





Diffuse interfaces with compressible fluids, phase transition and capillarity

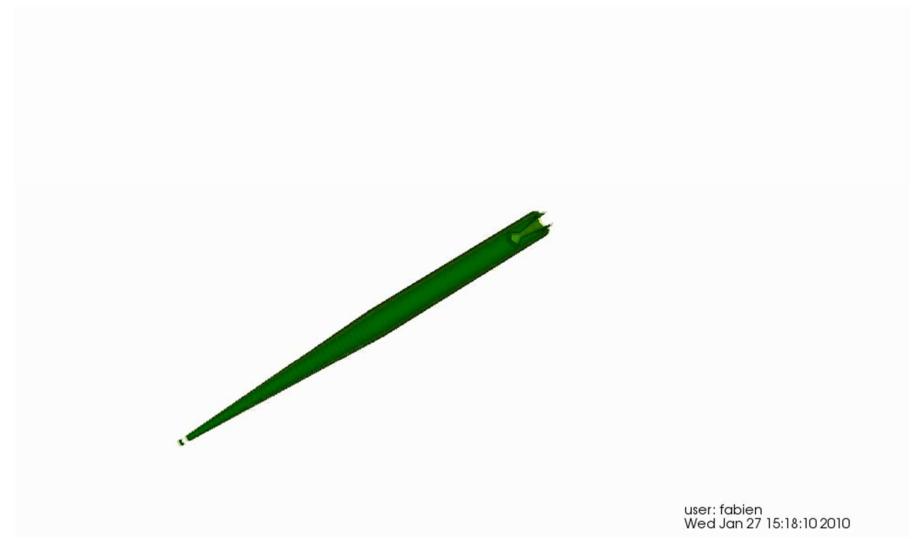
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Aims of the "diffuse interface" approach

- Solve liquid and gas flows with real density jumps at arbitrary speeds, separated by interfaces.
- Consider compressibility of both phases.
- Consider surface tension, heat diffusion and phase transition.
- Address waves propagation (possibly shocks).

Example: Underwater supercavitating missile (400 km/h) 2 interfaces are present: liquid-vapor and gas-vapor



Petitpas, Massoni, Saurel and Lapébie, 2009, Int. J. Mult. Flows

Preliminary remarks

- The 'diffuse interfaces' under consideration come from numerical diffusion (not capillary nor viscous regularization),
- These interfaces are captured with an hyperbolic flow solver.
- The numerical diffusion can be reduced (1-2 points work in progress).
- All fluids are considered compressible with a convex EOS.
- The 'Noble-Abel-stiffened-gas' EOS is a good prototype example:

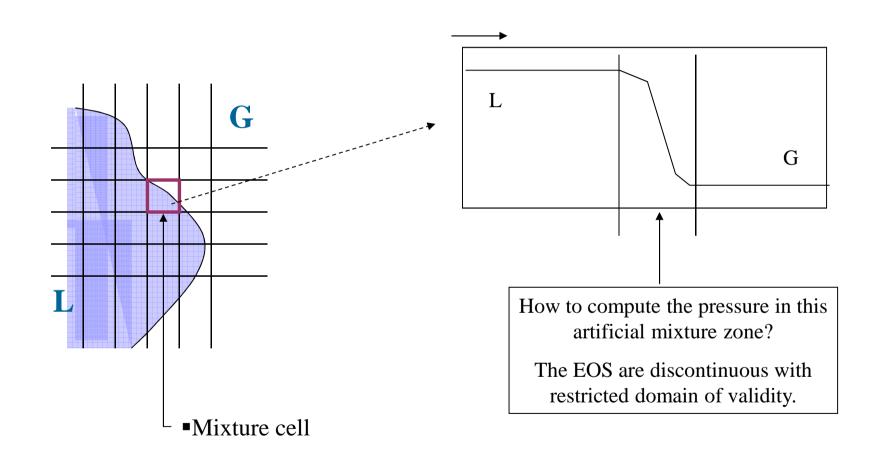
$$p_k = (\gamma_1 - 1) \frac{\rho_k (e_k - q_k)}{1 - \rho_k b_k} - \gamma_k p_{\infty k} \qquad k = 1, 2$$
(Le Metayer-Saurel, POF, 2016)

It is both an improved SG formulation and simplified van der

Waals formulation $(p_{\infty k} = \text{cst. instead of } p_{\infty k} = a\rho^2)$

- → well defined sound speed
- The liquid and vapour constants are coupled through the phase diagram (and saturation curves).

Diffuse interfaces of simple contact (with compressible fluids)



Starting point of the diffuse interfaces method: Consider mixture cells through a total non-equilibrium twophase model with 2 velocities, 2 temperatures, 2 pressures

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

Each phase evolves in its own sub-volume.

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

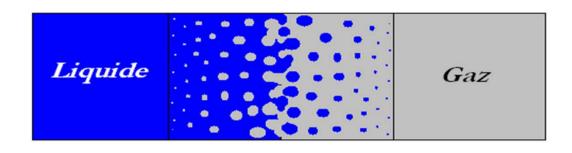
The pressure equilibrium condition is replaced by a PDE with relaxation → hyperbolicity is preserved.

