Numerical Simulation with Finite Volume of Dynamic Liquid-Vapor Phase Transition

G. Faccanoni* — S. Kokh* — G. Allaire**

DEN/DANS/DM2S, Commissariat à l'Énergie Atomique, Saclay, 91191 Gif-sur-Yvette Cedex, France

{gloria.faccanoni, samuel.kokh}@cea.fr

**CMAP, École Polytechnique, CNRS, 91128 Palaiseau, France*

gregoire.allaire@cmap.polytechnique.fr

ABSTRACT. *The present work investigates the simulation of phase transition in compressible fluids. We postulate a local and instantaneous equilibrium with respect to phasic pressures, temperatures and chemical potentials when both phases are present. This hypothesis leads to the definition of an equilibrium equation of state (EOS) for the two-phase medium. While this thermodynamical assumption is classical, there is no explicit expression of the equilibrium EOS in the general case. We propose a simple mean to approximate this EOS when both phases are governed by a "Stiffened Gas" EOS. Then we provide an implementation of this method within a Finite-Volume numerical scheme thanks to a two-step relaxation strategy.*

KEYWORDS: *phase transition, compressible flows, relaxation method*

1. Introduction

The simulation of phase change phenomena that take place in two-phase flows is an important issue that concerns many industrial applications such as the prediction of the boiling crisis for safety studies of nuclear power plants. The present work focuses on possible and simple means to deal with "Stiffened Gas" laws for simulating dynamical phase change within a Finite Volume Method framework far from the critical point. We first introduce the model examined in this paper, then we recall the basic thermodynamical tools that enable to construct the equation of state (EOS) of the two-phase system in section 1.1 and 1.2. This EOS is implicitly defined by a non-linear system. We then present an approximate solution of this system which is valid in the case when both phases are modelled as "Stiffened Gas". This approximation process is implemented into a numerical scheme that is presented in section 2. Finally we present numerical results in section 3.

1.1. *Characterization of the two-phase media*

We suppose both phases to be compressible fluids equipped with an EOS given by a function $(\tau_\alpha, \varepsilon_\alpha) \mapsto s_\alpha$ whose Hessian matrix is always negative definite and where τ_α, ε_α and s_α denote respectively the specific volume, the specific internal energy and the specific entropy of the fluid $\alpha = 1, 2$. We then define classically the temperature $T_\alpha = 1/(\partial s_\alpha / \partial \varepsilon_\alpha)_{\tau_\alpha}$, the pressure $P_\alpha = T_\alpha \cdot (\partial s_\alpha / \partial \tau_\alpha)_{\varepsilon_\alpha}$ and the chemical potential $g_\alpha = \varepsilon_\alpha + P_\alpha \tau_\alpha - T_\alpha s_\alpha$ of the fluid $\alpha = 1, 2$. Finally we note $y_1 = y$ (resp. $y_2 = 1 - y$) the mass fraction of phase 1 (resp. 2). We suppose both phases to have the same velocity $\mathbf{u}$.

The two-phase medium is characterized by the total density $\varrho = 1/(y\tau_1 + (1 - y)\tau_2)$ and the total specific internal energy $\varepsilon = y\varepsilon_1 + (1 - y)\varepsilon_2$ with $y \in [0, 1]$.

The mass transfer is modelled assuming that there is an instantaneous equilibrium at each point of the domain with respect to pressure, temperature and chemical potential between both phases. This hypothesis allows to define a new EOS $(\tau = 1/\varrho, \varepsilon) \mapsto P^{\mathrm{eq}}$ for the medium describing the liquid-vapor thermodynamical equilibrium wich will be detailed in section 1.2.

