

The assumption $\frac{dv_1}{dv_2} = \text{cst}$ **can be checked with the 7 eqs. model**

seems also valid for strong shocks



Resolution of the 7 equations model shows a quasi-linear dependence of the two specific volumes inside the shock layer.

Thus,

$$\hat{P}_1 = \hat{P}_2 = \hat{P}$$

The energy conservation for the mixture implies $\hat{P} = \frac{1}{2}(P_0 + P^*)$

Kinetic relation: Each phase follows its own Hugoniot

$$\boxed{e_k^* - e_{k0} + \frac{P^* + P_0}{2}\left(v_k^* - v_{k0}\right) = 0}$$

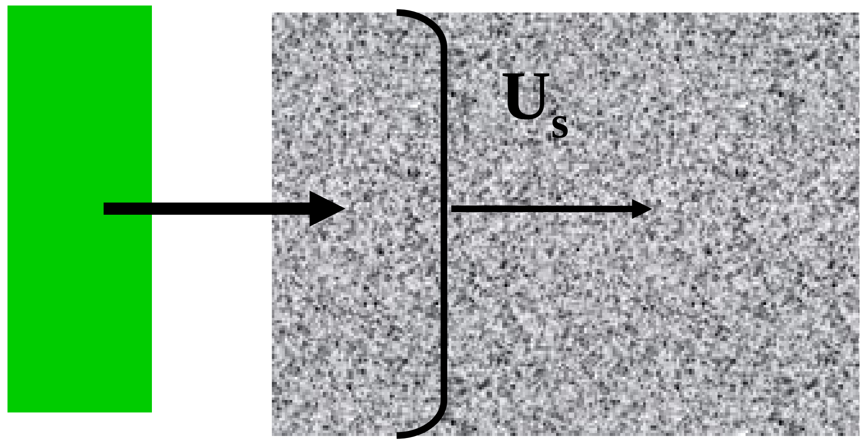
Saurel et al, Shock Waves J. , (2007)

Some properties

- Symmetric and conservative formulation
- Entropy inequality is fulfilled
- Single phase limit is recovered
- Validated for weak and strong shocks against more than 100 experimental data
- The mixture Hugoniot curve is tangent to mixture isentrope

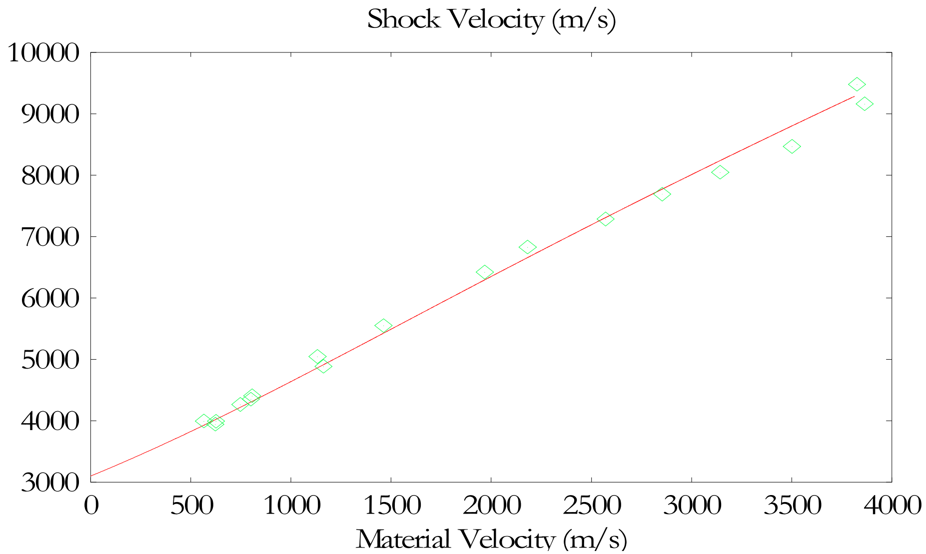
Validation

piston *Mixture of two solids*

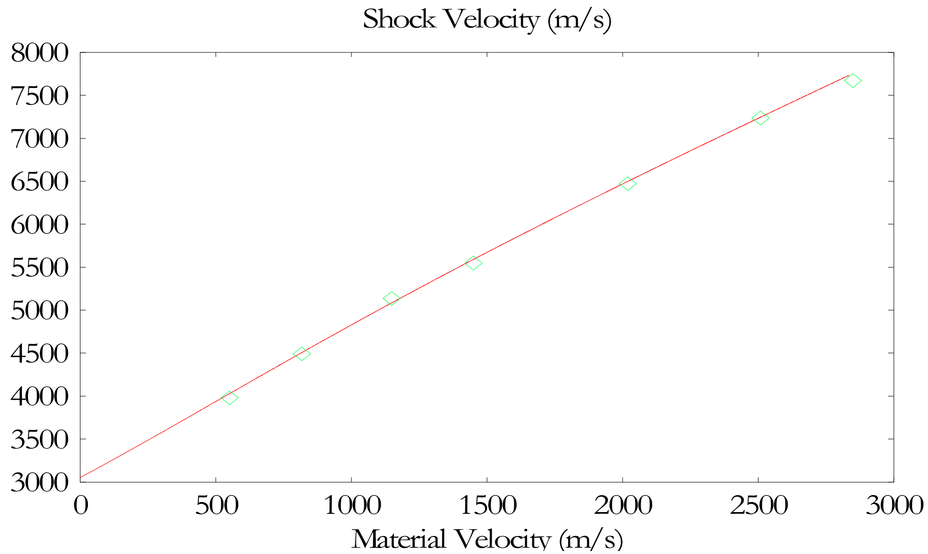


For each piston velocity the shock speed is recorded

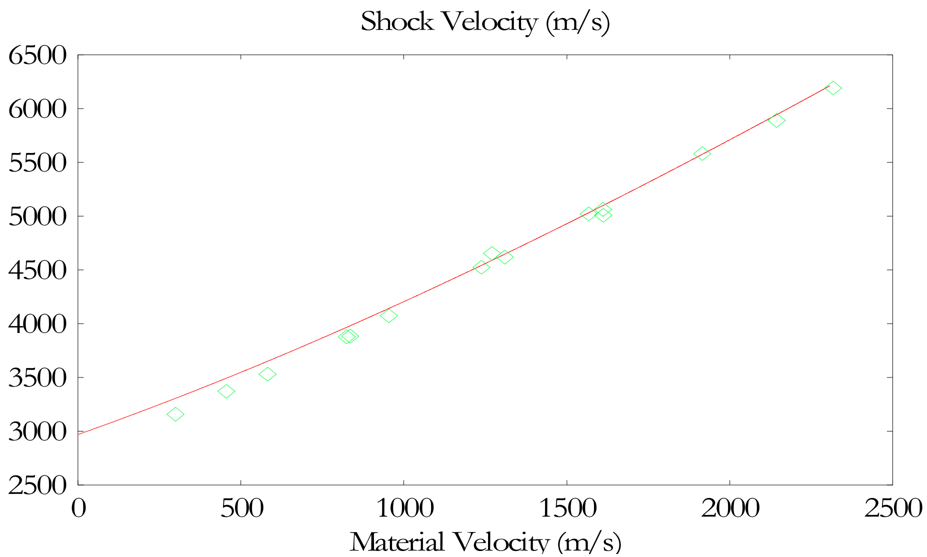
Experimental data (symbols) versus analytical model (lines)



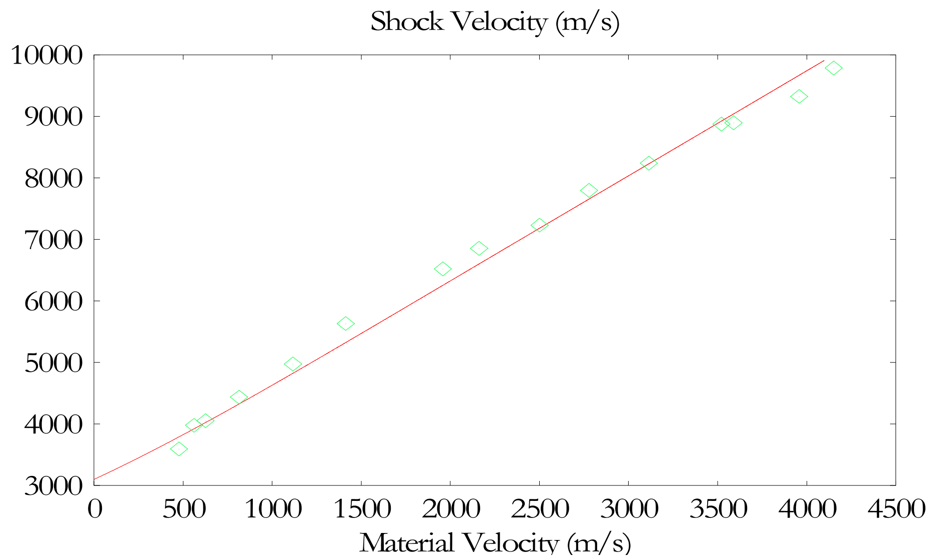
Epoxy-Spinel mixture



Paraffine-Enstatite mixture



Uranium-Molybdene mixture



Epoxy-Periclase mixture

We realized recently that Trunin (2001) (VNIIEF –Sarov) proposed the same relation, without justification, but with validations for more than 230 experimental tests done in Russia!