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

$$\frac{\partial \alpha_{l} \rho_{1} E_{1}}{\partial t} + \frac{\partial u_{1} (\alpha_{l} \rho_{1} E_{1} + \alpha_{l} p_{1})}{\partial x} = \overline{p}_{i} \overline{u}_{i} \frac{\partial \alpha_{k}}{\partial x} - \mu \overline{p}_{i}' (p_{1} - p_{2}) + \lambda \overline{u}_{i}' (u_{2} - u_{1})$$

3 symmetric equations are used for the second phase.

Fulfill interface conditions of equal pressures and equal velocities → stiff relaxation



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

'bubbles' expansion or contraction forces mechanical equilibrium locally:

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

Similar relaxation is done for velocities (Saurel and Abgrall, JCP, 1999)

This trick enables fulfilment of interface conditions.

In other words...

This method deals with 2 steps:

- -Solve the 7 equations model without relaxation terms during a time step → 2 velocities and 2 pressures are computed in the mixture zone.
- -Relax (reset) the 2 velocities and pressures to their equilibrium values:

$$\begin{split} &\frac{\partial \alpha_1}{\partial t} = \mu(p_1 - p_2) \\ &\frac{\partial \alpha_1 \rho_1}{\partial t} = 0 \\ &\frac{\partial \alpha_1 \rho_1 u_1}{\partial t} = \lambda(u_2 - u_1) \\ &\frac{\partial \alpha_1 \rho_1 E_1}{\partial t} = -\mu \overline{p}_i'(p_1 - p_2) + \lambda \overline{u}_i'(u_2 - u_1) \end{split}$$

Solve this ODE system in the limit

$$\lambda \to +\infty$$

$$\mu \to +\infty$$

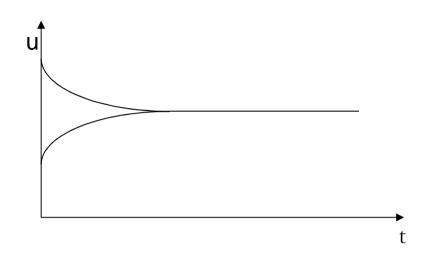
This ODE system is replaced by two algebraic systems.

Example with velocity relaxation

We have to solve:

$$\begin{split} &\frac{\partial \alpha_1 \rho_1}{\partial t} = 0 \\ &\frac{\partial \alpha_1 \rho_1 u_1}{\partial t} = \lambda (u_2 - u_1) \\ &\frac{\partial \alpha_2 \rho_2}{\partial t} = 0 \\ &\frac{\partial \alpha_2 \rho_2 u_2}{\partial t} = -\lambda (u_2 - u_1) \end{split}$$

At relaxed state $u_1^* = u_2^* = u^*$



Summing the two momentum equations results in:

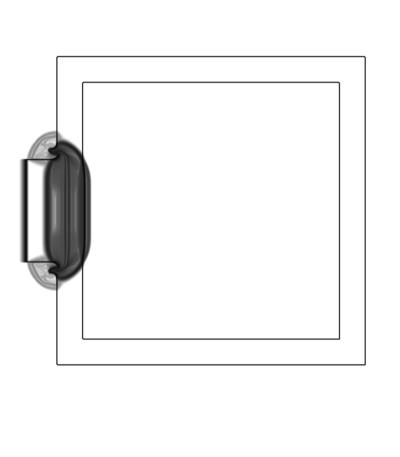
$$\frac{\partial(\alpha_1\rho_1u_1 + \alpha_2\rho_2u_2)}{\partial t} = 0$$

Integrating this equation between the end of the propagation step and the relaxed step results in:

$$\begin{aligned} & \left(\alpha_{1}\rho_{1}u_{1}+\alpha_{2}\rho_{2}u_{2}\right)^{*} = \left(\alpha_{1}\rho_{1}u_{1}+\alpha_{2}\rho_{2}u_{2}\right)^{0} \\ & \text{Thus:} \qquad u^{*} = \frac{\left(\alpha_{1}\rho_{1}u_{1}+\alpha_{2}\rho_{2}u_{2}\right)^{0}}{\left(\alpha_{1}\rho_{1}+\alpha_{2}\rho_{2}\right)^{*}} = \frac{\left(\alpha_{1}\rho_{1}u_{1}+\alpha_{2}\rho_{2}u_{2}\right)^{0}}{\left(\alpha_{1}\rho_{1}+\alpha_{2}\rho_{2}\right)^{0}} \end{aligned}$$

The same type of procedure is done for pressure relaxation.

Computational example: Impact of copper projectile at 5 km/s on a copper tank filled with water, surrounded by air.



Very robust but quite complicated if interface only are under consideration. Helpful when velocity disequilibrium effects are under consideration.

Reduced model with single pressure and single velocity but two temperatures

- Faster computations
- Add physical effects easily (surface tension, phase transition)...

$$\lambda, \mu = 1/\epsilon \rightarrow +\infty$$
 Relaxation coefficients are assumed stiff.

$$f = f^{\circ} + \varepsilon f^{1}$$
 Each flow variable evolves with small perturbations around an equilibrium state.