If we neglect all dissipative phenomena and local effects such as surface tension, the two-phase mixture with phase transition is governed by the compressible Euler equations with an "equilibrium EOS" denoted by $(\tau, \varepsilon) \mapsto P^{\mathrm{eq}}(\tau, \varepsilon)$:

$$
\begin{cases}
\partial_t \varrho + \mathrm{div}(\varrho \mathbf{u}) = 0, \\
\partial_t (\varrho \mathbf{u}) + \mathrm{div}(\varrho \mathbf{u} \otimes \mathbf{u} + P^{\mathrm{eq}} \, \mathrm{Id}) = \mathbf{0}, \\
\partial_t (\varrho \varepsilon + \varrho \, |\mathbf{u}|^2 /2) + \mathrm{div}((\varrho \varepsilon + \varrho \, |\mathbf{u}|^2 /2 + P^{\mathrm{eq}})\mathbf{u}) = 0.
\end{cases}
\tag{1}
$$

Some mathematical properties of this system are discussed in [ALL 07, JAO 01, MEN 89, VOS 05]. We remark that these equations are valid in pure phase area as well as when both phases are present. In the next section we will recall the thermodynamical construction scheme for $(\tau, \varepsilon) \mapsto P^{\mathrm{eq}}$. Then we shall introduce simple means for approximating the equilibrium EOS that aim to deal efficiently with "Stiffened Gas". In section 2 we shall provide a simple two-step relaxation algorithm that allows to use this approximate EOS within a Finite Volume scheme framework.

1.2. *Equilibrium EOS: definition of the "Saturated States"*

Let us first briefly recall the lines that allow to define the equilibrium EOS $(\tau, \varepsilon) \mapsto P^{\mathrm{eq}}$. Under classical thermodynamical assumptions that we shall not detail here (see e.g. [CAL 85, ALL 07, HEL 05, HEL 06]) one can introduce an equilibrium entropy $(\tau, \varepsilon) \mapsto s^{\mathrm{eq}}$ for the two-phase system by setting

$$
s^{\mathrm{eq}}(\tau, \varepsilon) = \sup \left\{ \; y s_1(\tau_1, \varepsilon_1) + (1 - y)s_2(\tau_2, \varepsilon_2) \; \middle| \; \begin{matrix} \tau = y\tau_1 + (1-y)\tau_2 \\ \varepsilon = y\varepsilon_1 + (1-y)\varepsilon_2 \\ 0 < y < 1 \end{matrix} \; \right\}
$$

Then the pressure P^{eq} is defined, for given (τ, ε), by $P^{\mathrm{eq}}(\tau, \varepsilon) = (\partial s^{\mathrm{eq}}/\partial \tau)_\varepsilon / (\partial s^{\mathrm{eq}}/\partial \varepsilon)_\tau$. When both phases are present at the equilibrium, *i.e.* when the maximizer $(\tau_1^*, \varepsilon_1^*, \tau_2^*, \varepsilon_2^*, y^*)$ of $ys_1 + (1-y)s_2$ is such that $0 < y^* < 1$, then the phases are said to be "at saturation" and the phasic variables $(\tau_1^*, \varepsilon_1^*, \tau_2^*, \varepsilon_2^*, y^*)$ can equivalently be defined (cf. [ALL 07, HEL 05, HEL 06]) as the solution of the system (2) with the condition (3):

$$\left\{ \begin{array}{ll} (\tau, \varepsilon) = y(\tau_1, \varepsilon_1) + (1-y)(\tau_2, \varepsilon_2); & \text{(2a)} \\[2mm] (P_1, T_1)(\tau_1, \varepsilon_1) = (P_2, T_2)(\tau_2, \varepsilon_2), & \text{(2b)} \\[2mm] g_1(\tau_1, \varepsilon_1) = g_2(\tau_2, \varepsilon_2), & \text{(2c)} \end{array} \right.$$

$$y \in (0, 1). \tag{3}$$

Far from the critical point, without breaking the thermodynamical coherence, we can reasonably assume that the functions $(T_\alpha, P_\alpha) \mapsto \tau_\alpha$, $\alpha = 1, 2$ verify, for any $P > 0$ and $T > 0$, that $\tau_1(P, T) \geq \tau_2(P, T)$.

