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Axisymmetric Level Set model of Leidenfrost effect

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December 20, 2013

Abstract

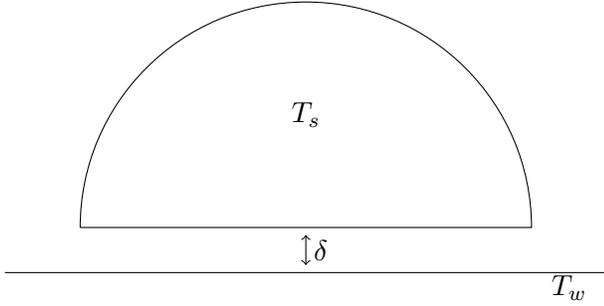
We propose a level-set model of phase change and apply it to the study of the Leidenfrost effect. The new ingredients used in this model are twofold: first we enforce by penalization the droplet temperature to the saturation temperature in order to ensure a correct mass transfer at interface, and second we propose a careful differentiation of the capillary interface with respect to a moving interface with phase change. We perform some numerical tests in the axisymmetric case and show that our numerical method, while not avoiding well known numerical caveats of diffuse interface methods, behave quite well in the limit of numerical interface width going to zero in comparison to an analytical formula.

1 Introduction

While heating water in a pan, small vapor bubbles are created and detach from the bottom at some frequency. This frequency increases as the temperature difference between the pan bottom and water increases, up to the point when a vapor layer is created. This layer acts as a barrier for the heat flux which reduces dramatically the phase change rate. For a physical study of the boiling crisis and Leidenfrost effect we refer to [1] and [2].

The Leidenfrost effect also occurs when a droplet falls slowly on a support heated at a temperature significantly hotter than the liquid's boiling point, so that an insulating vapor layer is created and prevents that droplet to burn out instantly. The random release of vapor under the droplet creates a motion. One challenge is to be able to somehow control the droplet motion through this vapor release. One way to do so is to use a heated supporting surface with a sawtooth shaped texture [3, 4]. The overall phenomenon is rather complicated since surface tension, phase change and compressible effects are coupled. Therefore we decided to start with a simple yet actually relevant model.

In this paper we will indeed focus on a Level Set method to deal with this phase change model, and consider first the case of an axisymmetric droplet. Therefore we do not study its horizontal motion, but rather its vertical motion and the balance between the gravity force and the pressure forces generated by the vapor layer, which is created by the phase change. We devised an even simpler model where we assumed that the temperature inside the droplet can be considered as constant and equal to the saturation temperature. To validate this model we will compare the result from its numerical simulation with some analytical results. If we consider a hemispherical droplet of radius R at equilibrium at the saturation temperature, an estimation of the vapor layer thickness δ as well as the time t_v before the droplet completely vanishes, is given in [5], page 156:



$$\delta = R \left(\frac{9k_g \mu_g \Delta T}{8\rho_g(\rho_\ell - \rho_g)g\mathcal{L}R^3} \right)^{\frac{1}{4}}$$

$$t_v = 4 \left(\frac{2\mu_g}{9\rho_g g} \right)^{\frac{1}{4}} \left(\frac{(\rho_\ell - \rho_g)\mathcal{L}R_0}{k_g \Delta T} \right)^{\frac{3}{4}}$$

where ΔT is the temperature drop between the pan bottom and water, R_0 is the initial radius of the droplet in hemispherical shape (which corresponds to the radius of the initial spherical droplet times $\sqrt[3]{2}$), k_v is the vapor thermal conductivity, \mathcal{L} the heat of vaporization, ρ the density and μ_v the dynamical viscosity of vapor.

As an example we would consider a droplet of $2mm$ with a saturation temperature of $373K$ and a support heated at $530K$. With the above formulae, it takes about 44 minutes for the droplet to disappear, which is quite long. Therefore Roland Denis during his PhD made a more careful analysis and found an alternative formula (computation described in annex):

$$t_v = \frac{8}{5} R_0^{\frac{5}{4}} \rho_\ell \left(\frac{\mathcal{L}}{k_g \Delta T} \right)^{\frac{3}{4}} \left(\frac{9}{4} \frac{\mu_g}{\rho_g(\rho_\ell - \rho_g)g} \right)^{\frac{1}{4}} \quad (1)$$

and with this formula we find an extinction time of 59.6 seconds which seems more realistic. The variation of volume with time related to this analytic expression is given by (we still refer to annex):

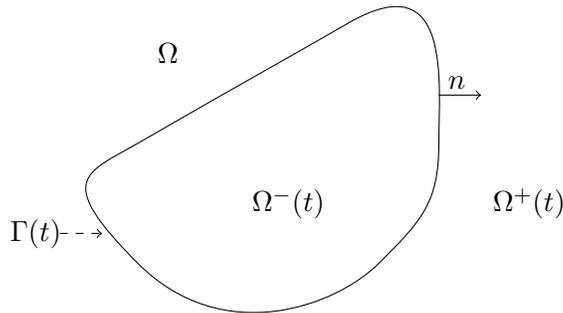
$$V(t) = V_0 \left(1 - \frac{t}{t_v} \right)^{\frac{12}{5}}. \quad (2)$$

Under a cylindrical droplet hypothesis, Bianche et al. obtain in [6] the following expression:

$$V(t) = V_0 \left(1 - \frac{t}{t_v} \right)^4 \quad \text{with} \quad t_v = 2 \left(\frac{4\rho_\ell a \mathcal{L}}{k_g \Delta T} \right)^{3/4} \left(\frac{3\mu_g}{\rho_g g} \right)^{1/4} R_0^{1/2} \quad (3)$$

where $a = \sqrt{\frac{\chi}{\rho_\ell g}}$ is the capillarity length and χ the surface tension.

2 Level Set modeling



The Level Set method [7, 8] is a classical interface capturing method. For the motion of a closed and bounded hypersurface $\Gamma(t)$ in an open set $\Omega \subset \mathbb{R}^d$ on some time interval $[0, T]$, this amounts to introduce an auxiliary function $\varphi : \Omega \times [0, T] \rightarrow \mathbb{R}$ whose zero level set coincides with $\Gamma(t)$:

$$\Gamma(t) = \{x \in \Omega; \varphi(x, t) = 0\}.$$

Starting from an initial position $\Gamma(0)$ captured by a function φ_0 , the motion of $\Gamma(t)$ with a velocity field $u : \Omega \times]0, T] \rightarrow \mathbb{R}^d$ corresponds to solve a transport equation for φ :

$$\begin{cases} \varphi_t + u \cdot \nabla \varphi = 0 & \text{on } \Omega \times]0, T], \\ \varphi = \varphi_0 & \text{on } \Omega \times \{0\}. \end{cases} \quad (4)$$

By convention we assume that x lies in the domain enclosed by $\Gamma(t)$, denoted by Ω^- (see picture) if and only if $\varphi(x) < 0$ and $x \in \Omega^+$ if and only if $\varphi(x) > 0$. Introducing the Heaviside function H defined by

$$\bar{H}(x) = \begin{cases} 0 & \text{if } x < 0 \\ 1 & \text{if } x \geq 0 \end{cases},$$

then

$$\bar{H}(\varphi(x, t)) = \begin{cases} 0 & \text{if } x \in \Omega^-(t) \\ 1 & \text{if } x \in \Omega^+(t) \end{cases}.$$

As $\bar{H}(\varphi)$ is also solution in the distributional sense of the same transport equation as φ , every quantity g with value g_1 inside $\Gamma(t)$ and g_2 outside $\Gamma(t)$, can be written as:

$$g(x, t) = g_1(x, t)(1 - \bar{H}(\varphi(x, t))) + g_2(x, t)\bar{H}(\varphi(x, t)). \quad (5)$$

However for numerical implementation one usually use a regularized version of this Heaviside function. First we introduce a cut-off function ζ , i.e. a nonnegative function with compact support and unit mass. It is well known that if $|\nabla \varphi| \geq \alpha > 0$ in a neighborhood of $\{\varphi = 0\}$ then

$$\frac{1}{\varepsilon} \zeta\left(\frac{\varphi}{\varepsilon}\right) |\nabla \varphi| \xrightarrow{\varepsilon \rightarrow 0} \delta_{\{\varphi=0\}},$$

in sense of bounded measures on Ω , so that for small ε :

$$\delta_\varepsilon(\varphi) := \frac{1}{\varepsilon} \zeta\left(\frac{\varphi}{\varepsilon}\right) |\nabla \varphi| \simeq \delta_{\{\varphi=0\}}.$$

However one has to take care that while $\delta_{\{\varphi=0\}}$ does not depend on the scale of φ , this is not the case of $\delta_\varepsilon(\varphi)$. This is one problem with Level Set method using this regularized approach: one needs to recover information on the distance to interface from the value of φ , but this is not direct. We will discuss that in section 4. For the regularization of \bar{H} , we just use the antiderivative H of ζ vanishing in -1 . There are many choice of function ζ . In this paper we used the more common given by:

$$\zeta(x) = \begin{cases} 0 & \text{if } x < -1 \\ \frac{1}{2}(1 + \cos(\pi x)) & \text{if } -1 \leq x \leq 1 \\ 0 & \text{if } x > 1 \end{cases} \quad H(x) = \begin{cases} 0 & \text{if } x < -1 \\ \frac{1}{2}(x + \frac{1}{\pi} \sin(\pi x) + 1) & \text{if } -1 \leq x \leq 1 \\ 1 & \text{if } x > 1 \end{cases}$$