Consequence

The pressure relaxation term becomes a differential one:

$$\frac{\partial \alpha_{1}}{\partial t} + \overline{u}_{1} \frac{\partial \alpha_{1}}{\partial x} = \mu(p_{1} - p_{2})$$

$$\mu(p_{1} - p_{2}) \rightarrow \frac{\left(\rho_{2}c_{2}^{2} - \rho_{1}c_{1}^{2}\right)}{\left(\frac{\rho_{1}c_{1}^{2}}{\alpha_{1}} + \frac{\rho_{2}c_{2}^{2}}{\alpha_{2}}\right)} \frac{\partial u}{\partial x}$$

Kapila et al., POF, 2001

$$\frac{\partial \alpha_{1}}{\partial t} + u \frac{\partial \alpha_{1}}{\partial x} = \frac{(\rho_{2}c_{2}^{2} - \rho_{1}c_{1}^{2})}{\rho_{1}c_{1}^{2}} \frac{\partial u}{\partial x}$$

$$\frac{\partial \alpha_{1}\rho_{1}}{\partial t} + \frac{\partial \alpha_{1}\rho_{1}u}{\partial x} = 0$$

$$\frac{\partial \alpha_{2}\rho_{2}}{\partial t} + \frac{\partial \alpha_{2}\rho_{2}u}{\partial x} = 0$$

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

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

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

$$p = p(\rho, e, \alpha_1, Y_1) = \frac{\rho\left(e - (Y_1q_1 + Y_2q_2)\right) - \left(\frac{\alpha_1\gamma_1p_{\infty 1}(1 - \rho_1b_1)}{\gamma_1 - 1} + \frac{\alpha_2\gamma_2p_{\infty 2}(1 - \rho_2b_2)}{\gamma_2 - 1}\right)}{\frac{\alpha_1(1 - \rho_1b_1)}{\gamma_1 - 1} + \frac{\alpha_2(1 - \rho_2b_2)}{\gamma_2 - 1}}$$

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

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

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

Two-phase shock relations are given in Saurel et al., Shock Waves, 2007.

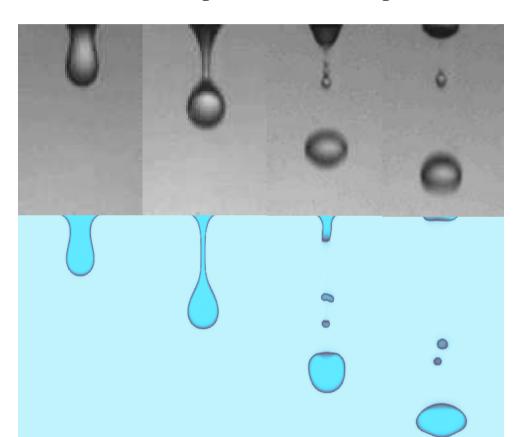
Capillary effects can be added (Perigaud and Saurel, JCP, 2005)

- Compressibilty is considered as well as surface tension.
- Thermodynamics and capillarity are decoupled: no need to enlarge the interface.
- Two Gibbs identities are used: $de_k = T_k ds_k pdv_k$ and $de_{\sigma} = \sigma dS$
- There is no capillary lenght to resolve: Jump conditions deal with capillarity as they deal with shocks (genuine property of the conservative formulation),

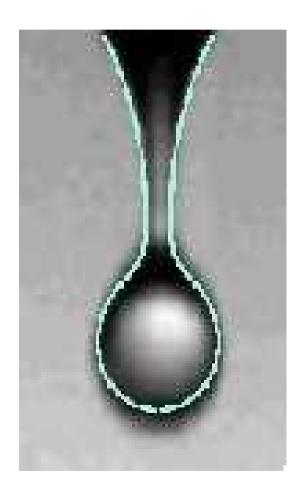
Falling droplet from the roof

(computations done in 2004)

Qualitative comparisons (2D computations)



Quantitative comparisons (2D axi)



Phase transition

Examination of the mixture entropy production suggests (Saurel et al., JFM, 2008)

$$\frac{\partial \alpha_1 \rho_1}{\partial t} + \operatorname{div}(\alpha_1 \rho_1 \vec{\mathbf{u}}) = \rho \nu (g_2 - g_1)$$
$$\frac{\partial \alpha_2 \rho_2}{\partial t} + \operatorname{div}(\alpha_2 \rho_2 \vec{\mathbf{u}}) = -\rho \nu (g_2 - g_1)$$

Phase transition is modeled as a Gibbs free energy relaxation process.

$$\frac{\partial \rho u}{\partial t} + \operatorname{div}(\rho u \otimes u) + \operatorname{grad}(p) = 0$$

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

But two kinetic parameters are now present.