We now detail how to compute in practice the pressure P^{eq}: let $(\tau_1^*, \varepsilon_1^*, \tau_2^*, \varepsilon_2^*, y^*)$ be sought as the solution of (2), we either have one of the following three possibilities:

1. if $(\tau_1^*, \varepsilon_1^*, \tau_2^*, \varepsilon_2^*, y^*)$ verifies both (2) and (3) then $\tau_2^* < \tau < \tau_1^*$, $y^* = \frac{\tau - \tau_2^*}{\tau_1^* - \tau_2^*}$ and we set $P^{\mathrm{eq}}(\tau, \varepsilon) = P_1(\tau_1^*, \varepsilon_1^*) = P_2(\tau_2^*, \varepsilon_2^*)$,
2. otherwise
   (a) if $s_1(\tau, \varepsilon) > s_2(\tau, \varepsilon)$ then we set $y^* = 1$ and $P^{\mathrm{eq}}(\tau, \varepsilon) = P_1(\tau, \varepsilon)$,
   (b) if $s_1(\tau, \varepsilon) < s_2(\tau, \varepsilon)$ then we set $y^* = 0$ and $P^{\mathrm{eq}}(\tau, \varepsilon) = P_2(\tau, \varepsilon)$.

In the first case, we have a uniquely defined equilibrium state between both phases and $(\tau_1^*, \varepsilon_1^*, \tau_2^*, \varepsilon_2^*, y^*)$ can be parametrized[1] by a single thermodynamical variable P or T. This result is classical [CAL 85] and allows to define the coexistence curve $T \mapsto P = P^{\mathrm{sat}}(T)$. The last two cases correspond to a pure phase $\alpha = 1$ or $\alpha = 2$ state and the system (2) has therefore no solution or the condition (3) fails.

Unfortunately, in the general case the strong non-linearity of system (2)-(3) can seriously affect its numerical resolution. Therefore we propose a strategy to approximate its possible solution. First we remark that solving (2) is equivalent to seek (T, P) such that

$$\frac{\tau - \tau_2(P, T)}{\tau_1(P, T) - \tau_2(P, T)} = \frac{\varepsilon - \varepsilon_2(P, T)}{\varepsilon_1(P, T) - \varepsilon_2(P, T)}, \qquad T \mapsto P = P^{\mathrm{sat}}(T). \tag{4}$$

We then consider the following alternative strategy: instead of (4) we impose the variable T to verify

$$\frac{\tau - \tau_2(P, T)}{\tau_1(P, T) - \tau_2(P, T)} = \frac{\varepsilon - \varepsilon_2(P, T)}{\varepsilon_1(P, T) - \varepsilon_2(P, T)}, \qquad T \mapsto P = \widehat{P}^{\mathrm{sat}}(T), \tag{5}$$

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1. Relations (2b) allow to write volumes τ_α and internal energies ε_α as functions of the same pressure P and temperature T. Then from relations (2a) we obtain that y is a function of P and T and finally we have that solving the system (2) is equivalent to seek (T, P) such that

$$\frac{\tau - \tau_2(P, T)}{\tau_1(P, T) - \tau_2(P, T)} = \frac{\varepsilon - \varepsilon_2(P, T)}{\varepsilon_1(P, T) - \varepsilon_2(P, T)}, \qquad g_1(P, T) = g_2(P, T).$$

Phase	c_v [J/(kg·K)]	γ	π [Pa]	q [J/kg]	m [J/(kg·K)]
Liquid	1816.2	2.35	10^9	-1167.056×10^3	-32765.55596
Vapor	1040.14	1.43	0	2030.255×10^3	-33265.65947

Table 1. *Parameters for water and steam with a "Stiffened Gas" EOS.*

where $T \mapsto \widehat{P}^{\mathrm{sat}}$ is a simple and convenient approximation for $T \mapsto P^{\mathrm{sat}}$. For example, given a set of points $\mathfrak{A} = \left\{ (T^i, P^{\mathrm{sat}}(T^i)) \right\}_i$, one can define $\widehat{P}^{\mathrm{sat}}$ thanks to a least square approximation of $\mathfrak{A}$.