Thanks to this regularization we replace (5) by its continuous counterpart,

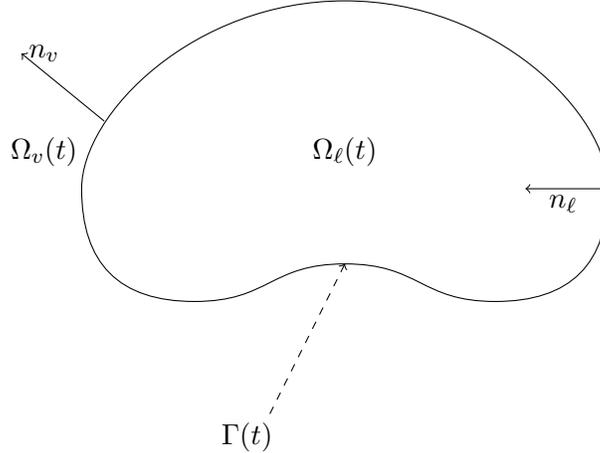
$$g(x, t) = g_1(x, t)\left(1 - H\left(\frac{\varphi(x, t)}{\varepsilon}\right)\right) + g_2(x, t)H\left(\frac{\varphi(x, t)}{\varepsilon}\right) \quad (6)$$

where $\varepsilon > 0$ controls the width of interface.

Before stepping to the phase change problem, we recall that geometrical information is quite easily obtained from the Level Set function. With our conventions the exterior normal N to the domain enclosed by Γ and its curvature κ are given by:

$$N(x, t) = \frac{\nabla\varphi(x, t)}{|\nabla\varphi(x, t)|} \quad \kappa = \operatorname{div} N = \operatorname{div} \frac{\nabla\varphi}{|\nabla\varphi|}. \quad (7)$$

3 Phase Change model



The phases densities are the following:

- liquid density: ρ_ℓ , assumed constant,
- dry vapor: $\rho_g < \rho_\ell$, assumed constant,
- wet vapor: $\rho(x, t) = \rho_\ell(1 - H(\frac{\varphi(x, t)}{\varepsilon})) + \rho_g H(\frac{\varphi(x, t)}{\varepsilon})$,

where φ is the level-set function capturing the phase change interface.

Remark 1. *The two incompressibility assumptions are different in nature: indeed the liquid is considered as incompressible because its density undergoes very small variations, whereas the dry vapor, which is far from the droplet, will not undergo compression in this phenomenon.*

From the above definitions we therefore have three identified regions:

- **Liquid:** $\Omega_\ell(t) = \{x \in \mathbb{R}^3 \mid \varphi(x, t) < -\varepsilon\}$,
- **Vapor:** $\Omega_v(t) = \{x \in \mathbb{R}^3 \mid -\varepsilon < \varphi(x, t) < \varepsilon\}$,
- **Dry vapor:** $\Omega_g(t) = \{x \in \mathbb{R}^3 \mid \varphi(x, t) > \varepsilon\}$.

3.1 Conservation equations

Mass conservation Writing the conservation of ρ alone is not sufficient since we need to account for the phase change between liquid and vapor. Arguing as in Allaire *et al* [9] which consider two compressible fluids with no phase change, we write the mass conservation of each phase, with opposite source terms:

$$\begin{aligned} \partial_t \left(\rho_\ell \left(1 - H \left(\frac{\varphi}{\varepsilon} \right) \right) \right) + \operatorname{div} \left(\rho_\ell \left(1 - H \left(\frac{\varphi}{\varepsilon} \right) \right) u \right) &= -\Phi_m |\nabla \varphi| \frac{1}{\varepsilon} \zeta \left(\frac{\varphi}{\varepsilon} \right), \\ \partial_t \left(\rho_g H \left(\frac{\varphi}{\varepsilon} \right) \right) + \operatorname{div} \left(\rho_g H \left(\frac{\varphi}{\varepsilon} \right) u \right) &= +\Phi_m |\nabla \varphi| \frac{1}{\varepsilon} \zeta \left(\frac{\varphi}{\varepsilon} \right). \end{aligned} \quad (8)$$

where Φ_m denotes the mass flux across the interface. We assumed $\Phi_m > 0$ when vaporization occurs, and $\Phi_m < 0$ when liquefaction takes place. Summing these two equations give the conservation for ρ . Note the smeared interfacial exchange term whose limit gives, as recalled in the first section, a Dirac mass. Under our assumptions, ρ_g and ρ_ℓ are constant and can be set in the source term. The two equations are not equivalent since u is not divergence free, in the wet vapor domain Ω_v . However, after dividing (8) by ρ_ℓ (resp. ρ_g) and summing, we can find $\operatorname{div} u$ as a function of Φ_m and write the two equivalent equations:

$$\partial_t \rho + \operatorname{div}(\rho u) = 0 \quad \operatorname{div} u = \Phi_m \left(\frac{1}{\rho_g} - \frac{1}{\rho_\ell} \right) |\nabla \varphi| \frac{1}{\varepsilon} \zeta \left(\frac{\varphi}{\varepsilon} \right). \quad (9)$$

This is roughly the same model as the one proposed by Juric and Tryggvason [10]. Of course up to now we did not define Φ_m , which should be related to the latent heat of vaporization since it measures the net flux of molecules from one phase to the other (see also [11]).

Interface motion As u is not divergence free around the interface (unless there is no phase change), the above conservation equations are not equivalent to the corresponding transport equations. This means that the interface velocity differs from u and thus, a correction due to the phase change arises. In order to emphasize this velocity correction, we sum the two equations in (8), divide each part respectively by ρ_ℓ and ρ_g , and take apart the velocity divergence, to get:

$$\partial_t H \left(\frac{\varphi}{\varepsilon} \right) + \operatorname{div} \left(H \left(\frac{\varphi}{\varepsilon} \right) u \right) = -\frac{\rho_\ell}{\rho_g - \rho_\ell} \operatorname{div} u.$$

Expanding the divergence term and using the density definition give us:

$$\partial_t H \left(\frac{\varphi}{\varepsilon} \right) + u \cdot \nabla H \left(\frac{\varphi}{\varepsilon} \right) = \frac{\rho}{\rho_\ell - \rho_g} \operatorname{div} u. \quad (10)$$

Expressing the derivatives of H in term of the cut-off function ζ and thanks to the velocity divergence expression (9), we obtain:

$$\frac{1}{\varepsilon} \zeta \left(\frac{\varphi}{\varepsilon} \right) [\partial_t \varphi + u \cdot \nabla \varphi] = \frac{\rho}{\rho_g \rho_\ell} \Phi_m |\nabla \varphi| \frac{1}{\varepsilon} \zeta \left(\frac{\varphi}{\varepsilon} \right)$$

which, as $|\nabla \varphi| = \frac{\nabla \varphi}{|\nabla \varphi|} \cdot \nabla \varphi$, is equivalent to

$$\frac{1}{\varepsilon} \zeta \left(\frac{\varphi}{\varepsilon} \right) \left[\partial_t \varphi + \left(u - \frac{\rho}{\rho_g \rho_\ell} \Phi_m \frac{\nabla \varphi}{|\nabla \varphi|} \right) \cdot \nabla \varphi \right] = 0.$$

The bracketed term expresses a transport equation for the Level-Set function that occurs only in the interfacial zone. As usual in the Level-Set methodology, we extend its validity on the whole domain and we finally assume that the following transport equation holds:

$$\partial_t \varphi + (u + V) \cdot \nabla \varphi = 0 \quad (11)$$

where the velocity correction V is given by :

$$V = -\frac{\rho}{\rho_g \rho_\ell} \Phi_m \frac{\nabla \varphi}{|\nabla \varphi|}.$$

Capillary forces As the interface velocity is affected by the phase change, we have to derive the capillary force in that case. We first recall the transport equation (10) on H :

$$\partial_t H \left(\frac{\varphi}{\varepsilon} \right) + u \cdot \nabla H \left(\frac{\varphi}{\varepsilon} \right) = \frac{\rho}{\rho_\ell - \rho_g} \operatorname{div} u.$$

As the surface tension energy depends essentially on $\nabla H \left(\frac{\varphi}{\varepsilon} \right)$, let us compute its time variations t . Differentiating the transport equation on $H \left(\frac{\varphi}{\varepsilon} \right)$ gives

$$\left(\nabla H \left(\frac{\varphi}{\varepsilon} \right) \right)_t + u \cdot \nabla \left(\nabla H \left(\frac{\varphi}{\varepsilon} \right) \right) + \nabla u^T \nabla H \left(\frac{\varphi}{\varepsilon} \right) = \frac{\nabla \rho}{\rho_\ell - \rho_g} \operatorname{div} u + \frac{\rho}{\rho_\ell - \rho_g} \nabla (\operatorname{div} u)$$