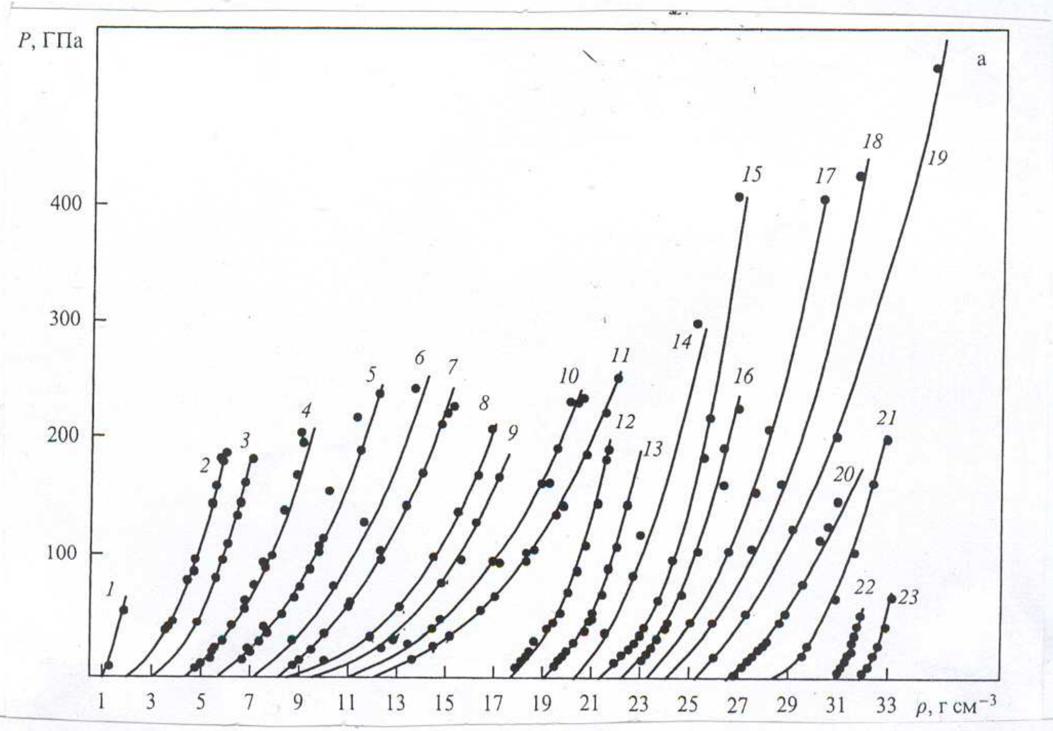
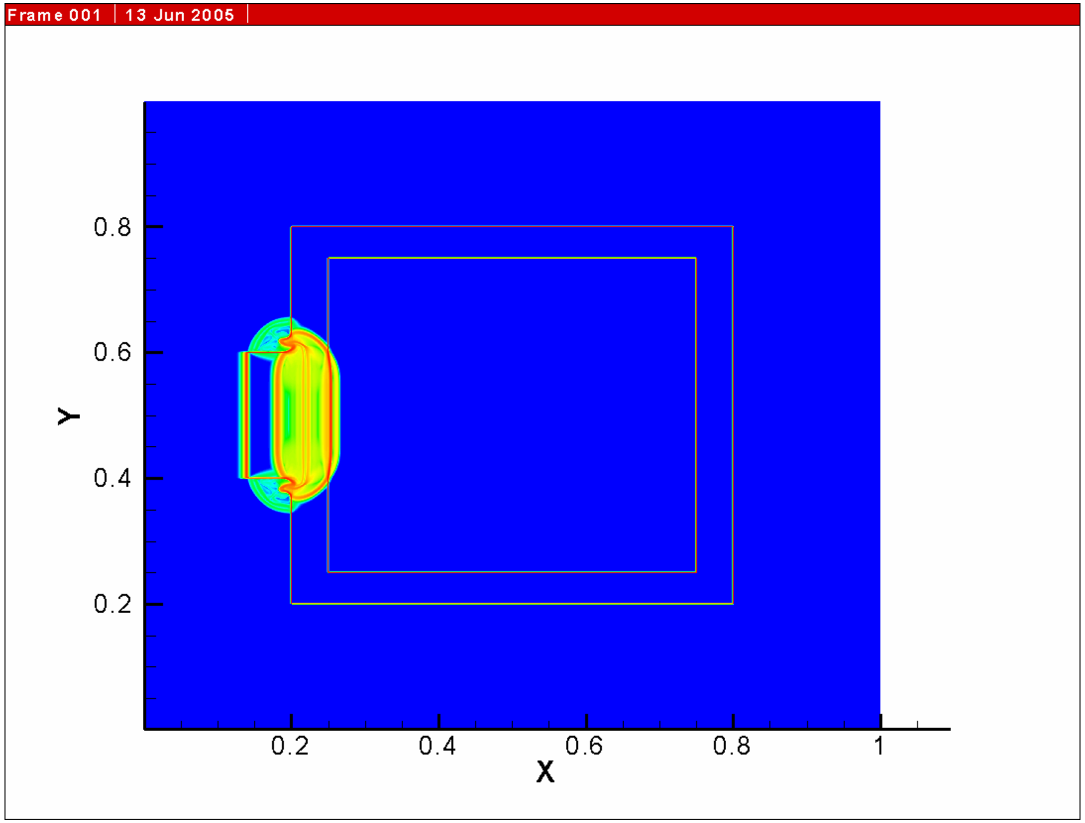


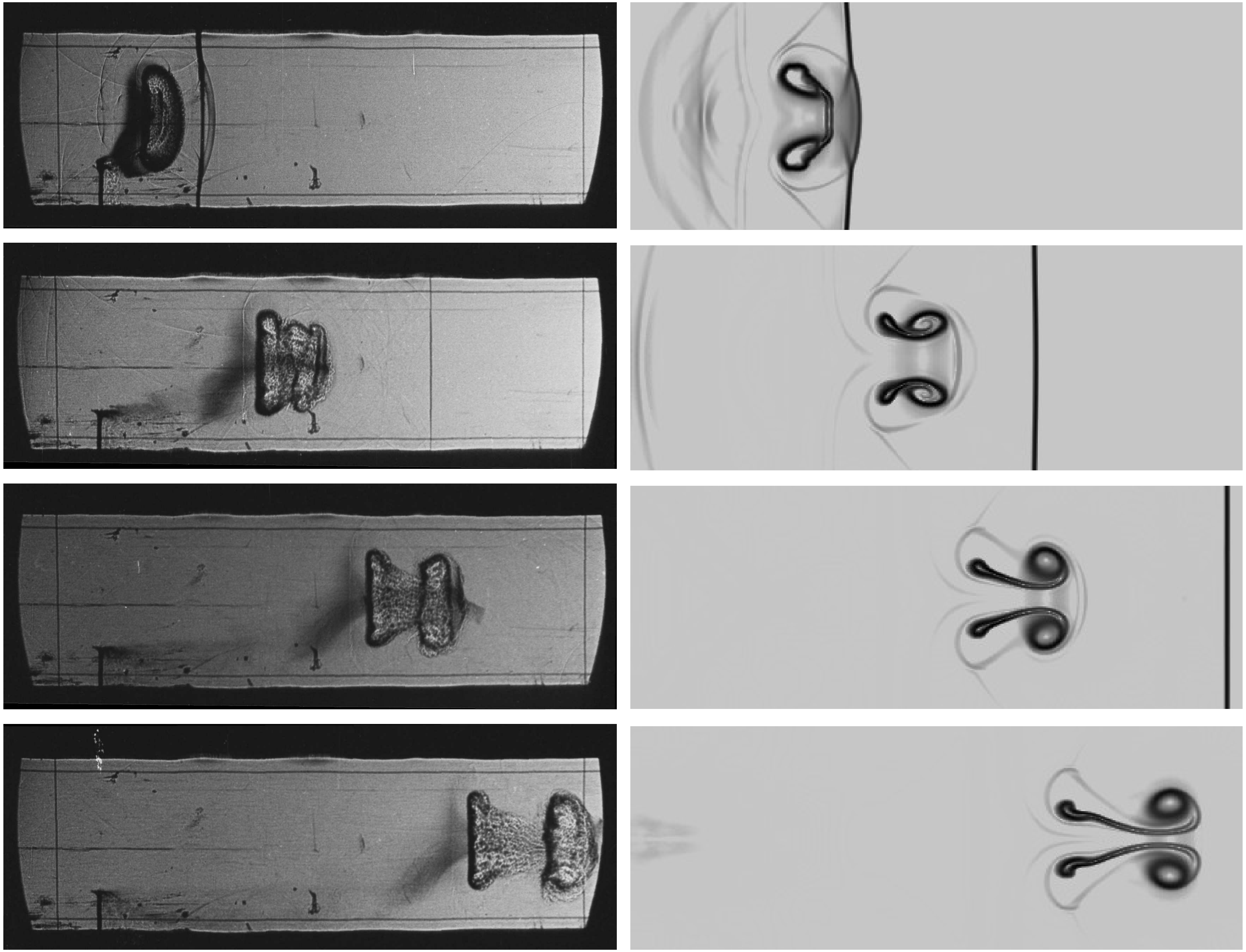
Рис. 11. (а) Ударные адиабаты металлических сплавов: *1* — Be(68 %)–Al(32 %), *2* — Fe(90 %)–Ni(10 %), *3* — Fe(74 %)–Ni(26 %), *4* — Cu(74,5 %)–W(25,5 %), *5* — Cu(45 %)–W(55 %), *6* — Cu(32 %)–W(68 %), *7* — Cu(24 %)–W(76 %), *8* — Au(90,7 %)–Ge(9,3 %), *9* — Au(92,1 %)–Ge(7,9 %), *10* — U(86,6 %)–Rh(13,4 %), *11* — U(91,7 %)–Mo(8,3 %), *12* — Fe(60 %)–Co(40 %), *13* — Fe(90 %)–W(10 %), *14* — Ti(70 %)–Mo(30 %), *15* — Fe(49 %)–Cu(51 %), *16* — Ni(50 %)–Cu(50 %), *17* — Ta(5 %)–Nb(95 %), *18* — Ta(30 %)–Nb(70 %), *19* — Re(60 %)–Mo(40 %), *20* — Ti(34,3 %)–Zr(65,7 %), *21* — Co(64,5 %)–Ni(35,5 %), *22* — Mg(85 %)–Li(14 %)–Al(1 %), *23* — Mg(88 %)–Li(12 %). (б) $P-\rho$-диаграмма карбидов металлов: *1* — SiC, *2* — TiC, *3* — ZrC, *4* — NbC ($\rho + 2$), *5* — TaC, *6* — WC ($\rho + 2$). (в) Сравнительная сжимаемость гидридов и образующих их металлов.

The pressure range is 1 atm – 5 000 000 atms !

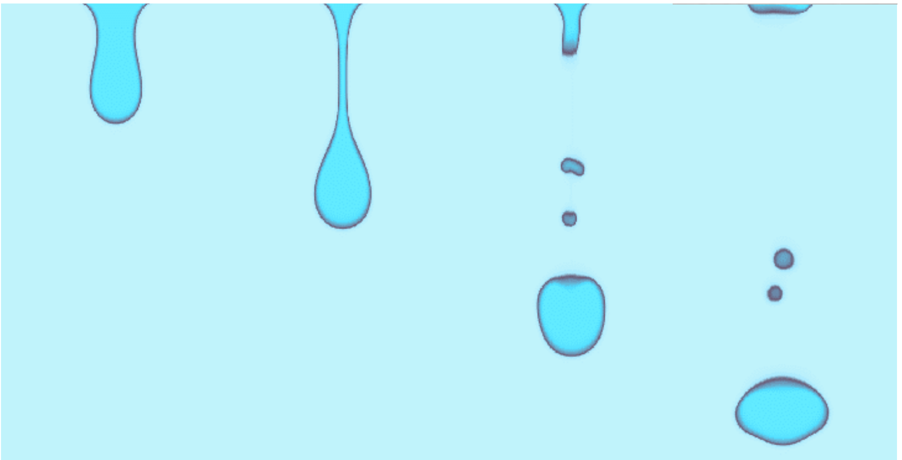
With the 5 equations model and associated shock relations, it is possible to solve interface problems. Example of the impact of a projectile over a copper tank filled with water. Numerical issues will be addressed at the end.



Shock/bubble interaction: experiments (IUSTI-left) computations (right)



Modeling capillary effects



→ We are seeking for a compressible flow model with surface tension

Modeling capillary effects

- Continuum Surface Force CSF [Brackbill *et al.* , JCP, 1992]
  - Allows numerical diffusion of the interfaces
  - Surface force $\rightarrow$ volume force
  - Developed in the incompressible flow context

- With compressible fluids, the volume fraction cannot be used for the curvature computation: it varies across shocks and rarefactions.

Thus, the mass fraction Y is used:

$$\vec{F}_{\sigma} = -\sigma \kappa \vec{\nabla} Y \qquad \text{where} \qquad \kappa = \mathrm{div}\left(\frac{\vec{\nabla} Y}{\left| \vec{\nabla} Y \right|} \right)$$

the mass fraction Y varies only across interfaces and is constant across shocks and rarefaction waves.