In the sequel we consider both phases to be governed by a "Stiffened Gas" EOS: $(\tau_\alpha, \varepsilon_\alpha) \mapsto s_\alpha = c_{v_\alpha} \ln(\varepsilon_\alpha - q_\alpha - \pi_\alpha \tau_\alpha) + c_{v_\alpha}(\gamma_\alpha - 1) \ln \tau_\alpha + m_\alpha$ where the constants $c_{v_\alpha} > 0$, $\gamma_\alpha > 1$, π_α and m_α are coefficients that describe the thermodynamical properties of the phase $\alpha = 1, 2$. According to the definition we have

$$(P,T) \mapsto \varepsilon_\alpha = c_{v_\alpha} T \frac{P + \pi_\alpha \gamma_\alpha}{P + \pi_\alpha} + q_\alpha, \quad (P,T) \mapsto \tau_\alpha = c_{v_\alpha}(\gamma_\alpha - 1) \frac{T}{P + \pi_\alpha}. \quad (6)$$

If $q_\alpha \neq 0$ for at least one α, we did not find any explicit expression for the coexistence curve.

We provide below an example function $T \mapsto \widehat{P}^{\mathrm{sat}}$ for water. The "Stiffened Gas" parameters c_{v_α}, γ_α, π_α and m_α (displayed in Table 1) are those proposed by [LEM 04]. We consider the set of points $\mathfrak{A} = \left\{ (T^i = 278 + 4i, P^{\mathrm{sat}}(T^i)) \right\}_{i=0}^{83}$ where temperature and pressure are expressed in SI units. The value $P^{\mathrm{sat}}(T^i)$ is computed by solving numerically $g_1(P, T^i) = g_2(P, T^i)$. In this particular case, we chose to seek for $T \mapsto \ln(\widehat{P}^{\mathrm{sat}})$ as a polynomial. We obtained good approximation results with a 8th degree polynomial that leads to set the following approximation

$$T \mapsto \widehat{P}^{\mathrm{sat}} = \exp\left(\sum_{k=0}^{8} a_k T^k \right) \quad (7)$$

with

$a_0 = -110.562041$	$a_1 = 1.411518$	$a_2 = -0.808758 \times 10^{-2}$
$a_3 = 0.290760 \times 10^{-4}$	$a_4 = -0.687431 \times 10^{-7}$	$a_5 = 0.107095 \times 10^{-9}$
$a_6 = -0.106089 \times 10^{-12}$	$a_7 = 0.606689 \times 10^{-16}$	$a_8 = -0.152683 \times 10^{-19}$

Finally, given (τ, ε), we propose to compute the pressure value of the equilibrium EOS by solving system (5) thanks to a fixed point algorithm, where $T \mapsto \widehat{P}^{\mathrm{sat}}$ is given by (7) (see Figure 1).

In order to check the accuracy of this strategy, we consider a sequence of states $\{(\tau, \varepsilon)^{i,j}\}_{i,j}$ computed as follows: let $(T^i = 278 + 4i)_{i=0}^{83}$, $(y^j = j/15)_{j=0}^{15}$; let $(\tilde{\tau}_\alpha, \tilde{\varepsilon}_\alpha)^{i,j}$ be the approximated solution of the system $(P, T, g)_1(\tau_1, \varepsilon_1) = (P, T, g)_2(\tau_2, \varepsilon_2)$ provided by Maple with the function `fsolve` (with 40 digits precision) and where $(\tau_\alpha, \varepsilon_\alpha)^{i,j}$ verify (6); we set $(\tau, \varepsilon)^{i,j} = y^j (\tilde{\tau}_1, \tilde{\varepsilon}_1)^{i,j} + (1 - y^j)(\tilde{\tau}_2, \tilde{\varepsilon}_2)^{i,j}$. Let $(\widehat{T}^{i,j}, \widehat{y}^{i,j})$ be the approximated solution of (5) associated with $(\tau, \varepsilon)^{i,j}$ obtained by Maple with the function `fsolve`. We obtain