Taking the scalar product with $\nabla H \left(\frac{\varphi}{\varepsilon} \right)$, and using $\nabla \rho = -(\rho_\ell - \rho_g) \nabla H \left(\frac{\varphi}{\varepsilon} \right)$ we obtain

$$\begin{aligned} \frac{1}{2} \partial_t \left(\left| \nabla H \left(\frac{\varphi}{\varepsilon} \right) \right|^2 \right) + \frac{1}{2} u \cdot \nabla \left(\left| \nabla H \left(\frac{\varphi}{\varepsilon} \right) \right|^2 \right) + \nabla H \left(\frac{\varphi}{\varepsilon} \right)^T \nabla u^T \nabla H \left(\frac{\varphi}{\varepsilon} \right) \\ = - \left| \nabla H \left(\frac{\varphi}{\varepsilon} \right) \right|^2 \operatorname{div} u + \frac{\rho}{\rho_\ell - \rho_g} \nabla H \left(\frac{\varphi}{\varepsilon} \right) \cdot \nabla (\operatorname{div} u). \end{aligned}$$

Restricting ourselves on the interface layer $|\varphi| < \varepsilon$ and using $\nabla H \left(\frac{\varphi}{\varepsilon} \right)^T \nabla u^T \nabla H \left(\frac{\varphi}{\varepsilon} \right) = \nabla H \left(\frac{\varphi}{\varepsilon} \right) \otimes \nabla H \left(\frac{\varphi}{\varepsilon} \right) : \nabla u$, we obtain after dividing by $|\nabla H \left(\frac{\varphi}{\varepsilon} \right)|$,

$$\begin{aligned} \partial_t \left| \nabla H \left(\frac{\varphi}{\varepsilon} \right) \right| + u \cdot \nabla \left| \nabla H \left(\frac{\varphi}{\varepsilon} \right) \right| \\ = - \frac{\nabla H \left(\frac{\varphi}{\varepsilon} \right) \otimes \nabla H \left(\frac{\varphi}{\varepsilon} \right)}{\left| \nabla H \left(\frac{\varphi}{\varepsilon} \right) \right|} : \nabla u - \left| \nabla H \left(\frac{\varphi}{\varepsilon} \right) \right| \operatorname{div} u + \frac{\rho}{\rho_\ell - \rho_g} \nabla (\operatorname{div} u) \cdot \frac{\nabla H \left(\frac{\varphi}{\varepsilon} \right)}{\left| \nabla H \left(\frac{\varphi}{\varepsilon} \right) \right|} \end{aligned}$$

Note that in the above expression of $\frac{\nabla H \left(\frac{\varphi}{\varepsilon} \right)}{\left| \nabla H \left(\frac{\varphi}{\varepsilon} \right) \right|} = \frac{\nabla \varphi}{|\nabla \varphi|}$ since we are on the layer $|\varphi| < \varepsilon$. Finally,

$$\partial_t \left| \nabla H \left(\frac{\varphi}{\varepsilon} \right) \right| + \operatorname{div} \left(\left| \nabla H \left(\frac{\varphi}{\varepsilon} \right) \right| u \right) = -\frac{1}{\varepsilon} \zeta \left(\frac{\varphi}{\varepsilon} \right) \frac{\nabla \varphi \otimes \nabla \varphi}{|\nabla \varphi|} : \nabla u + \frac{\rho}{\rho_\ell - \rho_g} \nabla (\operatorname{div} u) \cdot \frac{\nabla \varphi}{|\nabla \varphi|}. \quad (12)$$

Moreover we note that outside $|\varphi| < \varepsilon$ both members of this formula are zero thanks to (9) and since ζ is \mathcal{C}^1 . Thus this formula holds in Ω . The capillary energy is defined by

$$E_c = \int_{\{\varphi=0\}} \chi \, dS = \lim_{\varepsilon \rightarrow 0} \int_{\Omega} \chi |\nabla \varphi| \frac{1}{\varepsilon} \zeta \left(\frac{\varphi}{\varepsilon} \right) \, dx$$

where χ is the surface tension coefficient. In this paper we assume that χ is constant. The case of temperature dependent capillary coefficient will be addressed in a forthcoming work. We consider the regularized capillary energy for our problem:

$$E_c^\varepsilon = \int_{\Omega} \chi |\nabla\varphi| \frac{1}{\varepsilon} \zeta\left(\frac{\varphi}{\varepsilon}\right) dx = \chi \int_{\Omega} \left| \nabla H\left(\frac{\varphi}{\varepsilon}\right) \right| dx,$$

and compute its time derivative using formula (12):

$$\frac{dE_c^\varepsilon}{dt} = \chi \int_{\Omega} \partial_t \left(\left| \nabla H\left(\frac{\varphi}{\varepsilon}\right) \right| \right) dx = -\chi \int_{\Omega} \frac{1}{\varepsilon} \zeta\left(\frac{\varphi}{\varepsilon}\right) \frac{\nabla\varphi \otimes \nabla\varphi}{|\nabla\varphi|} : \nabla u - \frac{\rho}{\rho_\ell - \rho_g} \nabla(\operatorname{div} u) \cdot \frac{\nabla\varphi}{|\nabla\varphi|} dx.$$

Integrate by parts the first term and since $\frac{1}{\varepsilon} \zeta\left(\frac{\varphi}{\varepsilon}\right)$ vanishes on $\partial\Omega$, we get

$$\frac{dE_c^\varepsilon}{dt} = -\chi \int_{\Omega} -\operatorname{div} \left(\frac{1}{\varepsilon} \zeta\left(\frac{\varphi}{\varepsilon}\right) \frac{\nabla\varphi \otimes \nabla\varphi}{|\nabla\varphi|} \right) \cdot u - \frac{\rho}{\rho_\ell - \rho_g} \nabla(\operatorname{div} u) \cdot \frac{\nabla\varphi}{|\nabla\varphi|} dx.$$

After integrating twice by parts to isolate u in the second part (using $\operatorname{div} u = 0$ on $\partial\Omega$ for the first one, and $(u \cdot n) \operatorname{div} \frac{\nabla\varphi}{|\nabla\varphi|} = 0$ on $\partial\Omega$ for the second) we obtain

$$\frac{dE_c^\varepsilon}{dt} = -\chi \int_{\Omega} \left[-\operatorname{div} \left(\frac{1}{\varepsilon} \zeta\left(\frac{\varphi}{\varepsilon}\right) \frac{\nabla\varphi \otimes \nabla\varphi}{|\nabla\varphi|} \right) - \nabla \left(\operatorname{div} \left(\frac{\rho}{\rho_\ell - \rho_g} \frac{\nabla\varphi}{|\nabla\varphi|} \right) \right) \right] \cdot u dx.$$

Therefore we have to consider boundary conditions on u and φ such that $(u \cdot n) \operatorname{div} \frac{\nabla\varphi}{|\nabla\varphi|} = 0$ on $\partial\Omega$. For homogeneous Dirichlet boundary conditions on u this is straightforwardly verified. However for Neumann-type boundary conditions, one has to take φ on the boundary such that the curvature of its level sets is zero. For a flat boundary, it suffices to take as boundary condition for φ a linear extrapolation of the interior values, for instance. Or to simply reset φ to the minimum between φ and the distance to a point just outside de boundary. If the boundary is $y = 1$, and the interface width 2ε , this amounts to reset $\varphi(x, y)$ to $\min(\varphi(x, y), 1 + 3\varepsilon - y)$.

As the time variation of energy equals minus the power of the corresponding force,

$$\frac{dE_c^\varepsilon}{dt} = - \int_{\Omega} F_c \cdot u dx$$

we recover the capillary force:

$$F_c(x, t) = -\chi \left[\operatorname{div} \left(\frac{1}{\varepsilon} \zeta\left(\frac{\varphi}{\varepsilon}\right) \frac{\nabla\varphi \otimes \nabla\varphi}{|\nabla\varphi|} \right) + \nabla \left(\operatorname{div} \left(\frac{\rho}{\rho_\ell - \rho_g} \frac{\nabla\varphi}{|\nabla\varphi|} \right) \right) \right]. \quad (13)$$

Conservation of momentum We write that the material derivative of momentum equals the sum of applied forces, which encompass the volume forces (gravity), and the capillary force we just derived:

$$(\rho u)_t + \operatorname{div}(\rho u \otimes u) = \rho g + \operatorname{div} \sigma - \chi \operatorname{div} \left(\frac{\nabla\varphi \otimes \nabla\varphi}{|\nabla\varphi|} \frac{1}{\varepsilon} \zeta\left(\frac{\varphi}{\varepsilon}\right) \right) - \chi \nabla \left(\operatorname{div} \left(\frac{\rho}{\rho_\ell - \rho_g} \frac{\nabla\varphi}{|\nabla\varphi|} \right) \right) \quad (14)$$

with $\sigma = \mu(\nabla u + \nabla u^T) + (\lambda \operatorname{div} u - p)\mathbb{I}$. We point out that the gradient term as to be taken into account, in contrast with the incompressible case where a gradient has zero work (under homogeneous or periodic boundary conditions). However we will see below that up to the redefinition of pressure, it could be dropped from the final equations.