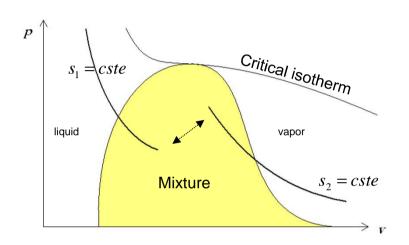
$$\frac{\partial \alpha_{1}}{\partial t} + \vec{u}.grad(\alpha_{1}) = \frac{(\rho_{2}c_{2}^{2} - \rho_{1}c_{1}^{2})}{\rho_{1}c_{1}^{2} + \rho_{2}c_{2}^{2}} div(\vec{u}) + \rho v(g_{2} - g_{1}) \frac{\frac{c_{1}^{2}}{\alpha_{1}} + \frac{c_{2}^{2}}{\alpha_{2}}}{\frac{\rho_{1}c_{1}^{2}}{\alpha_{1}} + \frac{\rho_{2}c_{2}^{2}}{\alpha_{2}}} + H(T_{2} - T_{1}) \frac{\frac{\Gamma_{1}}{\alpha_{1}} + \frac{\Gamma_{2}}{\alpha_{2}}}{\frac{\rho_{1}c_{1}^{2}}{\alpha_{1}} + \frac{\rho_{2}c_{2}^{2}}{\alpha_{2}}}$$

Pressure relaxation

Phase change

Heat exchange

The model involves two entropies

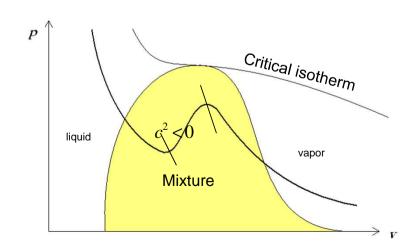


Phase transition connects the two isentropes through a kinetic path (mass source terms).

Sound speed is defined everywhere:

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

• Very different of the van der Waals (and variants) approaches



With VdW phase transition is modeled as a kinetic path and sound speed is undefined

$$c^2 = -v^2 \frac{\partial p}{\partial v} \Big|_{s} < 0$$

→ III posed model.

Thermodynamic closure

Each fluid is governed by the NASG EOS (Le Metayer and Saurel, Phys.

Fluids, 2016)
$$p_{k}(\rho_{k}, e_{k}) = (\gamma_{k} - 1) \frac{\rho_{k}(e_{k} - q_{k})}{1 - \rho_{k}b_{k}} - \gamma_{k}p_{\infty k}$$
short distances repulsion

With the help of Gibbs identity and Maxwell relations:

$$e(P,T) = \frac{P + \gamma p_{\infty}}{P + p_{\infty}} C_V T + q$$

$$v(P,T) = \frac{(\gamma - 1)C_VT}{P + P_{\infty}} + b$$

$$h(P,T) = \gamma C_V T + bP + q$$

$$g(P,T) = (\gamma C_v - q')T - C_v T \ln \frac{T^{\gamma}}{(p + p_{\infty})^{\gamma - 1}} + bP + q$$

EOS parameters

Each fluid EOS requires 6 parameters:

$$\gamma$$
, P_{∞} , C_{V} , b , q , q'

The liquid and gas saturation curves are used

$$h_{k}(P,T) \qquad | \setminus h_{k,sat}(T) \longrightarrow \gamma_{k}C_{V,k}$$

$$v(P,T) \qquad | \setminus V_{k,sat}(T) \longrightarrow P_{\infty,k}, C_{V,k}$$

$$L_{V}(T) \qquad | \setminus L_{V,sat}(T) \longrightarrow q_{g}, q_{l}$$

$$ln(p) = A + \frac{B}{T} + Cln T + Dln(p + p_{\infty,l}) | \setminus P_{sat}(T) \longrightarrow q'_{g}, q'_{l}$$

$$T_{g} = T_{l}, p_{g} = p_{l}, g_{g} = g_{l}$$

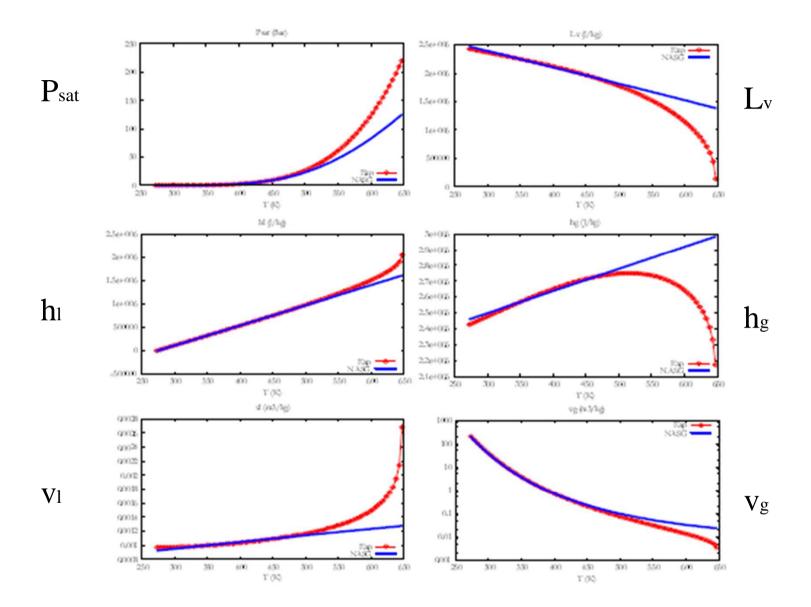


FIG. 6. Comparison between experimental (symbols) and NASG theoretical (lines) saturation curves for liquid water and steam with coefficients determined in the temperature range [300 – 500 K].