$$\max_{0 \le i \le 83} \left| P^{\mathrm{sat}}(T^i) - \widehat{P}^{\mathrm{sat}}(T^i) \right| < 67.2 \text{ Pa}, \quad \max_{0 \le i \le 83} \frac{\left| P^{\mathrm{sat}}(T^i) - \widehat{P}^{\mathrm{sat}}(T^i) \right|}{P^{\mathrm{sat}}(T^i)} < 1.8 \times 10^{-5},$$
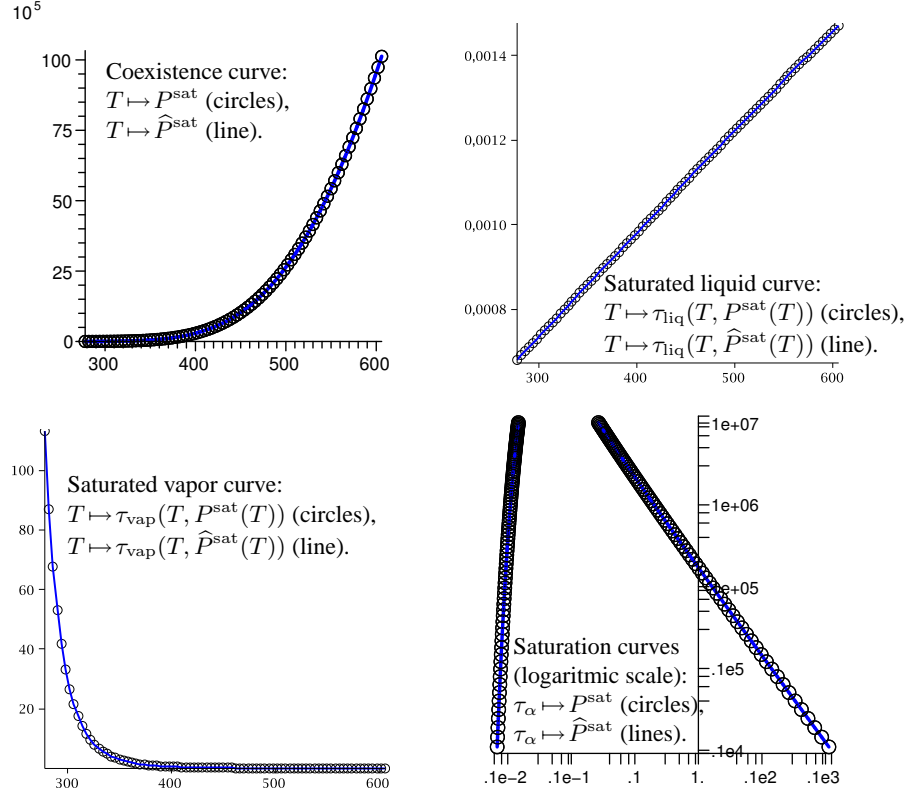
Figure 1. *Exact (circles) and approximate (lines) pressure and volumes at saturation as functions of temperature and saturation dome.*

$$\max_{\substack{0\leq i\leq 83 \\ 0\leq j\leq 15}} \left| T^i - \widehat{T}^{i,j} \right| < 1.2 \times 10^{-3} \text{ K}, \qquad \max_{\substack{0\leq i\leq 83 \\ 0\leq j\leq 15}} \frac{\left| T^i - \widehat{T}^{i,j} \right|}{T^i} < 2.4 \times 10^{-6},$$

$$\max_{\substack{0\leq i\leq 83 \\ 0\leq j\leq 15}} \left| y^j - \widehat{y}^{i,j} \right| < 1.9 \times 10^{-6}.$$

This allows us to check that the thermodynamical values associated with the saturated states are recovered with a good accuracy by the approximation (5) (see Figure 1).