Energy conservation From the fact that the latent heat of vaporization \mathcal{L} defines the enthalpy jump through the phase interface and assuming that the phase change occurs at constant pressure p_{sat} , we define the internal energy and total energy by

$$\mathcal{E}_I = c_v(T - T_{\text{sat}}) + \left(\mathcal{L} + \left(\frac{1}{\rho_\ell} - \frac{1}{\rho_g} \right) p_{\text{sat}} \right) H \left(\frac{\varphi}{\varepsilon} \right) \quad \mathcal{E}_T = \mathcal{E}_I + \frac{|u|^2}{2} + \frac{1}{\rho} \chi |\nabla \varphi| \frac{1}{\varepsilon} \zeta \left(\frac{\varphi}{\varepsilon} \right) \quad (15)$$

where c_v is the specific heat capacity at constant volume, \mathcal{L} the latent heat of vaporization, T_{sat} the saturation temperature. We later use the notation $\mathcal{L}_e := \mathcal{L} + \left(\frac{1}{\rho_\ell} - \frac{1}{\rho_g} \right) p_{\text{sat}}$.

We write that the variation of total energy balances the energy flux and the energy source ([11], p.15, equation (2-6)):

$$\partial_t(\rho \mathcal{E}_T) + \text{div}(\rho \mathcal{E}_T u) = -\text{div} \mathbb{J} + \rho \Psi. \quad (16)$$

The energy fluxes in our system correspond to surface constraints, which are of viscous and capillary types, and to the heat flux q that we classically assume to follow a Fourier's law $q = -k(\varphi) \nabla T$. We get

$$\mathbb{J} = -k(\varphi) \nabla T - \sigma \cdot u + \chi \frac{1}{\varepsilon} \zeta \left(\frac{\varphi}{\varepsilon} \right) \frac{\nabla \varphi \otimes \nabla \varphi}{|\nabla \varphi|} \cdot u + \chi \text{div} \left(\frac{\rho}{\rho_\ell - \rho_g} \frac{\nabla \varphi}{|\nabla \varphi|} \right) u.$$

The source term is reduced to the gravity contribution, since there is no heat sources: $\Psi = g \cdot u$. Finally we obtained the following conservation equation:

$$\begin{aligned} \partial_t(\rho \mathcal{E}_T) + \text{div}(\rho \mathcal{E}_T u) = & \text{div}(k(\varphi) \nabla T) + \text{div}(\sigma \cdot u) - \text{div} \left(\chi \frac{1}{\varepsilon} \zeta \left(\frac{\varphi}{\varepsilon} \right) \frac{\nabla \varphi \otimes \nabla \varphi}{|\nabla \varphi|} \cdot u \right) \\ & - \text{div} \left(\chi \text{div} \left(\frac{\rho}{\rho_\ell - \rho_g} \frac{\nabla \varphi}{|\nabla \varphi|} \right) u \right) + \rho g \cdot u. \end{aligned} \quad (17)$$

Energy equation written in temperature Rather than solving for total energy we will find an equation for the temperature that we can more easily measure. Plugging the total energy expression into (17), we get for the kinematic energy

$$\partial_t \left(\rho \frac{u^2}{2} \right) + \text{div} \left(\rho \frac{u^2}{2} u \right) = (\partial_t(\rho u) + \text{div}(\rho u \otimes u)) \cdot u$$

whose expression is given by the momentum equation. Therefore

$$\begin{aligned} \partial_t \left(\rho \frac{u^2}{2} \right) + \text{div} \left(\rho \frac{u^2}{2} u \right) = & \rho g \cdot u + \text{div}(\sigma) \cdot u \\ & - \chi \text{div} \left(\frac{\nabla \varphi \otimes \nabla \varphi}{|\nabla \varphi|} \frac{1}{\varepsilon} \zeta \left(\frac{\varphi}{\varepsilon} \right) \right) \cdot u - \chi \nabla \left(\text{div} \left(\frac{\rho}{\rho_\ell - \rho_g} \frac{\nabla \varphi}{|\nabla \varphi|} \right) \right) \cdot u. \end{aligned} \quad (18)$$

Subtracting this equation and (12) to the conservation of total energy, we get the internal energy conservation:

$$\partial_t(\rho \mathcal{E}_I) + \text{div}(\rho \mathcal{E}_I u) = \text{div}(k(\varphi) \nabla T) + \sigma : \nabla u - \chi \text{div} \left(\frac{\rho}{\rho_\ell - \rho_g} \frac{\nabla \varphi}{|\nabla \varphi|} \text{div} u \right). \quad (19)$$

Let us stop on that equation to point out that capillary forces have a thermal contribution only if $\text{div} u$ is not zero. This could be justified because except in case of phase change, capillarity is a non

dissipative force (of elastic type). Replacing the internal energy by its expression (15) as a function of temperature will produce the temperature equation. We first note that

$$\partial_t \left(\rho H \left(\frac{\varphi}{\varepsilon} \right) \right) + \operatorname{div} \left(\rho H \left(\frac{\varphi}{\varepsilon} \right) u \right) = \rho \left(\partial_t H \left(\frac{\varphi}{\varepsilon} \right) + u \cdot \nabla H \left(\frac{\varphi}{\varepsilon} \right) \right) = \frac{\rho^2}{\rho_\ell \rho_g} \Phi_m |\nabla \varphi| \frac{1}{\varepsilon} \zeta \left(\frac{\varphi}{\varepsilon} \right)$$

and setting $\theta = T - T_{\text{sat}}$, we finally obtain

$$\begin{aligned} \partial_t(\rho c_V \theta) + \operatorname{div}(\rho c_V \theta u) &= \operatorname{div}(k(\varphi) \nabla \theta) - \frac{\rho^2}{\rho_g \rho_\ell} \Phi_m \mathcal{L}_\varepsilon |\nabla \varphi| \frac{1}{\varepsilon} \zeta \left(\frac{\varphi}{\varepsilon} \right) + \sigma : \nabla u \\ &\quad - \chi \operatorname{div} \left(\frac{\rho}{\rho_\ell - \rho_g} \frac{\nabla \varphi}{|\nabla \varphi|} \operatorname{div} u \right). \end{aligned} \quad (20)$$

3.2 A simplified model for the mass flux Φ_m

In order to close the above model, one needs to find a relation between Φ_m and other variables. The idea of our approach is to consider that the droplet is at constant temperature $T = T_{\text{sat}}$ (or $\theta = 0$), equal to the temperature of saturation. In the numerical scheme we will add a penalization term to ensure that this property holds true. Ensuring that the phase change indeed occurs at the saturation temperature is one of the big difficulty of phase change simulations. Our hope is that this penalization, which simplifies the expression of Φ_m , will also stabilize the whole model. Assuming that initially all the domain is at constant temperature equal to the liquid saturation temperature, the heating from below will lead to a raise of temperature of the surrounding fluid while the droplet will undergo phase change at constant temperature. Therefore a heat flux from outside the drop to inside will establish, which will be captured by the phase change layer for vaporization. We assume that this heat flux q follows a Fourier's law:

$$q = -k \nabla T.$$

Then, the assumption of constant temperature inside the droplet means that there is no heat flux inside, and therefore the heat flux jump across the interface is merely the outer heat flux. This also means that every part of the outer heat flux is used to vaporize the droplet, while none is used to raise its temperature. Let \mathcal{L} be the vaporization heat which is the heat required to transform a unit mass of liquid into vapor. Let us consider a small part ω of the interface layer $\{|\varphi| < \varepsilon\}$ with middle surface $\omega \cap \{\varphi = 0\}$ of measure $\delta\sigma$. The surface heat sink due to phase-change being smeared, the local heat balance equation on ω reads:

$$\operatorname{div} q = -\mathcal{L} \Phi_m \frac{1}{\varepsilon} \zeta \left(\frac{\varphi}{\varepsilon} \right) |\nabla \varphi|.$$

Note that

$$\int_\omega \frac{1}{\varepsilon} \zeta \left(\frac{\varphi}{\varepsilon} \right) |\nabla \varphi| dx = \int_{-\varepsilon}^\varepsilon \int_{\{|\varphi|=r\} \cap \omega} \frac{1}{\varepsilon} \zeta \left(\frac{\varphi}{\varepsilon} \right) d\sigma dr = \int_{-\varepsilon}^\varepsilon \frac{1}{\varepsilon} \zeta \left(\frac{r}{\varepsilon} \right) \left(\int_{\{|\varphi|=r\} \cap \omega} d\sigma \right) dr \longrightarrow \delta\sigma$$

when $\varepsilon \rightarrow 0$, so that integrating the local heat balance gives, neglecting the contribution of the heat flux tangential to the interface,

$$\Phi_m \delta\sigma \approx -\frac{1}{\mathcal{L}} \int_\omega \operatorname{div} q dx \approx -\frac{1}{\mathcal{L}} (q_i \cdot n_i \delta\sigma + q_o \cdot n_o \delta\sigma)$$

where q_i (resp. q_o) is the heat flux inside the droplet (resp. outside the droplet and interface layer), and n_i, n_o are the corresponding exterior normals. By assumption the temperature is constant inside the droplet therefore $q_i = 0$. Assuming linear variation of q inside the layer, q is equal to $q_o/2$ on the middle of the layer. Thus inside ω , we have

$$\Phi_m \approx -\frac{2q \cdot n}{\mathcal{L}} = \frac{2}{\mathcal{L}} k(\varphi) \nabla \theta \cdot \frac{\nabla \varphi}{|\nabla \varphi|}.$$