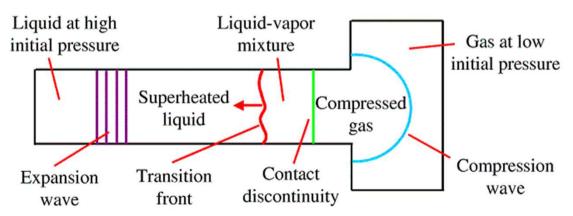
Data for water

Coefficients	Liquid phase	Vapor phase
$C_P(J/kg/K)$	4285	1401
$C_v(J/kg/K)$	3610	955
γ	1.19	1.47
$P_{\infty}(Pa)$	7028×10^5	0
$b(m^3/kg)$	6.61×10^{-4}	0
q(J/kg)	-1177788	2077616
q'(J/(kg.K))	0	14317

Kinetic parameters?

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

Evaporation front observations in expansion tubes (Simoes Moreira and Shepherd, JFM, 1999)

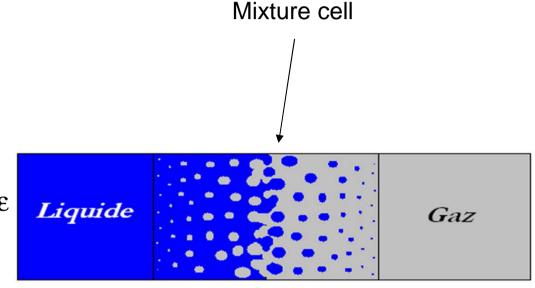


Existence of 4 waves: left expansion, evaporation front, contact discontinuity, right shock wave.

Local thermodynamic equilibrium is assumed at interfaces

Same idea as with contact interfaces:

$$v, H = \begin{cases} +\infty & \text{if } \epsilon < \alpha_k < 1 - \epsilon \\ 0 & \text{otherwise} \end{cases}$$
 Liquide



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

- → Thermodynamic equilibrium is forced locally.
- → Waves propagate on both sides of the front and produce metastable states that relax to equilibrium at interfaces only.
- → When heat diffusion is present metastable states result of heat transfer as well.

Stiff thermodynamic relaxation

The asymptotic solution when H and ν tend to infinity corresponds to the solution of the algebraic system:

$$e = Y_g e_g(T, P) + (1 - Y_g) e_L(T, P)$$

$$v = Y_g v_g(T, P) + (1 - Y_g) v_L(T, P)$$

$$g_g(T, P) = g_L(T, P) \Leftrightarrow T = T_{sat}(P)$$

$$T_g = T_L = T$$

$$P_g = P_L = P$$

$$e = Y_g e_g(P_{sat}) + (1 - Y_g) e_L(P_{sat})$$

$$v = Y_g v_g(P_{sat}) + (1 - Y_g) v_L(P_{sat})$$

Unknowns (P_{sat}, Y_g) $\rightarrow Y_g^{equilibrium}$

Non-linear system quite delicate to solve in particular when the states range from two-phase to single phase : Allaire, Faccanoni and Kokh, CRAS 2007

Le Metayer, Massoni and Saurel, ESAIM, 2013

Simple and fast equilibrium solver

(Chiapolino, Boivin, Saurel, IJNMF, 2016)

Single phase bounds:

If
$$(Y_1 \le \varepsilon \text{ and } T > T_{\text{sat}})$$
 then $Y_1^{\text{eq}} = \varepsilon \text{ (overheated vapor)}$

If
$$(Y_1 \ge 1 - \varepsilon \text{ and } T < T_{\text{sat}})$$
 then $Y_1^{\text{eq}} = 1 - \varepsilon \text{ (subcooled liquid)}$

$$\varepsilon < Y_1^{eq} < 1 - \varepsilon$$

Compute:
$$Y_l^m(p) = \frac{v - v_g(p)}{v_l(p) - v_g(p)}$$
, from the mixture mass definition,

$$Y_l^e(p) = \frac{e - e_g(p)}{e_l(p) - e_g(p)}.$$

 $Y_l^e(p) = \frac{e - e_g(p)}{e_l(p) - e_g(p)}$. from the mixture energy definition.

These two estimates are equal only when $p=p_{sat}$ which is unknown.