2. Numerical Method

We propose in this section a two-step relaxation method that aims to simulate system (1) following similar lines as in [HEL 06, CAR 06]. We consider below the augmented system that is a relaxed version of (1):

$$\begin{cases} \partial_t \mathbf{W} + \mathrm{div}\, \mathbf{F}(\mathbf{W}, z) = \mathbf{R}(\mathbf{W}, z) \\ \partial_t z + \mathbf{u} \cdot \mathbf{grad}\, z = Q(\mathbf{W}, z) \end{cases} \tag{8}$$

where

$$\mathbf{W} = (z\varrho_1, (1-z)\varrho_2, \varrho\mathbf{u}, \varrho(\varepsilon + |\mathbf{u}|^2/2)),$$

$$\mathbf{F}(\mathbf{W}, z) = (z\varrho_1\mathbf{u}, (1-z)\varrho_2\mathbf{u}, \varrho\mathbf{u} \otimes \mathbf{u} + P\,\mathrm{Id}, (\varrho(\varepsilon + |\mathbf{u}|^2/2) + P)\mathbf{u}),$$

$$\mathbf{R}(\mathbf{W}, z) = (\mu\left(g_2/T_2 - g_1/T_1\right), -\mu\left(g_2/T_2 - g_1/T_1\right), 0, 0),$$

$$Q(\mathbf{W}, z) = \nu\left(P_1/T_1 - P_2/T_2\right),$$

with the volume fraction z such that $\varrho = z\varrho_1 + (1-z)\varrho_2$, $P = zP_1 + (1-z)P_2$ and the closure $T_1 = T_2$.

Formally the equilibrium $\mu, \nu \to +\infty$ implies that $\mathbf{R}(\mathbf{W}, z) = \mathbf{0}$, $Q(\mathbf{W}, z) = 0$ which matches the equilibrium relations (2). We implement the following numerical strategy for approximating (1).

Step I: let $(\mathbf{W}, z)^n$ be the state variables of system (8) at $t = t^n$. The augmented variable $(\mathbf{W}, z)^n$ is updated to $(\mathbf{W}, z)^{n+1/2}$ by solving the system (8) with $\mathbf{R}(\mathbf{W}, z) = \mathbf{0}$, $Q(\mathbf{W}, z) = 0$. In our tests this step is achieved thanks to a Finite Volume Roe-like solver proposed in [ALL 02];

Step II: perform an approximated projection of the state $(\mathbf{W}, z)^{n+1/2}$ onto the equilibrium defined by $\mu, \nu \to +\infty$ by approaching the solution of $\mathbf{R}(\mathbf{W}, z) = \mathbf{0}$, $Q(\mathbf{W}, z) = 0$. This step is achieved by seeking the solution $(\widehat{T}, \widehat{y})$ of the system (5), thanks to a dichotomy algorithm. We then set

$$T^{n+1} = \widehat{T}, \qquad P^{n+1} = \widehat{P}^{\mathrm{sat}}(T^{n+1}), \qquad y^{n+1} = \widehat{y}$$

and

$$(\varrho, \mathbf{u}, \varepsilon)^{n+1} = (\varrho, \mathbf{u}, \varepsilon)^{n+1/2}, \qquad z^{n+1} = \begin{cases} 0 & \text{if } y^{n+1} = 0 \\ y^{n+1}\varrho^{n+1}\tau_1^{n+1} & \text{if } 0 < y^{n+1} < 1 \\ 1 & \text{if } y^{n+1} = 1 \end{cases}$$

which defines $(\mathbf{W}, z)^{n+1}$.

Let us remark that although the pressure P^{eq} is $\mathcal{C}^0$ regular but merely piecewise $\mathcal{C}^1$ regular, the two-step relaxation method did not generate spurious oscillations in the solutions of our tests.