In this formula for Φ_m we have assumed temperature constant inside the droplet and the heat flux orthogonal to the phase-change interface in the phase change layer. If the temperature outside the droplet is greater than T_{sat} , the temperature gradient points outward of the droplet, while q is inward, and thus $q \cdot n < 0$, which gives $\Phi_m > 0$. One way to ensure a constant temperature in the droplet is, from a numerical point of view, to add a penalization term in the temperature equation:

$$\begin{aligned} \partial_t(\rho c_V \theta) + \text{div}(\rho c_V \theta u) + \frac{1}{\eta} \left(1 - H\left(\frac{\varphi}{\varepsilon}\right)\right) \theta &= \text{div}(k(\varphi) \nabla \theta) - \frac{\rho^2}{\rho_g \rho_\ell} \Phi_m \mathcal{L}_e |\nabla \varphi| \frac{1}{\varepsilon} \zeta\left(\frac{\varphi}{\varepsilon}\right) \\ &+ \sigma : \nabla u - \chi \text{div}\left(\frac{\rho}{\rho_\ell - \rho_g} \frac{\nabla \varphi}{|\nabla \varphi|} \text{div} u\right) \end{aligned} \quad (21)$$

where $\eta > 0$ is a small parameter. Eliminating Φ_m in the equation gives:

$$\begin{aligned} \partial_t(\rho c_V \theta) + \text{div}(\rho c_V \theta u) + \frac{1}{\eta} \left(1 - H\left(\frac{\varphi}{\varepsilon}\right)\right) \theta &= \text{div}(k(\varphi) \nabla \theta) - \frac{2\rho^2}{\rho_g \rho_\ell} \frac{\mathcal{L}_e}{\mathcal{L}} k(\varphi) \nabla \theta \cdot \nabla \varphi \frac{1}{\varepsilon} \zeta\left(\frac{\varphi}{\varepsilon}\right) \\ &+ \sigma : \nabla u - \chi \text{div}\left(\frac{\rho}{\rho_\ell - \rho_g} \frac{\nabla \varphi}{|\nabla \varphi|} \text{div} u\right). \end{aligned} \quad (22)$$

In order to write an evolution equation for the temperature, we note that

$$\partial_t(\rho c_V \theta) + \text{div}(\rho c_V \theta u) = \rho c_V (\partial_t \theta + u \cdot \nabla \theta) + (c_{Vg} - c_{V\ell}) \frac{\rho^2 \theta}{\rho_g \rho_\ell} \Phi_m |\nabla \varphi| \frac{1}{\varepsilon} \zeta\left(\frac{\varphi}{\varepsilon}\right).$$

3.3 Final model

First formulation. Gathering the above equations we obtain the following complex fluid formulation of phase-change:

$$\left\{ \begin{array}{l} \partial_t \rho + \text{div}(\rho u) = 0 \\ \text{div} u = 2 \frac{\varepsilon}{\mathcal{L}} k(\varphi) \nabla \theta \cdot \nabla \varphi \frac{1}{\varepsilon} \zeta\left(\frac{\varphi}{\varepsilon}\right) \\ \partial_t(\rho u) + \text{div}(\rho u \otimes u) - \text{div} \sigma_T = \rho g \\ \rho c_V (\partial_t \theta + u \cdot \nabla \theta) + \frac{1}{\eta} \left(1 - H\left(\frac{\varphi}{\varepsilon}\right)\right) \theta - \text{div}(k(\varphi) \nabla \theta) + (\mathcal{L}_e + (c_{Vg} - c_{V\ell}) \theta) \frac{2\rho^2}{\rho_g \rho_\ell} \frac{k(\varphi) \nabla \theta}{\mathcal{L}} \cdot \nabla \varphi \frac{1}{\varepsilon} \zeta\left(\frac{\varphi}{\varepsilon}\right) = \mathcal{N} \\ \partial_t \varphi + u \cdot \nabla \varphi = \frac{2\rho}{\rho_\ell \rho_g \mathcal{L}} k(\varphi) \nabla \theta \cdot \nabla \varphi \end{array} \right. \quad (23)$$

with

$$\begin{aligned}
c &= \frac{1}{\rho_g} - \frac{1}{\rho_\ell} > 0, \quad \sigma = 2\mu D(u) + (\lambda \operatorname{div} u - p)\mathbb{I}, \\
\sigma_T &= \sigma - \chi \frac{1}{\varepsilon} \zeta \left(\frac{\varphi}{\varepsilon} \right) \nabla \varphi \otimes \nabla \varphi - \chi \operatorname{div} \left(\frac{\rho}{\rho_\ell - \rho_g} \frac{\nabla \varphi}{|\nabla \varphi|} \right) \mathbb{I} \\
\theta &= T - T_{\text{sat}} \\
c_V &\text{ is the specific heat capacity at constant volume (per unit of mass)} \\
\mathcal{N} &= \sigma : \nabla u - \chi \operatorname{div} \left(\frac{\rho}{\rho_\ell - \rho_g} \frac{\nabla \varphi}{|\nabla \varphi|} \operatorname{div} u \right)
\end{aligned}$$

Unknowns are: ρ , $u = (u_1, u_2, u_3)$, p , T , φ .

Another expression of surface tension. The surface tension is given by:

$$-\chi \operatorname{div} \left(\frac{\nabla \varphi \otimes \nabla \varphi}{|\nabla \varphi|} \frac{1}{\varepsilon} \zeta \left(\frac{\varphi}{\varepsilon} \right) \right) - \chi \nabla \left(\operatorname{div} \left(\frac{\rho}{\rho_\ell - \rho_g} \frac{\nabla \varphi}{|\nabla \varphi|} \right) \right).$$

Expanding the first term gives:

$$\begin{aligned}
\operatorname{div} \left(\frac{\nabla \varphi \otimes \nabla \varphi}{|\nabla \varphi|} \frac{1}{\varepsilon} \zeta \left(\frac{\varphi}{\varepsilon} \right) \right) &= \\
\operatorname{div} \left(\frac{\nabla \varphi \otimes \nabla \varphi}{|\nabla \varphi|} \right) \frac{1}{\varepsilon} \zeta \left(\frac{\varphi}{\varepsilon} \right) &+ |\nabla \varphi| \left(\frac{\nabla \varphi \otimes \nabla \varphi}{|\nabla \varphi|^2} - I \right) \nabla \left(\frac{1}{\varepsilon} \zeta \left(\frac{\varphi}{\varepsilon} \right) \right) + |\nabla \varphi| \nabla \left(\frac{1}{\varepsilon} \zeta \left(\frac{\varphi}{\varepsilon} \right) \right).
\end{aligned}$$

However $\left(\frac{\nabla \varphi \otimes \nabla \varphi}{|\nabla \varphi|^2} - I \right)$ is the projection on the tangent plane to $\{\varphi = 0\}$ while $\nabla \left(\frac{1}{\varepsilon} \zeta \left(\frac{\varphi}{\varepsilon} \right) \right)$ is normal to this plane. Therefore the corresponding term vanishes. Moreover

$$\operatorname{div} \left(\frac{\nabla \varphi \otimes \nabla \varphi}{|\nabla \varphi|} \right) \frac{1}{\varepsilon} \zeta \left(\frac{\varphi}{\varepsilon} \right) = \operatorname{div} \left(\frac{\nabla \varphi}{|\nabla \varphi|} \right) \nabla \varphi \frac{1}{\varepsilon} \zeta \left(\frac{\varphi}{\varepsilon} \right) + \nabla(\nabla \varphi) \frac{\nabla \varphi}{|\nabla \varphi|} \frac{1}{\varepsilon} \zeta \left(\frac{\varphi}{\varepsilon} \right).$$

Since

$$\nabla(\nabla \varphi) \frac{\nabla \varphi}{|\nabla \varphi|} = \nabla |\nabla \varphi|$$

we obtain

$$\operatorname{div} \left(\frac{\nabla \varphi \otimes \nabla \varphi}{|\nabla \varphi|} \frac{1}{\varepsilon} \zeta \left(\frac{\varphi}{\varepsilon} \right) \right) = \operatorname{div} \left(\frac{\nabla \varphi}{|\nabla \varphi|} \right) \nabla \varphi \frac{1}{\varepsilon} \zeta \left(\frac{\varphi}{\varepsilon} \right) + \nabla \left(|\nabla \varphi| \frac{1}{\varepsilon} \zeta \left(\frac{\varphi}{\varepsilon} \right) \right).$$