Momentum and energy contributions

- F_σ acts as a volume force as well as gravity $\rightarrow$ its power must be accounted for in the energy equation

$$
\left\{
\begin{array}{lll}
\dfrac{\partial \alpha}{\partial t} & + \vec{u}.\vec{\nabla}\alpha & = \dfrac{(\rho_2 c_2 - \rho_1 c_1)}{\dfrac{\rho_1 c_1^2}{\alpha_1} + \dfrac{\rho_2 c_2^2}{\alpha_2}} \mathrm{div}(u) \\
\dfrac{\partial \rho Y}{\partial t} & + \mathrm{div}(\rho Y \vec{u}) & = 0 \\
\dfrac{\partial \rho}{\partial t} & + \mathrm{div}(\rho \vec{u}) & = 0 \\
\dfrac{\partial \rho \vec{u}}{\partial t} & + \mathrm{div}(\rho \vec{u} \otimes \vec{u}) + \vec{\nabla} P & = \boxed{-\sigma \kappa \vec{\nabla} Y} \\
\dfrac{\partial \rho E}{\partial t} & + \mathrm{div}((\rho E + P)\vec{u}) & = \boxed{-\sigma \kappa \vec{\nabla} Y . \vec{u}}
\end{array}
\right.
$$

$$\kappa = \mathrm{div}\left(\frac{\vec{\nabla} Y}{\left| \vec{\nabla} Y \right|} \right)$$

Local curvature

Capillary effects

Conservative formulation (Perigaud and Saurel, JCP, 2005)

$$
\left\{
\begin{array}{lll}
\dfrac{\partial \alpha}{\partial t} & + \vec{u}.\vec{\nabla}\alpha - \dfrac{(\rho_2 c_2 - \rho_1 c_1)}{\dfrac{\rho_1 c_1^2}{\alpha_1} + \dfrac{\rho_2 c_2^2}{\alpha_2}} \mathrm{div}(u) & = 0 \\
\dfrac{\partial \rho Y}{\partial t} & + \mathrm{div}(\rho Y \vec{u}) & = 0 \\
\dfrac{\partial \rho}{\partial t} & + \mathrm{div}(\rho \vec{u}) & = 0 \\
\dfrac{\partial \rho \vec{u}}{\partial t} & + \mathrm{div}\left(P\bar{\bar{I}} + \rho \vec{u} \otimes \vec{u} - \sigma \left(\left|\vec{\nabla} Y\right| \bar{\bar{I}} - \dfrac{\vec{\nabla} Y \otimes \vec{\nabla} Y}{\left|\vec{\nabla} Y\right|} \right) \right) & = 0 \\
\dfrac{\partial \rho \left(e + \dfrac{\sigma \left|\vec{\nabla} Y\right|}{\rho} + \dfrac{1}{2} \vec{u}^2\right)}{\partial t} & + \mathrm{div}\left(\left(\rho \left(e + \dfrac{\sigma \left|\vec{\nabla} Y\right|}{\rho} + \dfrac{1}{2} \vec{u}^2\right) + P\right) \vec{u} - \sigma \left(\left|\vec{\nabla} Y\right| \bar{\bar{I}} - \dfrac{\vec{\nabla} Y \otimes \vec{\nabla} Y}{\left|\vec{\nabla} Y\right|} \right) . \vec{u} \right) & = 0
\end{array}
\right.
$$

Model’s features

- It is able to deal with arbitrary density ratios
- There is no interface length scale
- The same equations are solved everywhere → important for breakup and coalescence