Minmod

$$Y_l^m(p) = \frac{v - v_g(p)}{v_l(p) - v_g(p)},$$

$$Y_l^e(p) = \frac{e - e_g(p)}{e_l(p) - e_g(p)}.$$

compute the variations

$$\delta Y_1^m = Y_1^m - Y_1$$

$$\delta Y_1^e = Y_1^e - Y_1$$

Then compute the product $\delta Y_1^m.\delta Y_1^e$

If $(\delta Y_1^m.\delta Y_1^e > 0)$ then,

Take the minimum variation

$$\delta Y_1 = Min(\delta Y_1^m, \delta Y_1^e)$$

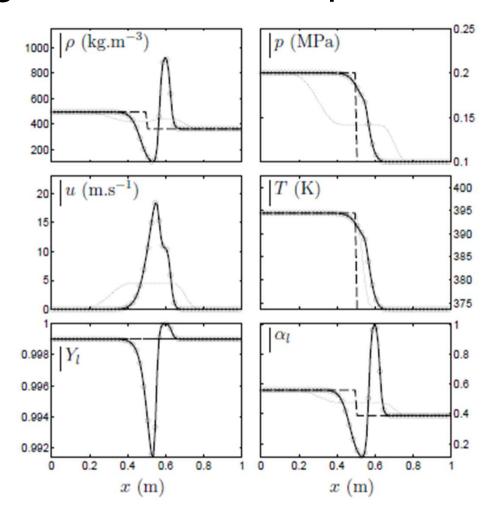
Otherwise,

Set the variation to zero

$$\delta Y_1 = 0$$

Update the mass fraction at equilibrium: $Y_1^{equ} = Y_1 + \delta Y_1$

Example: Shock tube computations with two liquid-gas mixtures and phase change

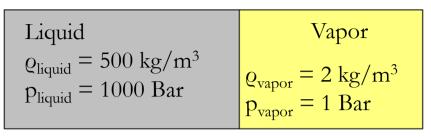


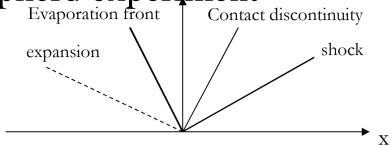
Symbols: Equilibrium computed with the Newton method.

Lines: Equilibrium computed with Minmod

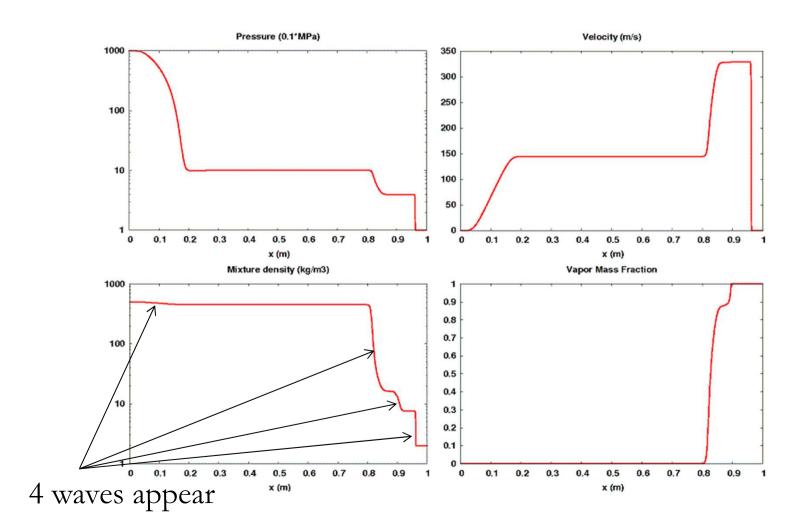
Dotted lines: Solution in temperature and pressure equilibrium without phase transition.

Back to the Simoes-Moreira Shepherd experiment Evaporation front Contact

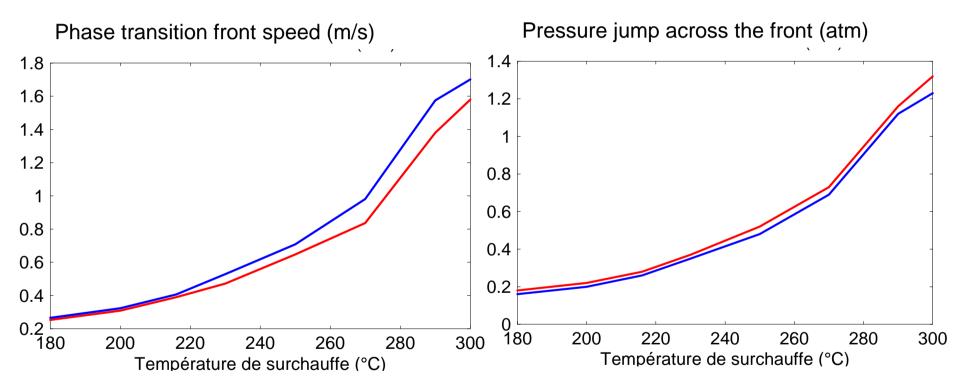




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Flashing front in an expansion tube (Moreira and Shepherd, JFM, 1999)