Gathering the gradient terms we get

$$-\chi \kappa(\varphi) \frac{1}{\varepsilon} \zeta \left(\frac{\varphi}{\varepsilon} \right) \nabla \varphi - \chi \nabla \left[\operatorname{div} \left(\frac{\rho}{\rho_\ell - \rho_g} \frac{\nabla \varphi}{|\nabla \varphi|} \right) + |\nabla \varphi| \frac{1}{\varepsilon} \zeta \left(\frac{\varphi}{\varepsilon} \right) \right], \quad (24)$$

which simplifies using $\nabla \rho = -(\rho_\ell - \rho_g) \nabla \varphi \frac{1}{\varepsilon} \zeta \left(\frac{\varphi}{\varepsilon} \right)$, to give the following alternative form:

$$-\chi \kappa(\varphi) \frac{1}{\varepsilon} \zeta \left(\frac{\varphi}{\varepsilon} \right) \nabla \varphi - \chi \nabla \left[\frac{\rho}{\rho_\ell - \rho_g} \kappa(\varphi) \right], \quad (25)$$

where $\kappa(\varphi)$ is the curvature given by:

$$\kappa(\varphi) = \operatorname{div} \left(\frac{\nabla \varphi}{|\nabla \varphi|} \right) \quad \text{In dimension 2: } \kappa = \frac{\partial_x^2 \varphi (\partial_y \varphi)^2 - 2 \partial_{xy}^2 \varphi \partial_x \varphi \partial_y \varphi + \partial_y^2 \varphi (\partial_x \varphi)^2}{|\nabla \varphi|^3} \quad (26)$$

Expanding the gradient term and using the expression for $\nabla \rho$ gives rise to the following simple form (equivalent to (13)) of the capillary force:

$$F_c = -\chi \frac{\rho}{\rho_\ell - \rho_g} \nabla \kappa(\varphi). \quad (27)$$

Remark 2. *One could be surprised that only the gradient of mean curvature seems to play a role in the capillary force, whereas the well known Laplace law states that the force is proportional to the curvature. This stems from the fact that in the incompressible case for Dirichlet conditions, gradients are irrelevant in terms of energy and therefore a constant $\kappa(\varphi)$ would just correspond to a modification of the pressure. This is not that case in the pseudo-compressible case under study, and the form (27) is not equivalent to the usual Laplace law.*

Second formulation Nethertheless, the form (27) has some drawbacks: indeed it is not localized in a neighborhood of the interface and therefore its implementation would require to compute the curvature of level sets of φ everywhere, which is highly undesirable since this curvature goes to infinity somewhere inside the droplet. As in the incompressible case, we could seek to absorb a gradient term into the pressure. It is indeed possible to introduce a pressure \tilde{p} defined by

$$\tilde{p} = p + \chi \frac{\rho}{\rho_\ell - \rho_g} \kappa(\varphi) \quad (28)$$

and set $\tilde{\sigma} = 2\mu D(u) + (\lambda \operatorname{div} u - \tilde{p})\mathbb{I}$, and $\tilde{F}_c = -\chi \kappa(\varphi) \frac{1}{\varepsilon} \zeta \left(\frac{\varphi}{\varepsilon} \right) \nabla \varphi$. Of course doing that we have to correct the \mathcal{N} reflecting the fact that gradient terms produce heat in the compressible interface. We obtain a model consisting of the system

$$\left\{ \begin{array}{l} \partial_t \rho + \operatorname{div}(\rho u) = 0 \\ \operatorname{div} u = 2 \frac{c}{\mathcal{L}} k(\varphi) \nabla \theta \cdot \nabla \varphi \frac{1}{\varepsilon} \zeta \left(\frac{\varphi}{\varepsilon} \right) \\ \partial_t(\rho u) + \operatorname{div}(\rho u \otimes u) - \operatorname{div} \tilde{\sigma} = \rho g - \chi \kappa(\varphi) \frac{1}{\varepsilon} \zeta \left(\frac{\varphi}{\varepsilon} \right) \nabla \varphi \\ \rho c_v (\partial_t \theta + u \cdot \nabla \theta) + \frac{1}{\eta} (1 - H \left(\frac{\varphi}{\varepsilon} \right)) \theta - \operatorname{div}(k(\varphi) \nabla \theta) + (\mathcal{L}_e + (c_{v_g} - c_{v_\ell}) \theta) \frac{2\rho^2}{\rho_g \rho_\ell} \frac{k(\varphi) \nabla \theta}{\mathcal{L}} \cdot \nabla \varphi \frac{1}{\varepsilon} \zeta \left(\frac{\varphi}{\varepsilon} \right) = \mathcal{N} \\ \partial_t \varphi + u \cdot \nabla \varphi = \frac{2\rho}{\rho_\ell \rho_g \mathcal{L}} k(\varphi) \nabla \theta \cdot \nabla \varphi \end{array} \right. \quad (29)$$

with

$$c = \frac{1}{\rho_\ell} - \frac{1}{\rho_g} < 0, \quad \tilde{\sigma} = 2\mu D(u) + (\lambda \operatorname{div} u - \tilde{p})\mathbb{I},$$

$$\theta = T - T_{\text{sat}},$$

c_v is the specific heat capacity at constant volume (per unit of mass),

$$\mathcal{N} = \tilde{\sigma} : \nabla u - \chi \nabla \left(\frac{\rho}{\rho_\ell - \rho_g} \operatorname{div} u \right) \cdot \frac{\nabla \varphi}{|\nabla \varphi|}.$$

As the capillary forces are fully expanded, this form is expected to be more stable. The hydrodynamic pressure p is easily recovered from \tilde{p} , if necessary.

4 Numerical simulation

4.1 Reinitiatization of φ

The drop interface is located by the zero level-set of φ which is advected by the velocity field u . Concerning the location of interface, only the zero level-set matters. However since we spread the singular force in a neighborhood of this interface, supposed to be of width 2ε , and defined by $-\varepsilon \leq \varphi \leq \varepsilon$, the slope of this function also comes into play. If φ is not a distance function, the width of this set could be different from 2ε , as illustrated on Fig.1 and Fig.2.

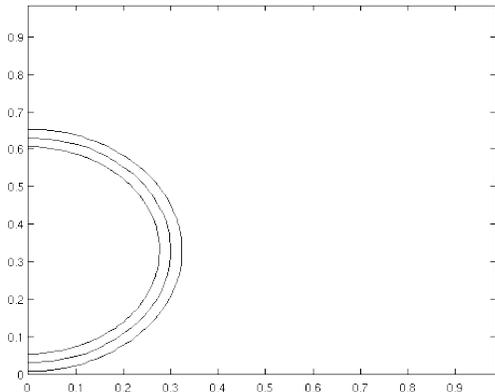


FIGURE 1: Level sets $-\varepsilon$, 0 and ε of φ at initial time.

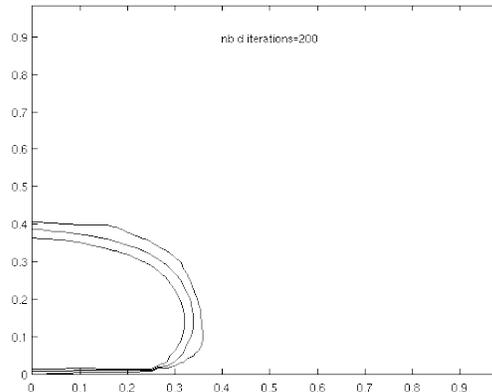


FIGURE 2: Level sets $-\varepsilon$, 0 and ε of φ after 200 iterations without reinitialization.

To circumvent this possible problem, we take φ_0 as a signed distance to the initial interface and solve the classical Hamilton-Jacobi equation to recover a distance function from φ_t at time t [8]. However we use this distance function only to apply the spreaded force, and start over with the non reinitialized φ so that no volume loss is induced and $|\nabla\varphi|$ still records the length variation of interface. Doing that, the spreaded interface keeps a constant width as illustrated on Fig.3.

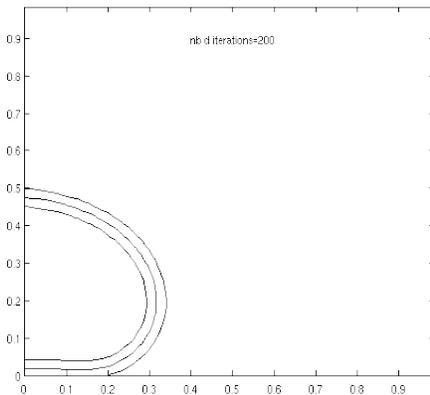


FIGURE 3: Level sets $-\varepsilon$, 0 and ε of φ after 200 iterations with reinitialization.