Surface tension effects with an annular explosion

$$\gamma_g = 1{,}4$$

$$P_{\infty g} = 0$$

$$\rho_g = 1\, kg/m^3$$

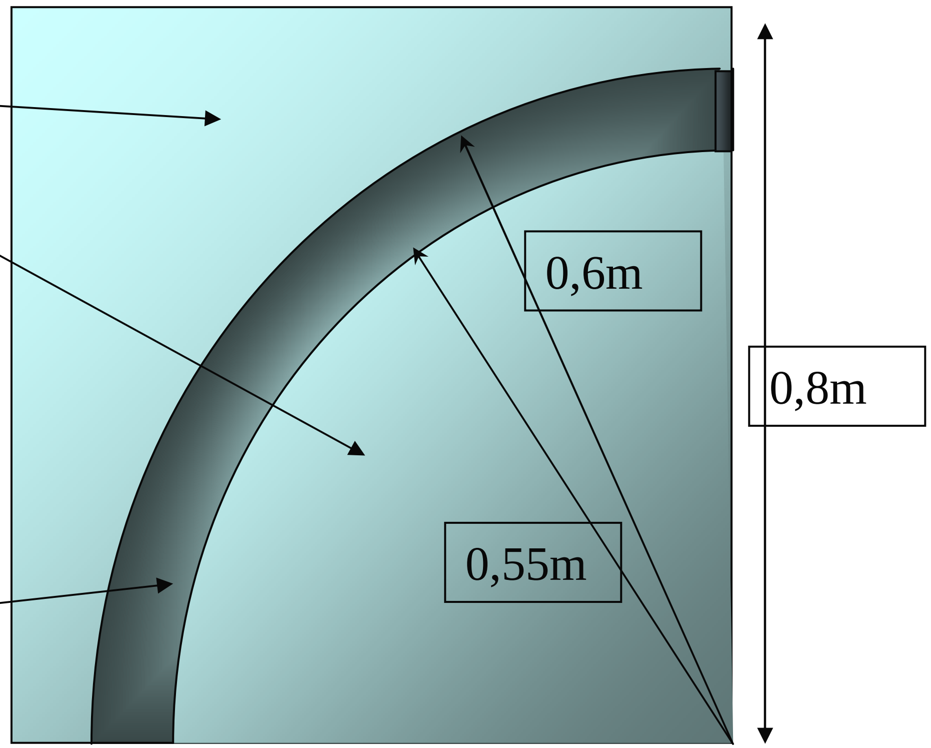
$$P_g = 10^5\, Pa$$

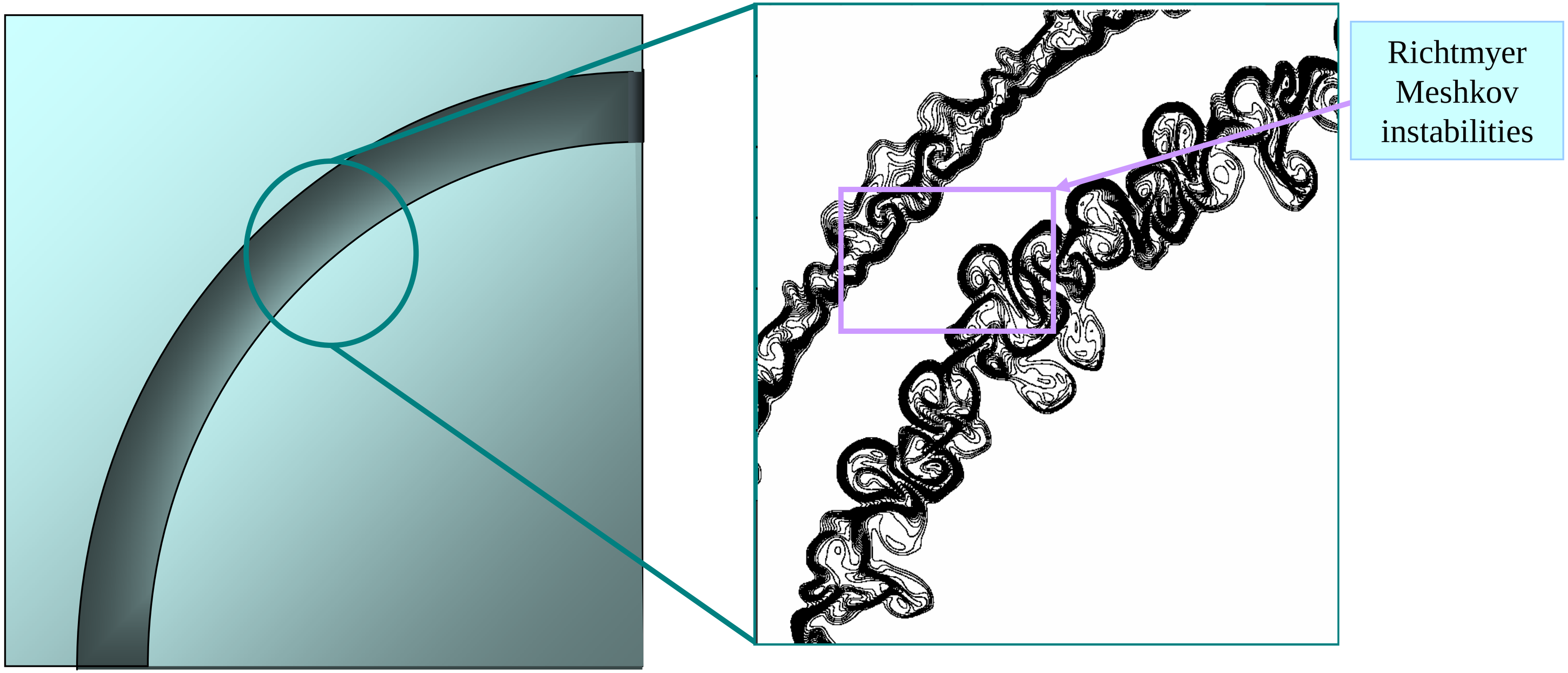
$$\gamma_l = 3$$

$$P_{\infty l} = 0$$

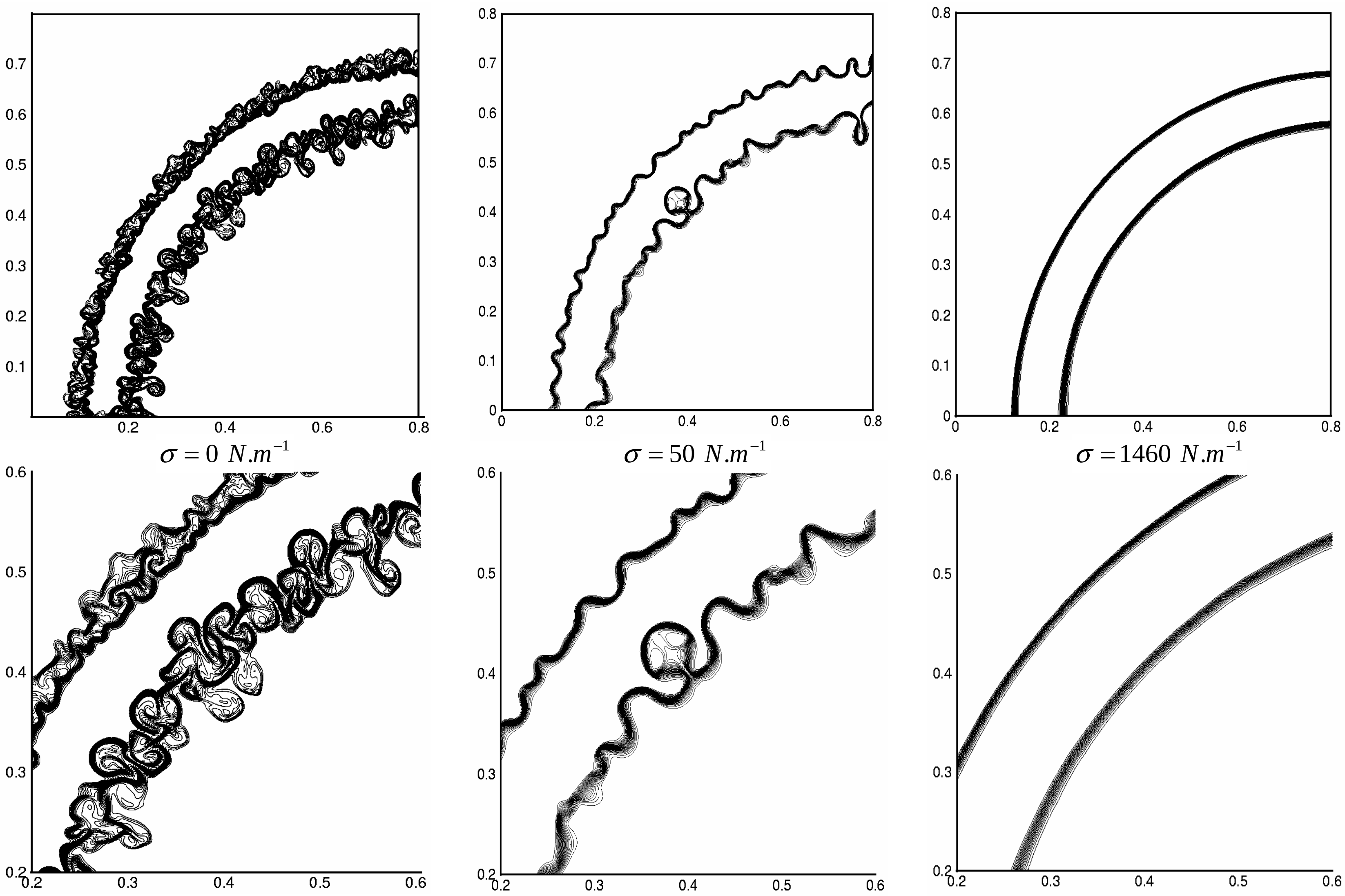
$$\rho_l = 50\, kg/m^3$$

$$P_l = 10^6\, Pa$$




Richtmyer
Meshkov
instabilities

Increasing surface tension coefficient

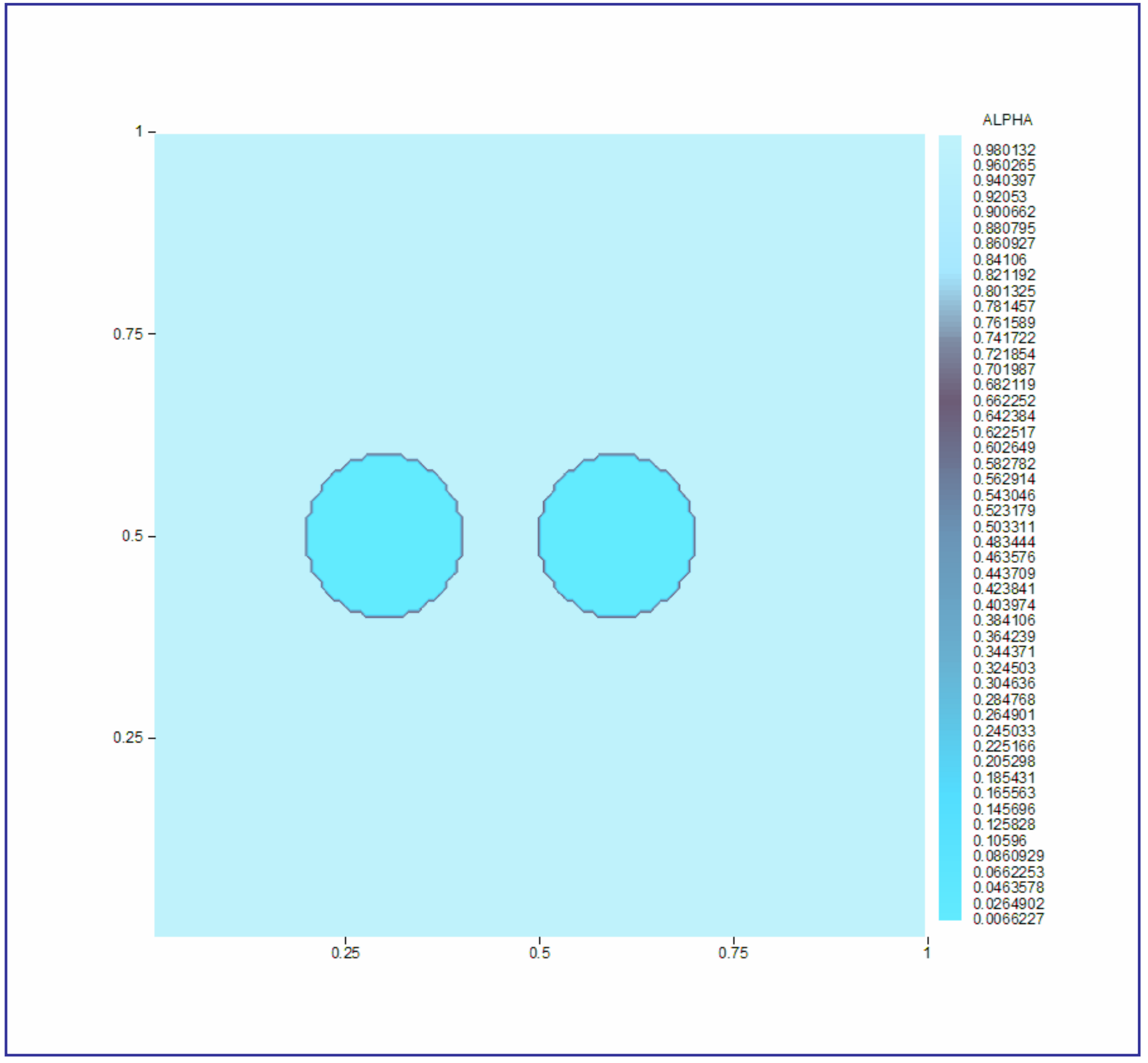


Quantitative comparison: Falling drop

Experiments done at IUSTI- shown with grey areas

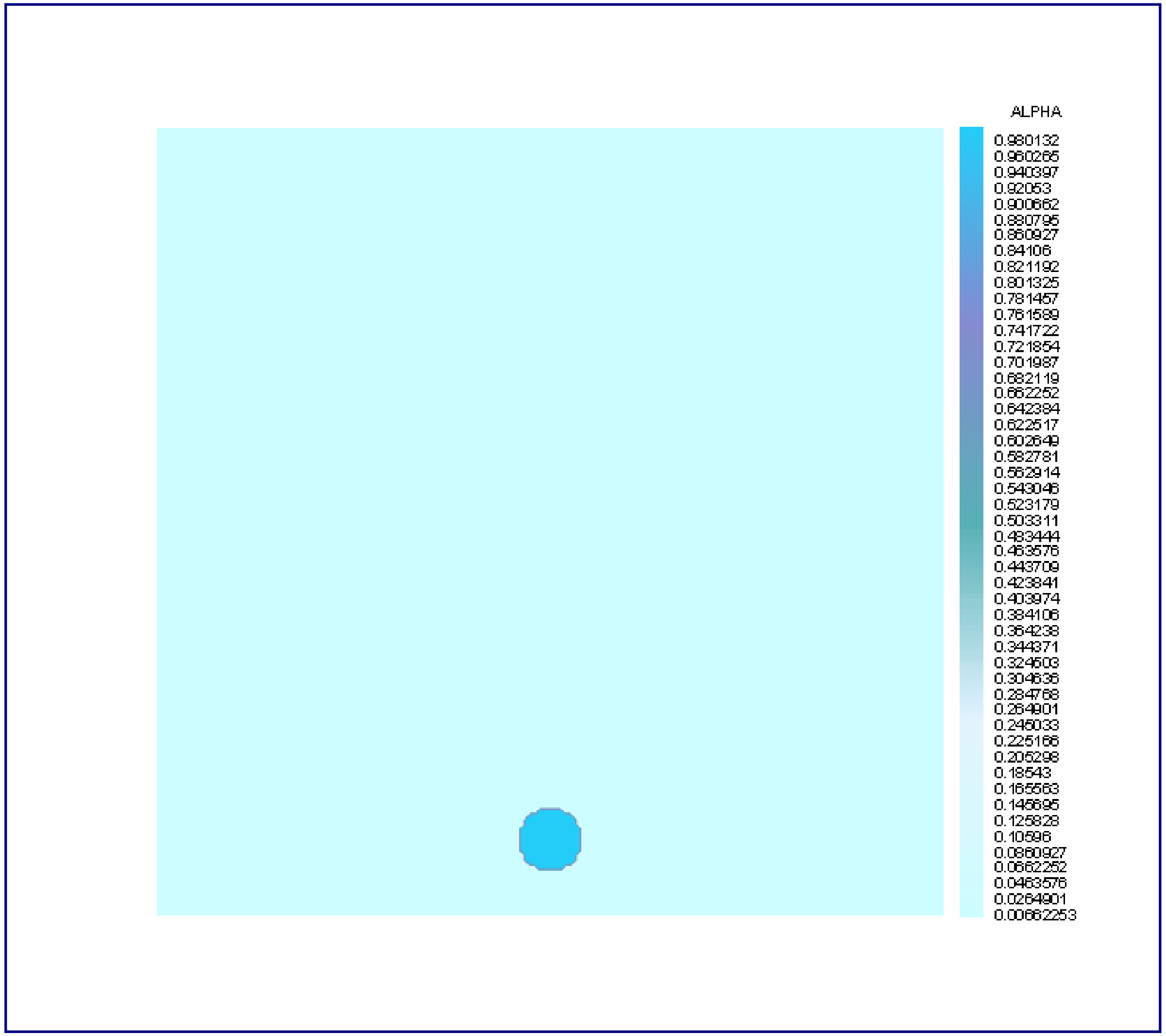
Computations shown with lines

Head-on collision of two liquid drops



Bubble explosion and collapse near a rigid wall

→ Surface erosion in cavitating systems



Next extension: Phase transition at interfaces

How to account for volume fraction variations due to mass transfer ?

- Mass transfer involves source terms in the mass equations:

$$\frac{\partial \alpha_1 \rho_1}{\partial t} + div(\alpha_1 \rho_1 \vec{u}) = \dot{m}_1 = \rho \dot{Y}_1$$

$$\frac{\partial \alpha_2 \rho_2}{\partial t} + div(\alpha_2 \rho_2 \vec{u}) = -\dot{m}_1 = -\rho \dot{Y}_1$$

$$\text{with } \dot{Y}_1 = \frac{dY_1}{dt} = \frac{d}{dt}\left(\frac{\alpha_1 \rho_1}{\rho}\right)$$

- Mass transfer also results in volume fraction variations:

$$\frac{d\alpha_1}{dt} = K div(\vec{u}) + AQ_1 + \frac{\dot{m}_1}{\rho_I}$$

The 'interfacial density' has to be determined.

Closure issues

The phase's entropy equations are examined.

$\frac{ds_1}{dt}$ and $\frac{ds_2}{dt}$ are determined as the solution of an algebraic system formed by:

- The energy conservation constraint
- The pressure equilibrium condition

$$\frac{ds_1}{dt} = \frac{H\left(T_2 - T_1\right)}{\alpha_1 \rho_1 T_1} + \frac{\rho \dot{Y}_1\left(h_1 - h_2\right)}{\rho_1 \Gamma_1 T_1\left(\frac{\alpha_1}{\Gamma_1} + \frac{\alpha_2}{\Gamma_2}\right)} + \frac{\rho \dot{Y}_1}{\alpha_1 \rho_1 T_1\left(\frac{\alpha_1}{\Gamma_1} + \frac{\alpha_2}{\Gamma_2}\right)} \left\{ \frac{\frac{\rho_1 c_1^2}{\alpha_1} + \frac{\rho_2 c_2^2}{\alpha_2}}{\rho_I} - \left(\frac{c_1^2}{\alpha_1} + \frac{c_2^2}{\alpha_2}\right) \right\}$$

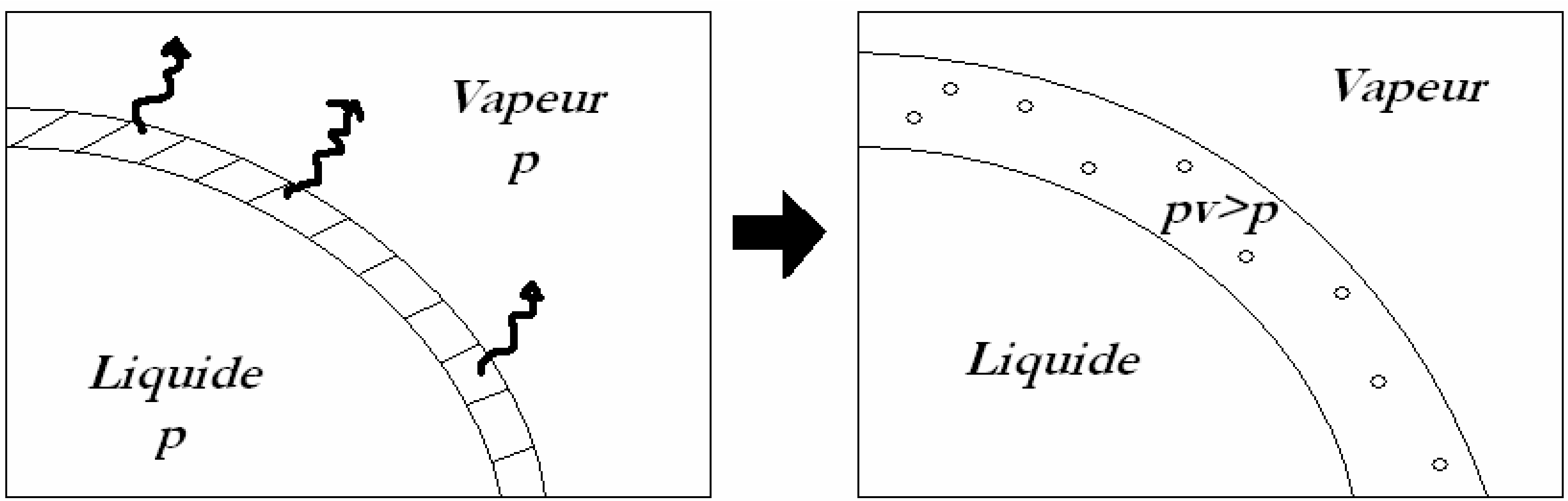
Heat exchanges

Chemical relaxation

Entropy production due to mechanical relaxation during mass transfer→ this relaxation occurs by the way of acoustic waves (isentropic)

Why mechanical relaxation during mass transfer is isentropic ?