3. Numerical Test: Compression of a Vapor Bubble

Our method is tested on the case of a vapor bubble compression (see Figure 2). We consider a 1 m side-length 2D square domain discretized over 300×300 cells mesh. A water vapor bubble is surrounded by liquid water in the center of the domain. The radius is initially $r = 0.2$ m. Both EOS used are "Stiffened Gas" type whose coefficients are given in Table 1. The initial temperature is fixed to $T_0 = 439$ K and the fluid is initially at rest ($\mathbf{u} = \mathbf{0}$) in the whole domain. Both phases are supposed to be at saturation at $t = 0$ therefore the densities for the liquid ϱ_{liq} and the vapor ϱ_{vap} are
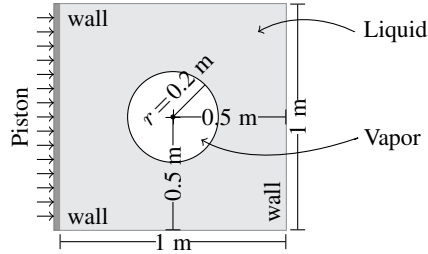
Figure 2. *Geometry of test "Compression of a Vapor Bubble"*

$\varrho_{\text{liq}} = 929.7941874$ kg/m^3, $\varrho_{\text{vap}} = 4.091902657$ kg/m^3, while the pressure is $P = P^{\text{sat}}(T_0) = 8.034337432 \times 10^5$ Pa for both phases. We suppose the left boundary to be a piston that moves towards right at constant speed by imposing a constant velocity $u_p = 30$ m/s in the fictitious cells. Other boundary conditions are reflective walls. Figure 3 shows the mass fraction y for time varying from $t = 0$ ms to $t = 3.30$ ms. The moving piston generates a pressure wave that compresses the vapor. As the pressure increases the vapor starts to condensate and the bubble shrinks.

4. Conclusion & Perspectives

In this paper we have examined a dynamical phase-change model for compressible flows. This model relies on a classical thermodynamical hypothesis of equilibrium between both phases. We introduced a simple process for approximating the computation of this equilibrium in the case both phases are modelled with "Stiffened Gas". We also proposed an implementation of this method coupled to a Finite Volume numerical solver within a two-step relaxation strategy.

When one deals with more realistic EOS, the resolution of the system (2) that determines the equilibrium between both phases may be more arduous because the experimental data $(\tau_\alpha, \varepsilon_\alpha) \mapsto (P_\alpha, T_\alpha, g_\alpha)$ for the pure phase $\alpha = 1, 2$ are not available for every point $(\tau_\alpha, \varepsilon_\alpha)$, therefore the pure phase EOS may be only partially defined. In this case one should propose an alternative approximation for (4) that circumvents this difficulty. Further investigations in order to achieve this task are already in progress.

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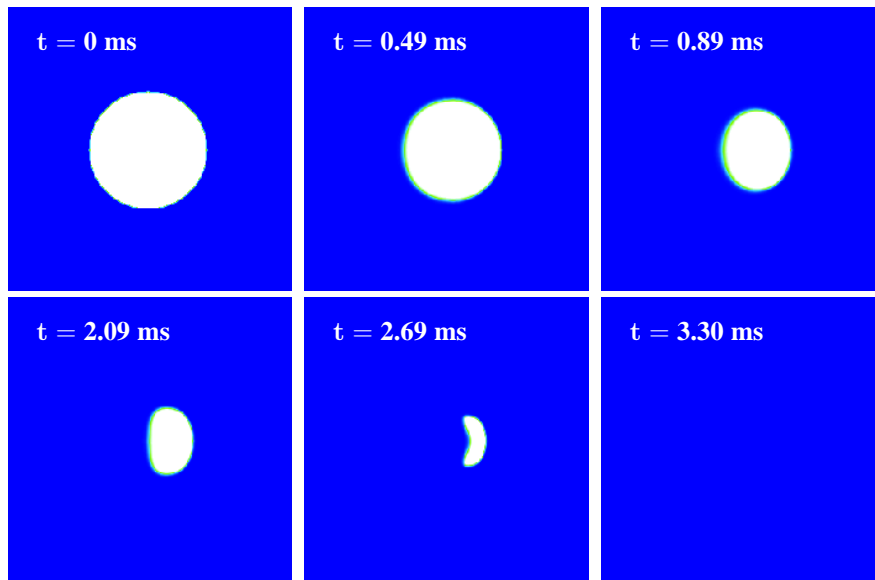
Figure 3. *Mass fraction profile.*

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