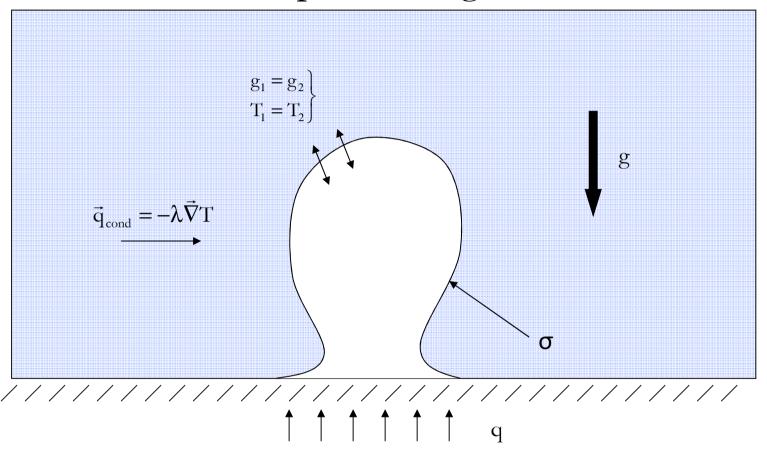
Experiments: blue

Computations: red

Saurel et al., JFM, 2008

Similar results were obtained by Zein, Hantke and Warnecke, JCP, 2010 Reduced model when heat diffusion is considered \rightarrow single temperature

Example: boiling flows



Reduced model in both mechanical and thermal equilibrium

$$\begin{split} \frac{\partial \rho Y_1}{\partial t} + \operatorname{div}(\rho Y_1 \vec{u}) &= \begin{cases} \rho \nu (g_2 - g_1) \\ 0 \end{cases} \\ \frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \vec{u}) &= 0 \\ \frac{\partial \rho \vec{u}}{\partial t} + \operatorname{div}(\rho \vec{u} \otimes \vec{u} + P\underline{I}) &= 0 \\ \frac{\partial \rho E}{\partial t} + \operatorname{div}((\rho E + P) \vec{u}) &= 0 \\ g_1 &= g_2 \\ T_1 &= T_2 \end{split}$$

The phases evolve with same pressure and same temperature but have different chemical potentials and evolve in their own subvolumes (very different of the Dalton law).

Conservative system ($\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} = 0$), comfortable for numerical resolution.

The model is reminiscent of the reactive Euler equations but the EOS is very different

$$P = \frac{1}{2} \left(A_1 + A_2 - \left(P_{\infty,1} + P_{\infty,2} \right) \right) + \sqrt{\frac{1}{4} \left(A_2 - A_1 - \left(P_{\infty,2} - P_{\infty,1} \right) \right)^2 + A_1 A_2}$$

$$A_{k} = \frac{Y_{k} (\gamma_{k} - 1) C_{vk}}{Y_{1} (\gamma_{1} - 1) C_{v1} + Y_{2} (\gamma_{2} - 1) C_{v,2}} (\rho (e - q) - P_{\infty,k})$$

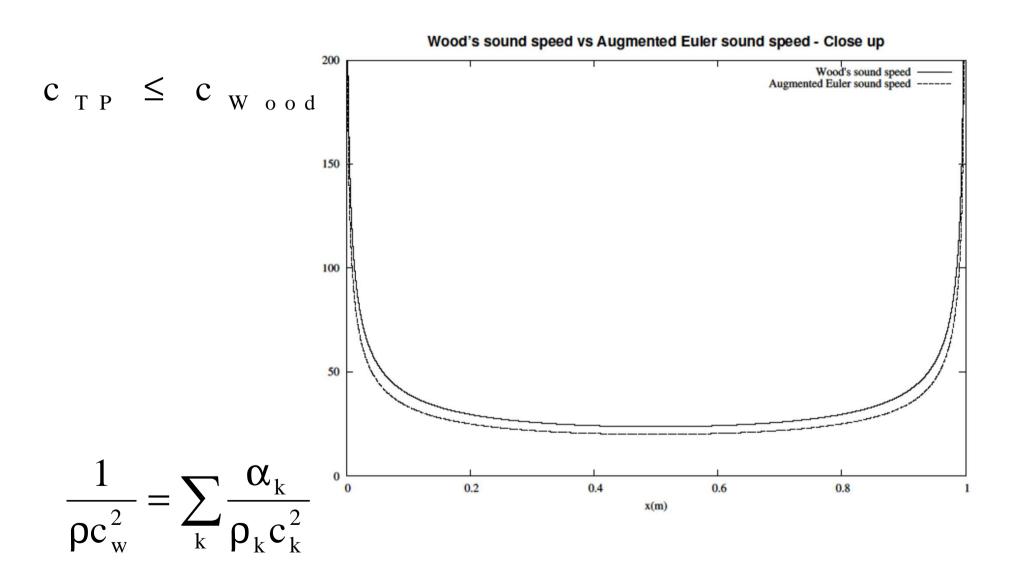
$$p_1 = p_2 = p$$
 $T_1 = T_2 = T$

1
2

$$e = Y_1 e_1(T, p) + Y_2 e_2(T, p)$$

$$v = Y_1 v_1(T, p) + Y_2 v_2(T, p)$$

The sound speed in lower than the previous one



Inserting heat diffusion and surface tension

$$\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \vec{\mathbf{u}}) = 0$$

Le Martelot, Saurel, Nkonga, IJMF, 2014

$$\frac{\partial \rho Y_1}{\partial t} + \operatorname{div}(\rho Y_1 \vec{u}) = \rho \nu (g_2 - g_1)$$