Example : Evaporation of a liquid layer in a closed vessel



Closure relations

- Examination of the phase's entropy equations → $\rho_I = \dfrac{\dfrac{\rho_1 c_1^2}{\alpha_1} + \dfrac{\rho_2 c_2^2}{\alpha_2}}{\dfrac{c_1^2}{\alpha_1} + \dfrac{c_2^2}{\alpha_2}}$
- Examination of the entropy inequality:

$$\frac{\partial \rho s}{\partial t} + \mathrm{div}\left(\rho s \vec{u}\right) \geq 0 \quad \text{with } s = Y_1 s_1 + Y_2 s_2$$

Results in: $$\frac{H\left(T_2 - T_1\right)^2}{\rho} + \left(\overline{g}_2 - \overline{g}_1\right) T_I \dot{Y}_1 \geq 0$$

Thus mass transfer is modeled as $$\dot{Y}_1 = \nu\left(\overline{g}_2 - \overline{g}_1\right)$$

$$g = h - Ts = \text{Gibbs free energy}$$

Summary of the flow model

- Volume fraction equation:

$$\frac{\partial \alpha_1}{\partial t}+\vec{u}.\mathrm{grad}(\alpha_1)=\frac{(\rho_2 c_2^2-\rho_1 c_1^2)}{\dfrac{\rho_1 c_1^2}{\alpha_1}+\dfrac{\rho_2 c_2^2}{\alpha_2}}\mathrm{div}(\vec{u})+\rho\nu(g_2-g_1)\frac{\dfrac{c_1^2}{\alpha_1}+\dfrac{c_2^2}{\alpha_2}}{\dfrac{\rho_1 c_1^2}{\alpha_1}+\dfrac{\rho_2 c_2^2}{\alpha_2}}+H(T_2-T_1)\frac{\dfrac{\Gamma_1}{\alpha_1}+\dfrac{\Gamma_2}{\alpha_2}}{\dfrac{\rho_1 c_1^2}{\alpha_1}+\dfrac{\rho_2 c_2^2}{\alpha_2}}$$

Mechanical relaxation

volume variations linked to mass transfer

heat exchanges

- Mass equations

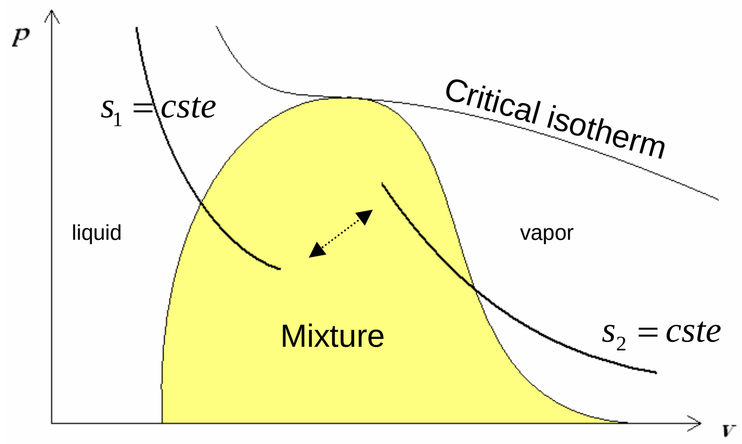
$$\frac{\partial \alpha_1\rho_1}{\partial t}+div(\alpha_1\rho_1\vec{u})=\rho\nu(g_2-g_1)$$

$$\frac{\partial \alpha_2\rho_2}{\partial t}+div(\alpha_2\rho_2\vec{u})=-\rho\nu(g_2-g_1)$$

- Momentum and energy

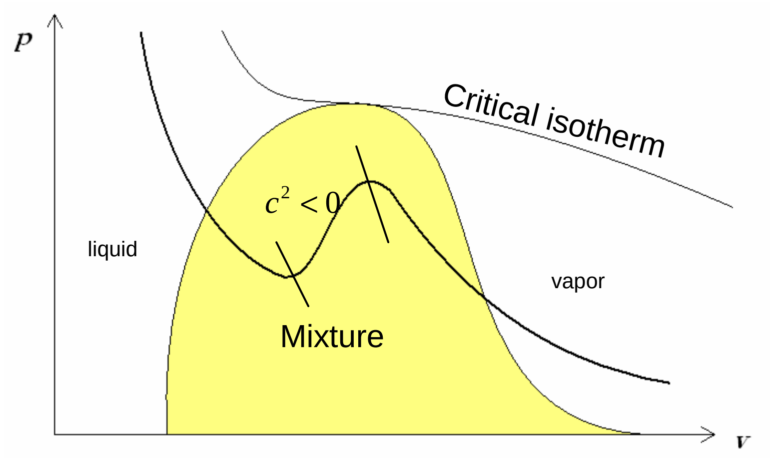
$$\frac{\partial \rho\vec{u}}{\partial t}+div(\rho\vec{u}\otimes\vec{u}+pI)=0 \qquad \frac{\partial \rho E}{\partial t}+div(\vec{u}(\rho E+p))=0$$

Remark: the model involves 2 temperatures and entropies



Hyperbolicity is preserved in the spinodal zone: the connection of the two isentropes is modeled as a **kinetic path**

- Very different of the Van der Waals model



Mass transfer is modeled as a **thermodynamic path**:

$$c^2 = -v^2 \left.\frac{\partial p}{\partial v}\right)_{s=cte} < 0$$

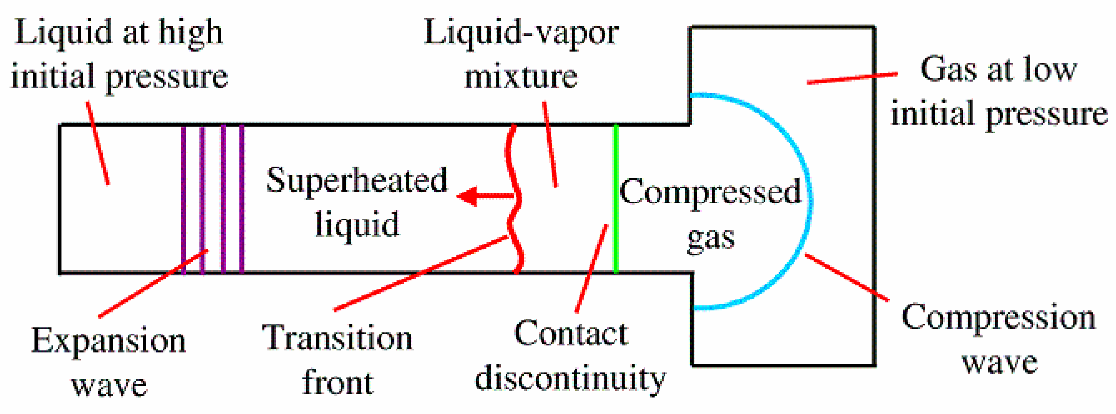
→ ill posed model

Kinetic parameters ?

- The model requires heat exchange (H) and evaporation kinetics (ν) relaxation parameters

How to chose them ?

- Evaporation front observed in expansion tubes

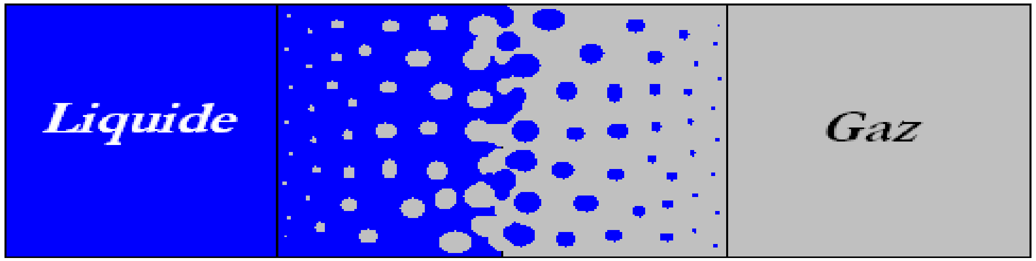


→ 4 waves are present in such experiment: left expansion, evaporation front, contact discontinuity, right shock wave.

Relaxation of metastable states at interfaces

At the interface when one of the fluids is metastable instantaneous relaxation is assumed:

$$\nu, H = \begin{cases} +\infty & \text{if} \quad \varepsilon < \alpha_k < 1-\varepsilon \\ 0 & \text{otherwise} \end{cases}$$



$$\varepsilon < \alpha_k < 1-\varepsilon$$

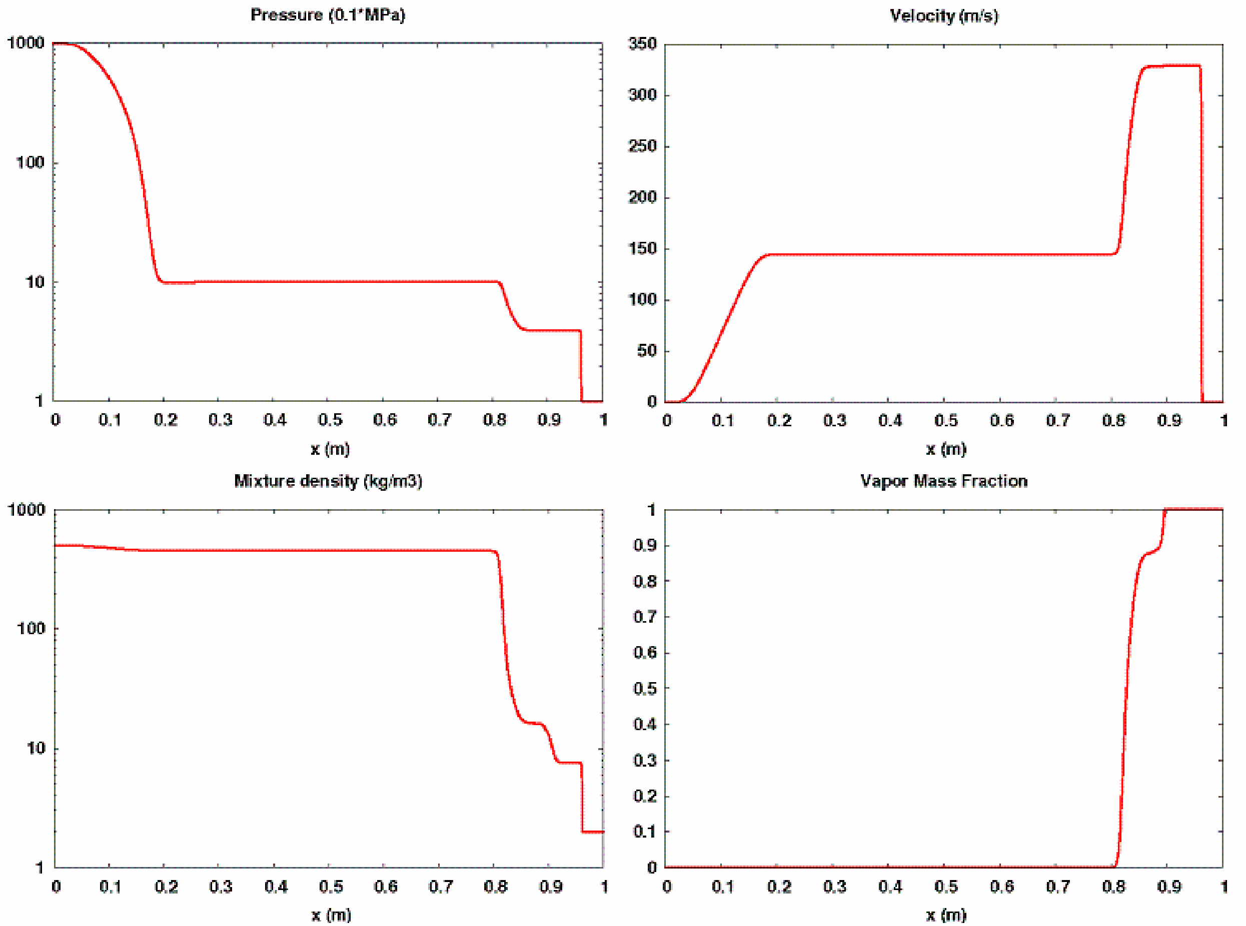
→ The interface is assumed at thermodynamic equilibrium