4.2 Time discretization

We developed an explicit scheme, where we neglected the heat generated by capillary and viscosity forces corresponding to \mathcal{N} in (29). This has been justified in [10]. Given $\rho^n, u^n, \tilde{p}^n, T^n, \Phi_m^n$ and φ^n at time iteration n , we compute iteration $n + 1$ by solving:

Advection of φ

$$\varphi^{n+1} = \varphi^n - \Delta t \left(u^n - \frac{\rho^n}{\rho_\ell \rho_g} \Phi_m^n \frac{\nabla \varphi^n}{|\nabla \varphi^n|} \right) \cdot \nabla \varphi^n. \quad (30)$$

Computation of ρ

$$\rho^{n+1} = \rho_\ell \left(1 - H \left(\frac{\varphi^{n+1}}{\varepsilon} \right) \right) + \rho_g H \left(\frac{\varphi^{n+1}}{\varepsilon} \right).$$

Temperature equation

$$\begin{aligned} \rho^{n+1} c_v(\varphi^{n+1}) \frac{\theta^{n+1} - \theta^n}{\Delta t} + \rho^{n+1} c_v(\varphi^{n+1}) u^n \cdot \nabla \theta^n + \frac{1}{\eta} \left(1 - H \left(\frac{\varphi^{n+1}}{\varepsilon} \right) \right) \theta^{n+1} - \operatorname{div} (k(\varphi^{n+1}) \nabla \theta^{n+1}) \\ = - (\mathcal{L}_e + (c_{vg} - c_{v\ell}) \theta^n) \frac{(\rho^{n+1})^2}{\rho_g \rho_\ell} \Phi_m^n |\nabla \varphi^{n+1}| \frac{1}{\varepsilon} \zeta \left(\frac{\varphi^{n+1}}{\varepsilon} \right). \end{aligned} \quad (31)$$

Interfacial mass flux

$$\Phi_m^{n+1} = \frac{2k(\varphi^{n+1}) \nabla \theta^{n+1}}{\mathcal{L}} \cdot \frac{\nabla \varphi^{n+1}}{|\nabla \varphi^{n+1}|}. \quad (32)$$

Solving Navier-Stokes equation Due to the fact that the divergence of velocity field is related to the interfacial mass flux which has been computed above, solving the Navier-Stokes equations can be performed using a slightly modified version of the classical Chorin projection algorithm in the incompressible case:

$$\begin{cases} \rho(\partial_t u + (u \cdot \nabla)u - \operatorname{div}(2\mu D(u)) - \lambda \nabla(\operatorname{div} u) + \nabla \tilde{p} = f \\ \operatorname{div} u = c \Phi_m |\nabla \varphi| \frac{1}{\varepsilon} \zeta \left(\frac{\varphi}{\varepsilon} \right) \end{cases} \quad (33)$$

In a first step we seek u^* solution of

$$\rho^{n+1} \left(\frac{u^* - u^n}{\Delta t} + (u^n \cdot \nabla) u^n \right) - \operatorname{div}(\mu^{n+1} D(u^*)) - \lambda \nabla(\operatorname{div} u^*) = \rho g - \chi \kappa(\varphi^{n+1}) \frac{1}{\varepsilon} \zeta \left(\frac{\varphi^{n+1}}{\varepsilon} \right) \nabla \varphi^{n+1} \quad (34)$$

In order to ensure the correct divergence condition, we compute the \tilde{p}^{n+1} from the Poisson equation:

$$\operatorname{div} \left(\frac{\nabla \tilde{p}^{n+1}}{\rho^{n+1}} \right) = - \frac{1}{\Delta t} \left(c \Phi_m^{n+1} |\nabla \varphi^{n+1}| \frac{1}{\varepsilon} \zeta \left(\frac{\varphi^{n+1}}{\varepsilon} \right) - \operatorname{div} u^* \right), \quad (35)$$

and then correct accordingly u^* to get u^{n+1} :

$$u^{n+1} = u^* - \Delta t \frac{\nabla \tilde{p}^{n+1}}{\rho^{n+1}}. \quad (36)$$

4.3 Spatial discretization in axisymmetrical case

Our test case will be to compare the analytical volume as a function of time for an evaporating droplet given in (2), with the one obtained from our numerical computations. Since we are not yet interested in drop motion (forthcoming work) we consider the axisymmetrical situation where we use classical cylindrical coordinates (r, θ, z) . All the problem reduces in the half r, z plane ($r \geq 0$) and the full 3D shape is obtained from a θ rotation.

We consider a discretization of m cells in the r direction and n in the z direction, with two mesh steps: $\Delta r = L_r/m$ and $\Delta z = L_z/n$ where L_r and L_z are the domain size in r et z direction. The time step is denoted by Δt , which leads to a time-space grid $(t_k, r_i, z_j) = (k\Delta t, (i - \frac{1}{2})\Delta r, (j - \frac{1}{2})\Delta z)$. For a function $g : \mathbb{R}^2 \rightarrow \mathbb{R}$ we denote by $g_{i,j}$ the approximating value of $g(r_i, z_j)$. The positioning of unknowns on the grid follows the MAC principles: the pressure is defined on nodes (i, j) , radial velocity between two horizontally aligned nodes $(i + \frac{1}{2}, j)$, and vertical velocity between two vertically aligned nodes $(i, j + \frac{1}{2})$ (Fig. 4). This way of positioning degrees of freedom ensure that the discrete operators defined thereafter verify a property such that no parasitic mode in the pressure appears. Moreover, in the projection method, the divergence of velocity field is exactly equal to the mass flux by construction since the discrete divergence of discrete gradient coincides with the discrete Laplacian used to solve the Poisson equation.

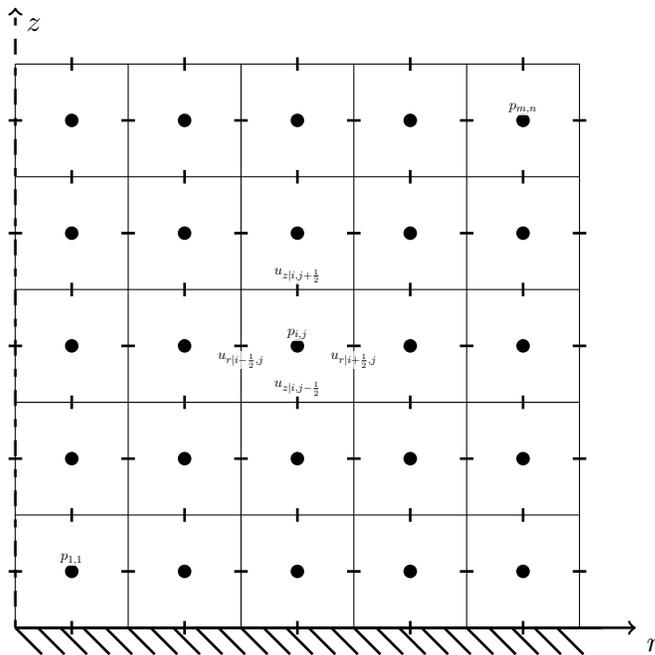


FIGURE 4: Position of discretization nodes for pressure (\tilde{p}), radial (u_r) and vertical (u_z) components of velocity.

On this grid, order two discretizations of first order derivatives of u_r with respect to r , u_z with respect to z are located on the pressures nodes while derivatives of \tilde{p} are located on the corresponding velocity nodes. That leads to a velocity divergence's discretization located on the same node as \tilde{p} . We

used the following expressions:

$$\begin{aligned}
(\operatorname{div} u)_{i,j} &\approx \frac{r_{i+\frac{1}{2},j} u_{r|i+\frac{1}{2},j} - r_{i-\frac{1}{2},j} u_{r|i-\frac{1}{2},j}}{r_{i,j} \Delta r} + \frac{u_{z|i,j+\frac{1}{2}} - u_{z|i,j-\frac{1}{2}}}{\Delta z} \\
(\partial_r \tilde{p})_{i+\frac{1}{2},j} &\approx \frac{\tilde{p}_{i+1,j} - \tilde{p}_{i,j}}{\Delta r} \\
(\partial_z \tilde{p})_{i,j+\frac{1}{2}} &\approx \frac{\tilde{p}_{i,j+1} - \tilde{p}_{i,j}}{\Delta z}
\end{aligned}$$

All other variables $(\rho, T, \varphi, \dots)$ are located on the pressure nodes.