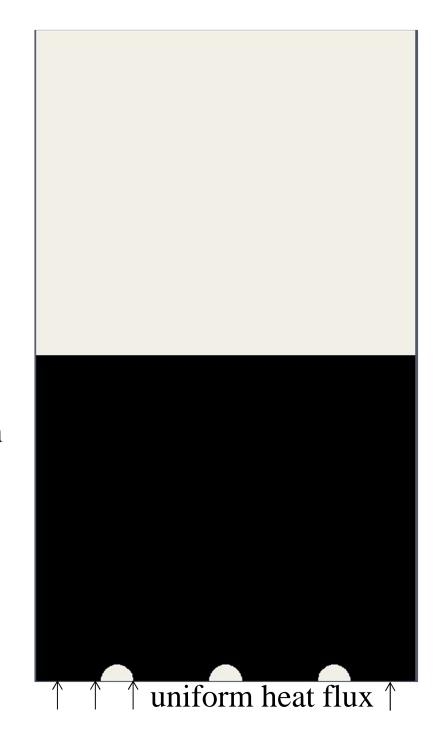
$$\frac{\partial \rho \vec{u}}{\partial t} + \text{div} \left(\rho \vec{u} \otimes \vec{u} + P \underline{I} - \sigma \left(|m| \underline{I} - \frac{m \otimes m}{|m|} \right) \right) = \rho \vec{g}$$

$$\frac{\partial \rho E + \sigma |m|}{\partial t} + \operatorname{div} \left((\rho E + P + \sigma |m|) \vec{u} - \sigma \left(|m| \underline{\underline{I}} - \frac{m \otimes m}{|m|} \right) \bullet \vec{u} + \alpha_1 q_1 + \alpha_2 q_2 \right) = \rho \vec{g} \bullet \vec{u}$$

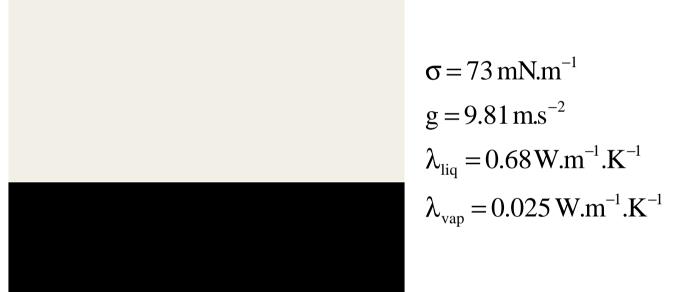
$$\mathbf{m} = \vec{\nabla} \mathbf{Y}_1$$

Computations done with an implicit low Mach hyperbolic solver.

Liquid initially at saturation temperature.

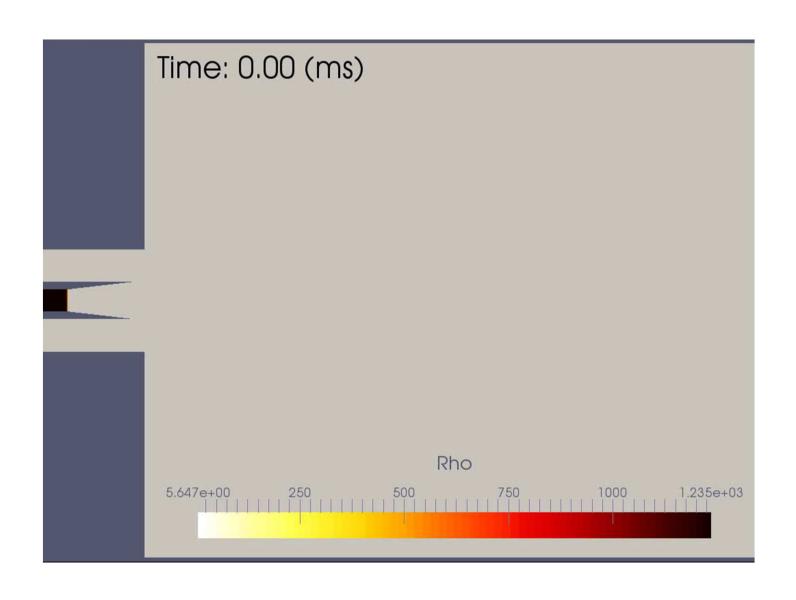


$$\sigma = 73 \text{ mN.m}^{-1}$$
 $g = 9.81 \text{ m.s}^{-2}$
 $\lambda_{\text{liq}} = 0.68 \text{ W.m}^{-1}.\text{K}^{-1}$
 $\lambda_{\text{vap}} = 0.025 \text{ W.m}^{-1}.\text{K}^{-1}$



Same computations without nucleation sites.

Another example: Atomization of O2 liquid jet surrounded by H2 vapour



Ongoing work:

- Extend the Minmod method for mass transfer to the presence of non condensable gas (liquid suspended in air for example): Chiapolino, Boivin, Saurel, Comp & Fluids, submitted
- Sharpen diffuse interfaces on unstructured meshes (Chiapolino and Saurel, SIAM, in preparation)