BUT

→ Acoustic precusors are present and produce metastable states

Shock tube with phase transition (relaxation) at the interface

Liquid at high pressure	Vapor at low pressure

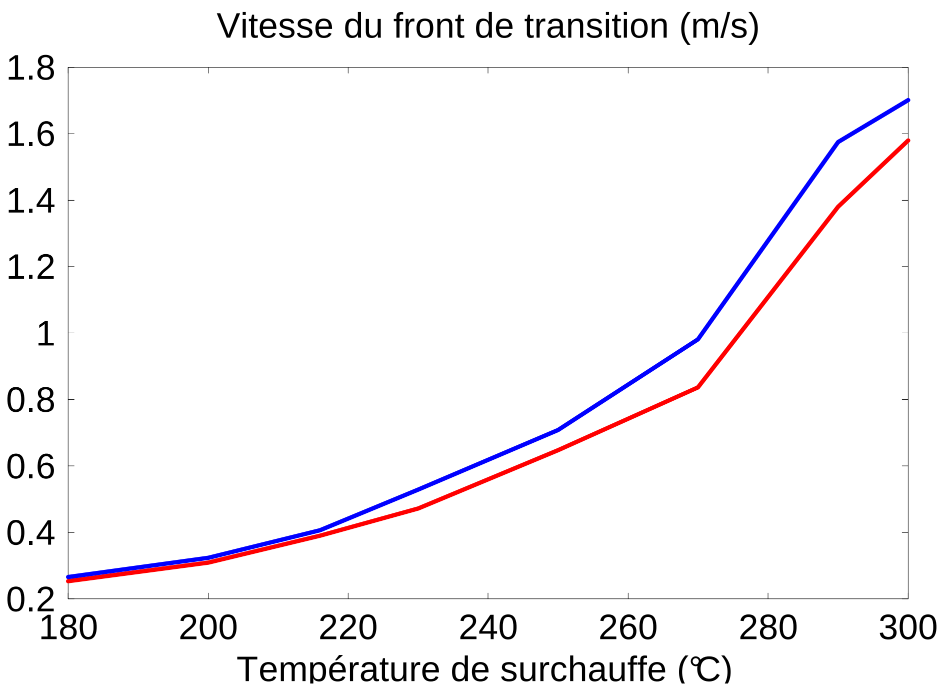


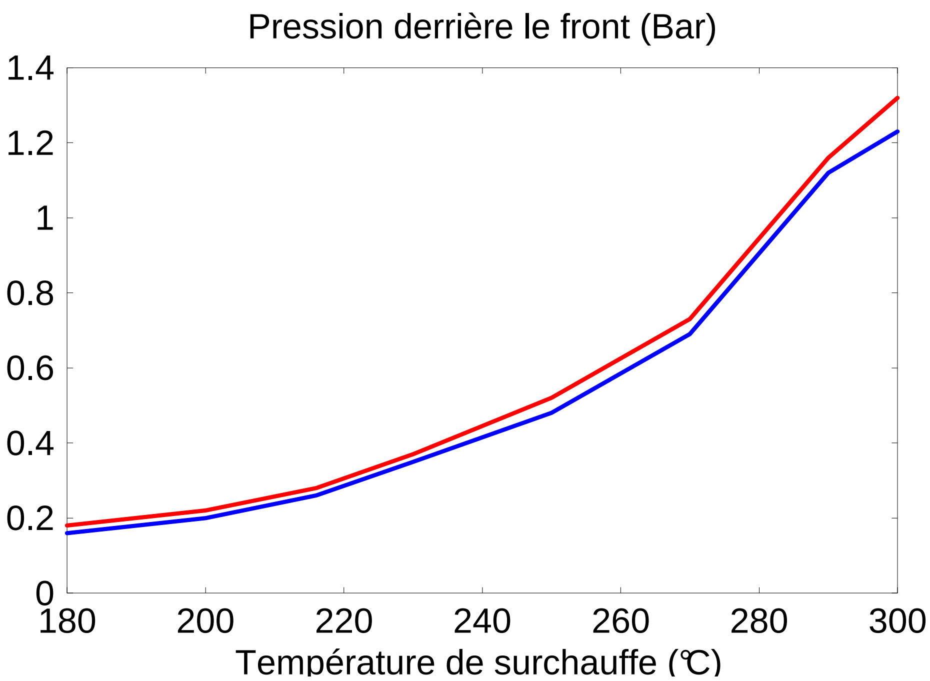
4 waves are observed

→ Relaxation terms are responsible for the appearance of an extra wave (evaporation front)

Validations for different initial liquid temperatures

- Caltech experiments in red: Simoes Moreira and Shepherd, JFM, 1999
- Computations in blue lines





Limit model

- The limit model solved at the interface when v and H tend to infinity corresponds to the mixture Euler equations:

$$\begin{cases} \dfrac{\partial \rho}{\partial t} + \dfrac{\partial \rho u}{\partial x} = 0 \\ \dfrac{\partial \rho u}{\partial t} + \dfrac{\partial (\rho u^2 + p)}{\partial x} = 0 \\ \dfrac{\partial \rho E}{\partial t} + \dfrac{\partial (\rho E + p) u}{\partial x} = 0 \end{cases}$$

$$\rho = \alpha_1 \rho_1 + \alpha_2 \rho_2$$
$$\rho E = \alpha_1 \rho_1 E_1 + \alpha_2 \rho_2 E_2$$

- Wave's speeds are: $u - c_{eq}$, u and $u + c_{eq}$

$$\text{Avec} \quad \frac{1}{\rho c_{eq}} = \frac{1}{\rho c_w} + T\left[\frac{\alpha_1 \rho_1}{C_{p,1}}\left(\frac{ds_1}{dp}\right)^2 + \frac{\alpha_2 \rho_2}{C_{p,2}}\left(\frac{ds_2}{dp}\right)^2\right]$$

$$\Rightarrow \quad \boxed{c_{eq} < c_{wood}}$$

$$\frac{1}{\rho c^2_{wood}} = \frac{\alpha_1}{\rho_1 c_1^2} + \frac{\alpha_2}{\rho_2 c_2^2}$$

Remarks

- The hyperbolic system with 5 equations connects two limit models:
  - a mechanical equilibrium model responsible for acoustic propagation and metastable states appearance
  - a thermodynamical equilibrium model used in order to match interface conditions

$$\begin{cases} \dfrac{d\alpha_1}{dt} = K\dfrac{\partial u}{\partial x} + AQ_1 + \dfrac{\dot{m}_1}{\rho_I} \\ \dfrac{\partial \alpha_1\rho_1}{\partial t} + \dfrac{\partial \alpha_1\rho_1 u}{\partial x} = \dot{m}_1 \\ \dfrac{\partial \alpha_2\rho_2}{\partial t} + \dfrac{\partial \alpha_2\rho_2 u}{\partial x} = -\dot{m}_1 \\ \dfrac{\partial \rho u}{\partial t} + \dfrac{\partial\left(\rho u^2 + p\right)}{\partial x} = 0 \\ \dfrac{\partial \rho E}{\partial t} + \dfrac{\partial\left(\rho E + p\right)u}{\partial x} = 0 \end{cases}$$

The model involves 5 waves:

u, u+c_w, u-c_w

u+c_{eq}, u-c_{eq} that appear as a result of relaxation terms

A physical result is obtained: The evaporation front speed in metastable liquids corresponds to those of acoustic waves of the relaxed system

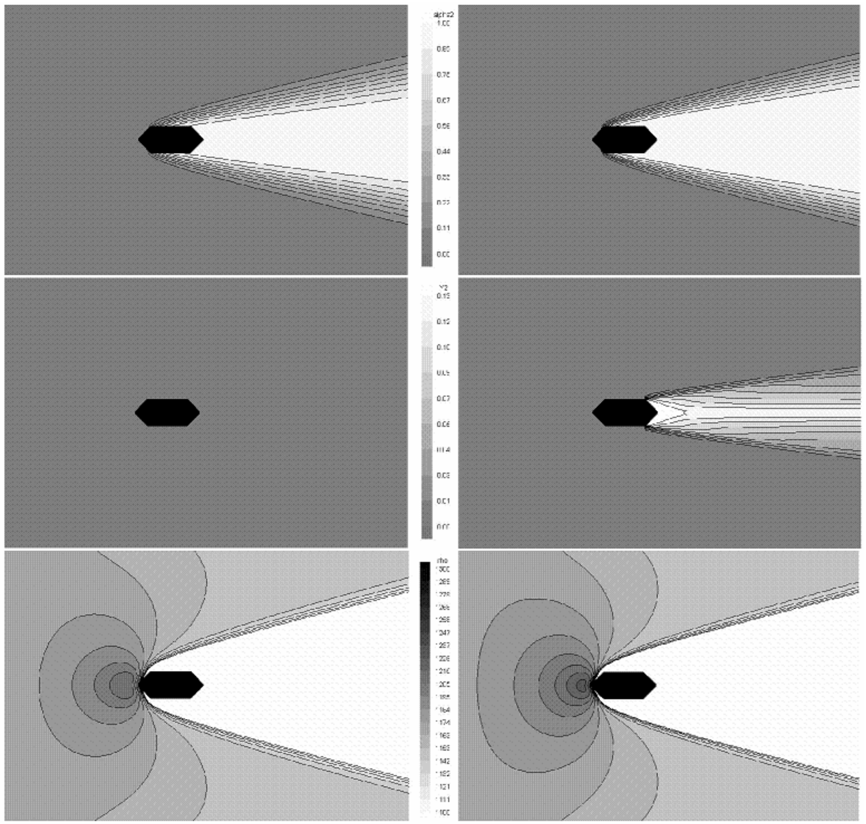
The 2 wave's speeds $u \pm c_{eq}$, correspond exactly to the Chapman Jouguet kinetic relation proposed by:

Thompson et al. JFM (1987)
Kurschat et al., JFM (1992)
Moreira & Shepherd, JFM (1999)

It is now demonstrated as an eigenvalue of the relaxed system.

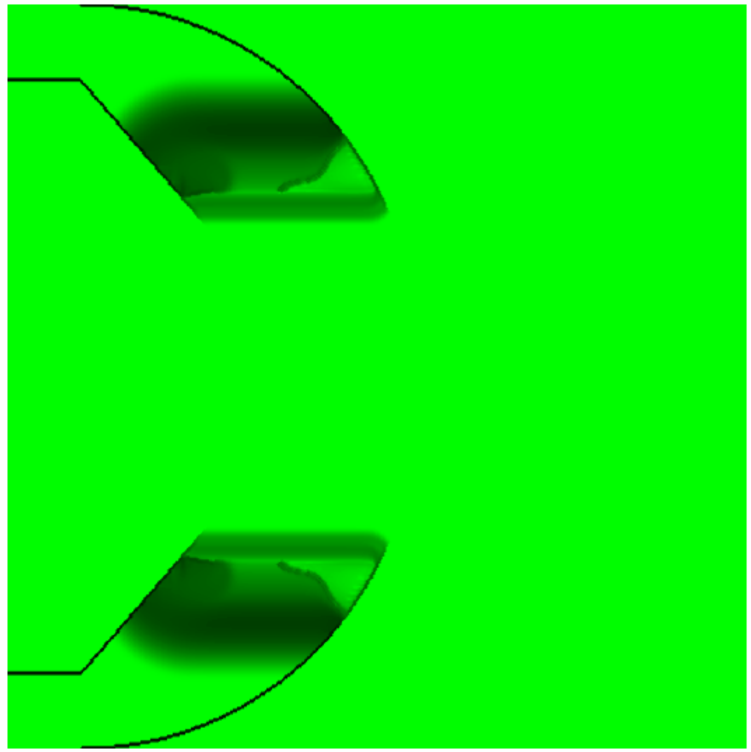
Application to cavitating flows

Hypervelocity underwater projectile



Without mass transfer With mass transfer

Fuel injection through nozzles:
Metastable states are accounted for

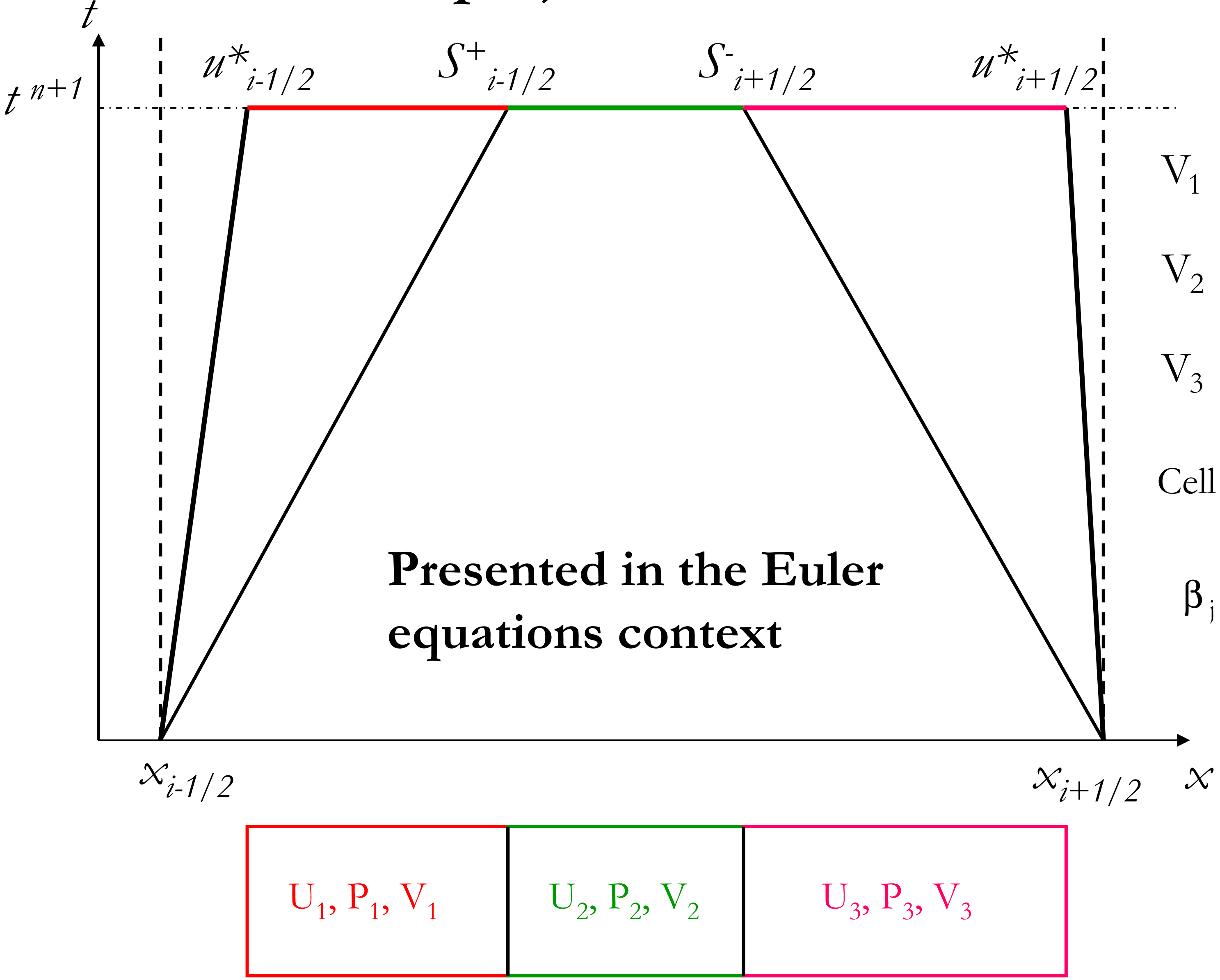


Numerical approximations

- Let us turn back to the basic 5 equations model without mass transfer and without capillary effects.
- The shock relations are known as well as Riemann invariants → the Riemann problem can be solved.
- How to average a non conservative variables in a given cell ?

$$\frac{\partial \alpha_1}{\partial t} + u \frac{\partial \alpha_1}{\partial x} = \frac{(\rho_2 c_2^2 - \rho_1 c_1^2)}{\frac{\rho_1 c_1^2}{\alpha_1} + \frac{\rho_2 c_2^2}{\alpha_2}} \frac{\partial u}{\partial x}$$

The relaxation-projection method: Saurel et al., JCP, 2007



$$V_1 = \Delta t(S^+_{i-1/2} - u^*_{i-1/2})$$

$$V_2 = \Delta x_i^{n+1} - V_1 - V_3$$

$$V_3 = \Delta t(u^*_{i+1/2} - S^-_{i+1:2})$$

Cell volume fractions def.

$$\beta_j = \frac{V_j}{\Delta x_i^{n+1}} \qquad j = 1,..,3$$

A relaxation system that replaces the use of the EOS

$$
\begin{cases}
\dfrac{\partial \beta_j}{\partial \tau} = \mu \beta_j (p_j - p_I) \\
\dfrac{\partial \beta_j \rho_j}{\partial \tau} = 0 \\
\dfrac{\partial \beta_j \rho_j u_j}{\partial \tau} = \lambda Y_j (u_I - u_j) \\
\dfrac{\partial \beta_j \rho_j E_j}{\partial \tau} = -p_I \mu \beta_j (p_j - p_I) + u_I \lambda Y_j (u_I - u_j)
\end{cases}
$$

Conservation and entropy inequality are preserved if:

$$
\begin{cases}
p_I = \sum_j \beta_j p_j \\
\mathrm{u_I} = \sum_{\mathrm{j}} \mathrm{Y_j u_j}
\end{cases}
$$

This system is derived with the Discrete Equations Method (DEM), Abgrall and Saurel, JCP, 2003.

Approximate integration of this system is possible in the limit $\tau \longrightarrow +\infty$

→ Algebraic non linear system solved with the Newton method.

Comparison with the Godunov method

- Conventional Godunov averages assume a single pressure, velocity and **temperature** in the cell. In the new method, we determine the **cell velocity and pressure are determined but several sub-cell temperatures remain.**
- The method guarantees conservation and volume fraction positivity
- The method does not use any flux and is valid for non conservative equations
- In the case of the ideal gas and the stiffened gas EOS with the Euler equations both methods are equivalent. Results are different for more complicated EOS (Mie-Gruneisen for example)
- The new method gives a cure to anomalous computation of some basic problems:

  - Sliding lines

  - Propagation of a density discontinuity in an uniform flow with Mie Gruneisen EOS.
- It can be used in Lagrange or Lagrange + Projection codes.

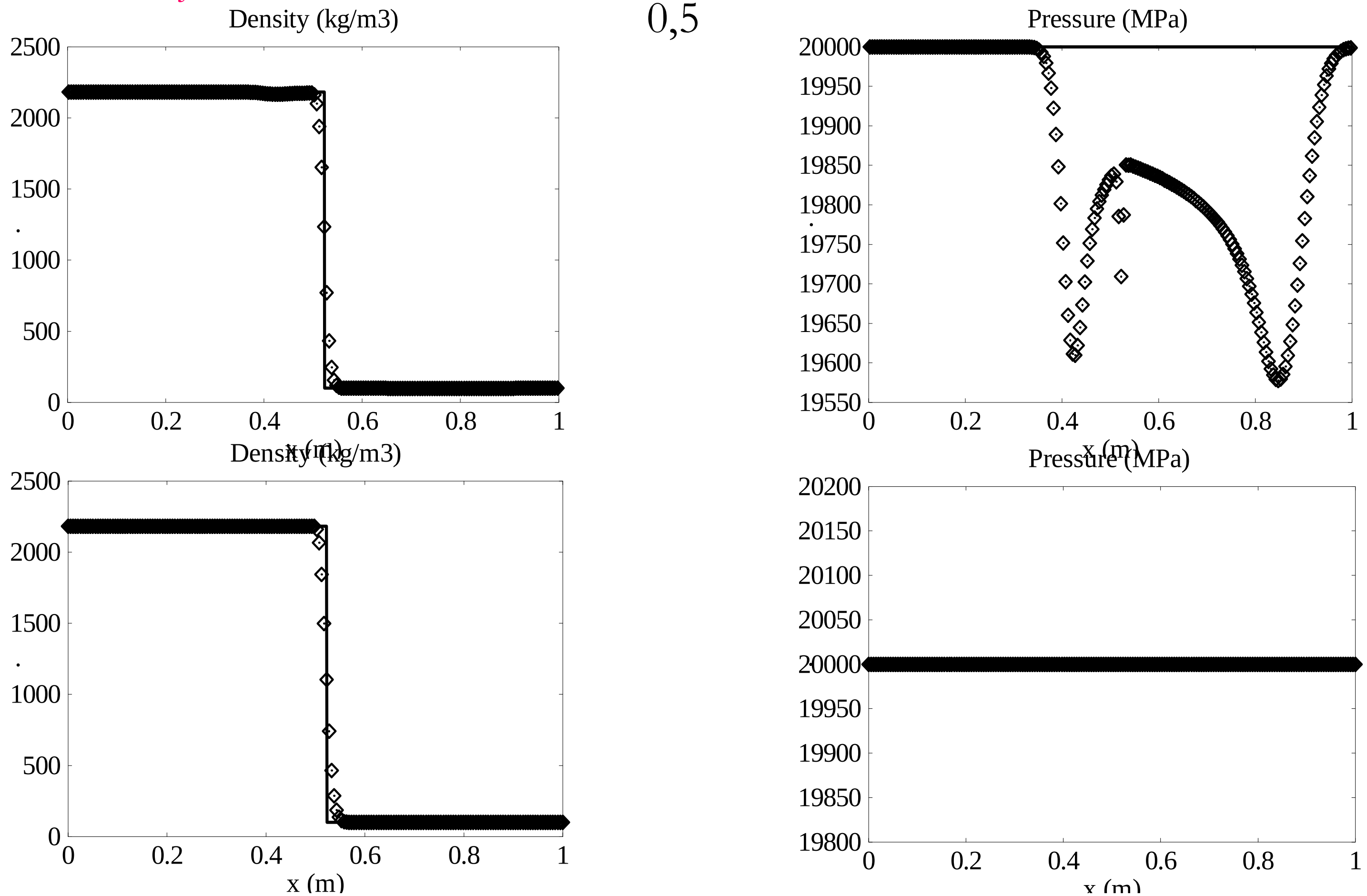
Propagation of a density discontinuity in a uniform flow with the Euler equations and JWL EOS

$P = P_{CJ} = 2\ 10^{10}$ Pa	$P = P_{CJ} = 2\ 10^{10}$ Pa
$u = 1000$ m/s	$u = 1000$ m/s
$\rho = \rho_{CJ} = 2182$ kg/m^3	$\rho = 100$ kg/m^3

0 0,5 1

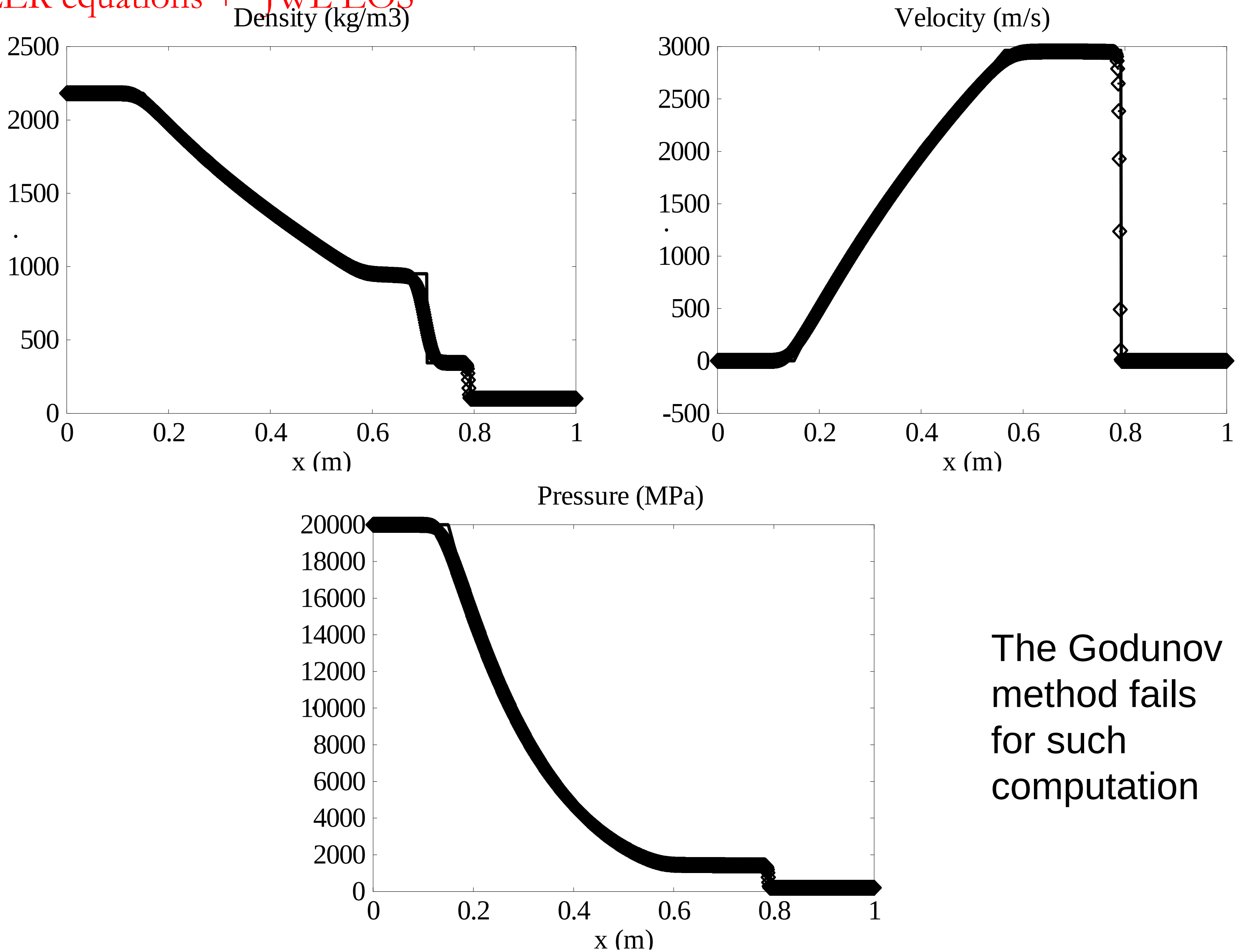
Godunov

New method



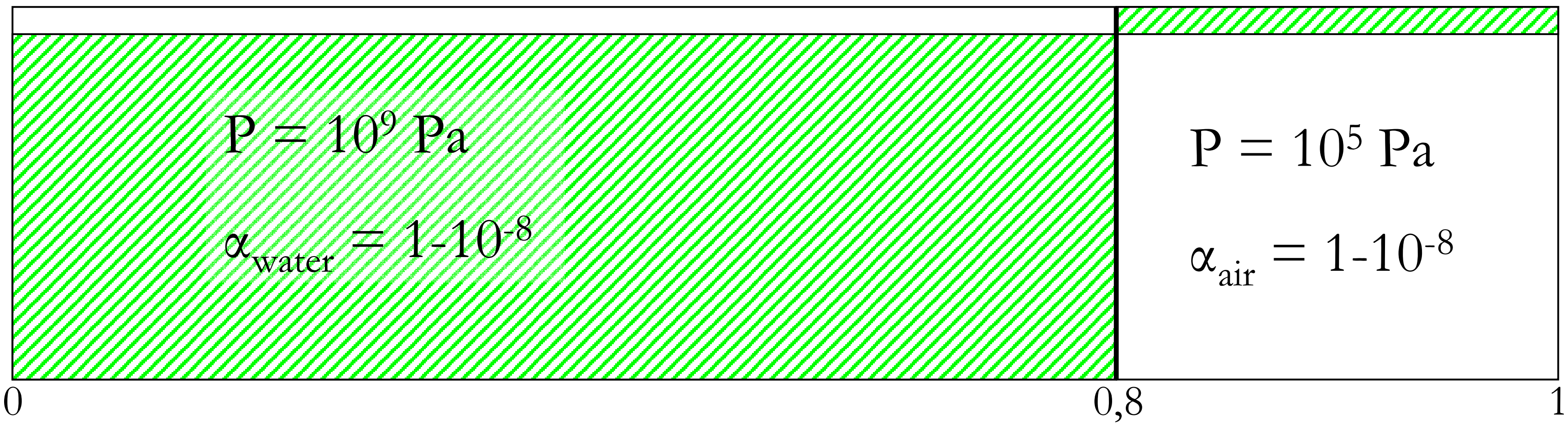
Shock tube problem in extreme conditions

EULER equations + JWL EOS



The Godunov method fails for such computation

Shock tube problem with almost pure fluids: Liquid-Gas interface with the 5 equations model

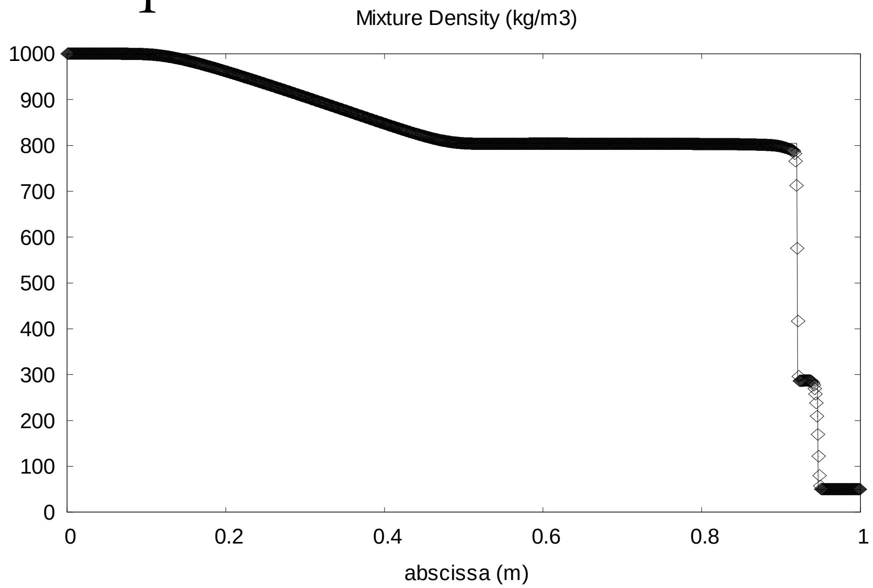


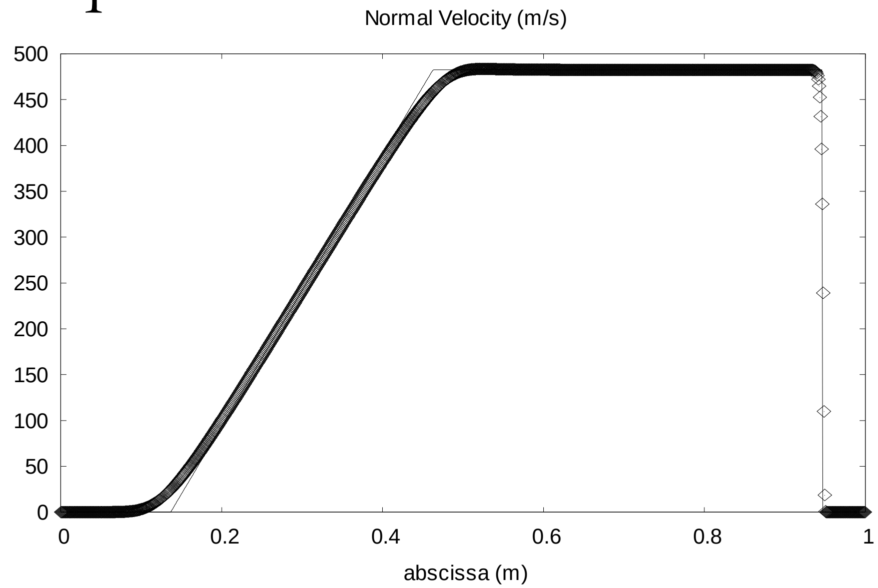
$\rho_{water} = 1000\ kg/m^3$

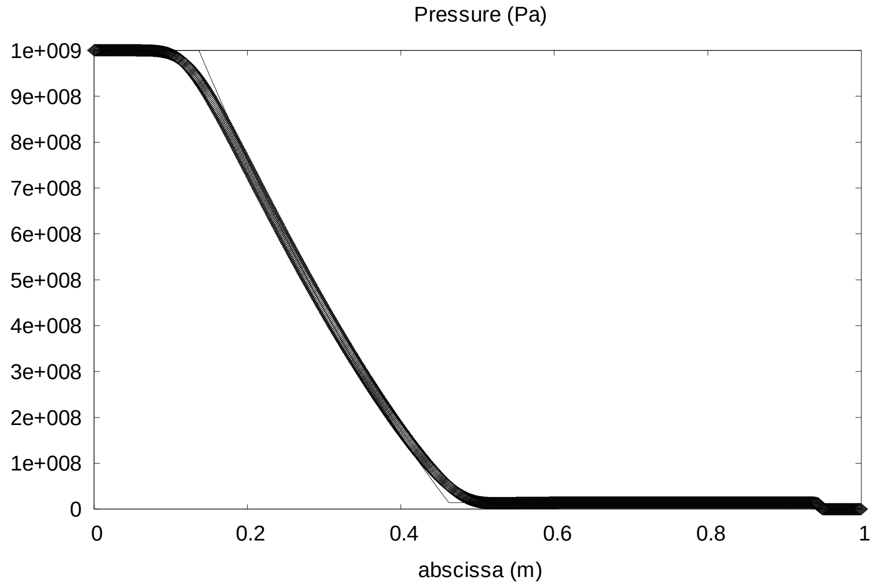
$\rho_{air} = 50\ kg/m^3$

Stiffened Gas EOS

Shock tube problem with almost pure fluids: Liquid-Gas interface with the 5 equations model







Perspectives

- Coupling capillary effects and phase transition.
- Eulerian elastic-plastic modeling in the context of this multiphase theory.

Thank you for your attention

```
ERROR: invalidrestore
OFFENDING COMMAND: restore

STACK:

-savelevel-
-savelevel-
0
0
```