In order to solve (35), we write the following discretization on pressure nodes:

$$\forall 2 \leq i \leq m-1, 2 \leq j \leq n-1$$

$$\begin{aligned}
\left(\operatorname{div} \left(\frac{\nabla \tilde{p}}{\rho} \right) \right)_{i,j} &\approx \frac{1}{r_{i,j} \Delta r} \left[\frac{r_{i+\frac{1}{2},j} (\partial_r \tilde{p})_{i+\frac{1}{2},j}}{\rho_{i+\frac{1}{2},j}} - \frac{r_{i-\frac{1}{2},j} (\partial_r \tilde{p})_{i-\frac{1}{2},j}}{\rho_{i-\frac{1}{2},j}} \right] \\
&\quad + \frac{1}{\Delta z} \left[\frac{(\partial_z \tilde{p})_{i,j+\frac{1}{2}}}{\rho_{i,j+\frac{1}{2}}} - \frac{(\partial_z \tilde{p})_{i,j-\frac{1}{2}}}{\rho_{i,j-\frac{1}{2}}} \right] \\
&\approx \frac{1}{\rho_{i+\frac{1}{2},j} \Delta r^2} \left(\frac{r_{i+\frac{1}{2},j}}{r_{i,j}} \right) (\tilde{p}_{i+1,j} - \tilde{p}_{i,j}) \\
&\quad - \frac{1}{\rho_{i-\frac{1}{2},j} \Delta r^2} \left(\frac{r_{i-\frac{1}{2},j}}{r_{i,j}} \right) (\tilde{p}_{i,j} - \tilde{p}_{i-1,j}) \\
&\quad + \frac{1}{\rho_{i,j+\frac{1}{2}} \Delta z^2} (\tilde{p}_{i,j+1} - \tilde{p}_{i,j}) \\
&\quad - \frac{1}{\rho_{i,j-\frac{1}{2}} \Delta z^2} (\tilde{p}_{i,j} - \tilde{p}_{i,j-1})
\end{aligned}$$

with

$$\rho_{i+\frac{1}{2},j} \approx \rho_\ell \left(1 - H \left(\frac{\varphi_{i+\frac{1}{2},j}}{\varepsilon} \right) \right) + \rho_g H \left(\frac{\varphi_{i+\frac{1}{2},j}}{\varepsilon} \right) \quad \text{and} \quad \varphi_{i+\frac{1}{2},j} \approx \frac{\varphi_{i,j} + \varphi_{i+1,j}}{2}$$

and likewise for $\rho_{i,j+\frac{1}{2}}$.

Factorizing by the pressure \tilde{p} , we get $\forall 2 \leq i \leq m-1, 2 \leq j \leq n-1$

$$a_{i,j}^\oplus \tilde{p}_{i+1,j} + a_{i,j}^\ominus \tilde{p}_{i-1,j} + b_{i,j}^\oplus \tilde{p}_{i,j+1} + b_{i,j}^\ominus \tilde{p}_{i,j-1} + c_{i,j} \tilde{p}_{i,j} = f_{i,j}$$

with

$$\begin{aligned}
a_{i,j}^{\oplus} &= \frac{1}{\rho_{i+\frac{1}{2},j} \Delta r^2} \frac{r_{i+\frac{1}{2},j}}{r_{i,j}}, \\
a_{i,j}^{\ominus} &= \frac{1}{\rho_{i-\frac{1}{2},j} \Delta r^2} \frac{r_{i-\frac{1}{2},j}}{r_{i,j}}, \\
b_{i,j}^{\oplus} &= \frac{1}{\rho_{i,j+\frac{1}{2}} \Delta z^2}, \\
b_{i,j}^{\ominus} &= \frac{1}{\rho_{i,j-\frac{1}{2}} \Delta z^2}, \\
c_{i,j} &= - \left(a_{i,j}^{\oplus} + a_{i,j}^{\ominus} + b_{i,j}^{\oplus} + b_{i,j}^{\ominus} \right), \\
f &= - \frac{1}{\Delta t} \left(c \Phi_m^{n+1} |\nabla \varphi^{n+1}| \frac{1}{\varepsilon} \zeta \left(\frac{\varphi^{n+1}}{\varepsilon} \right) - \operatorname{div} u^* \right).
\end{aligned}$$

On the boundaries, depending of boundary conditions (see below), we obtain:

- for $i = 1$, $2 \leq j \leq n - 1$, due to the axisymetry, we get $\partial_r p = 0$ that discretizes to $\tilde{p}_{0,j} = \tilde{p}_{1,j}$, therefore
$$a_{i,j}^{\oplus} \tilde{p}_{i+1,j} + b_{i,j}^{\oplus} \tilde{p}_{i,j+1} + b_{i,j}^{\ominus} \tilde{p}_{i,j-1} + \left(a_{i,j}^{\ominus} + c_{i,j} \right) \tilde{p}_{i,j} = f_{i,j}$$
- for $i = m$, $2 \leq j \leq n - 1$, we ensure a hydrostatic pressure that leads to the Dirichlet condition $p(L_r, z) = (L_z - z)g\rho_g$ that discretizes to $\frac{1}{2}\tilde{p}_{m,j} + \frac{1}{2}\tilde{p}_{m+1,j} = (n - j + \frac{1}{2}) \Delta z g\rho_g$. Therefore
$$a_{i,j}^{\ominus} \tilde{p}_{i-1,j} + b_{i,j}^{\oplus} \tilde{p}_{i,j+1} + b_{i,j}^{\ominus} \tilde{p}_{i,j-1} + \left(c_{i,j} - a_{i,j}^{\oplus} \right) \tilde{p}_{i,j} = f_{i,j} - 2a_{i,j}^{\oplus} \left(n - j + \frac{1}{2} \right) \Delta z g\rho_g$$
- for $2 \leq i \leq m - 1$, $j = 1$, Neumann condition $\partial_z p = 0$ discretizes to $\tilde{p}_{i,0} = \tilde{p}_{i,1}$, therefore
$$a_{i,j}^{\oplus} \tilde{p}_{i+1,j} + a_{i,j}^{\ominus} \tilde{p}_{i-1,j} + b_{i,j}^{\oplus} \tilde{p}_{i,j+1} + \left(b_{i,j}^{\ominus} + c_{i,j} \right) \tilde{p}_{i,j} = f_{i,j}$$
- for $2 \leq i \leq m - 1$, $j = n$, Dirichlet condition $p(r, L_z) = 0$ discretizes to $\frac{1}{2}\tilde{p}_{i,n} + \frac{1}{2}\tilde{p}_{i,n+1} = 0$, therefore
$$a_{i,j}^{\oplus} \tilde{p}_{i+1,j} + a_{i,j}^{\ominus} \tilde{p}_{i-1,j} + b_{i,j}^{\ominus} \tilde{p}_{i,j-1} + \left(c_{i,j} - b_{i,j}^{\oplus} \right) \tilde{p}_{i,j} = f_{i,j}$$

At the mesh corners, merging the appropriate boundary conditions give us the following equations :

$$\begin{aligned}
&a_{1,1}^{\oplus} \tilde{p}_{2,1} + b_{1,1}^{\oplus} \tilde{p}_{1,2} + \left(a_{1,1}^{\ominus} + b_{1,1}^{\ominus} + c_{1,1} \right) \tilde{p}_{1,1} = f_{1,1}, \\
&a_{1,n}^{\oplus} \tilde{p}_{2,n} + b_{1,n}^{\ominus} \tilde{p}_{1,n-1} + \left(a_{1,n}^{\ominus} + c_{1,n} - b_{1,n}^{\oplus} \right) \tilde{p}_{1,n} = f_{1,n}, \\
&a_{m,n}^{\ominus} \tilde{p}_{m-1,n} + b_{m,n}^{\ominus} \tilde{p}_{m,n-1} + \left(c_{m,n} - a_{m,n}^{\oplus} - b_{m,n}^{\oplus} \right) \tilde{p}_{m,n} = f_{m,n} - a_{m,n}^{\oplus} \Delta z g\rho_g, \\
&a_{m,1}^{\ominus} \tilde{p}_{m-1,1} + b_{m,1}^{\oplus} \tilde{p}_{m,2} + \left(b_{m,1}^{\ominus} + c_{m,1} - a_{m,1}^{\oplus} \right) \tilde{p}_{m,1} = f_{m,1} - 2a_{m,1}^{\oplus} \left(n - \frac{1}{2} \right) \Delta z g\rho_g.
\end{aligned}$$

5 Test case

We assume initially the droplet to be of hemi-circular shape centered on the z -axis, at rest and at saturation temperature (373K) and heated from below at 530K. The computational domain is taken

to be $\Omega =]0, L_r[\times]0, L_z[$, upon which we set:

$$\begin{aligned} u_0(r, z) &= 0, \\ \varphi_0(r, z) &= \sqrt{r^2 + (z - z_c)^2} - R^2, \\ \rho_0 &= \rho_g H_\epsilon(\varphi_0) + \rho_\ell (1 - H_\epsilon(\varphi_0)), \\ T_0 &= T_{\text{sat}}. \end{aligned}$$

5.1 Boundary conditions

We split the boundary $\partial\Omega$ in four parts which are: $\partial\Omega_B$ (bottom), $\partial\Omega_L$ (left), $\partial\Omega_R$ (right) and $\partial\Omega_T$ (top). For a considered quantity G : G_B , G_L , G_R and G_T stand for the corresponding values taken by this quantity on the above parts of $\partial\Omega$. We will denote by N a normal vector to $\partial\Omega$. With these notations we consider the following boundary conditions (we indicate boundary conditions for the pressure which are used in the projection method):

On $\partial\Omega_L$ (z axis), u_r has to vanish due to the axisymmetric case:

$$u_r = 0, \quad \partial_r u_z = 0, \quad \partial_r p = 0, \quad \partial_r \varphi = 0, \quad \partial_r T = 0.$$

On $\partial\Omega_B$:

$$u = 0, \quad \partial_z p = 0, \quad T = 530.$$

On $\partial\Omega_R$:

$$\partial_r u_z = 0, \quad \partial_r u_r = 0, \quad p = (L_z - z)\rho_g g, \quad \partial_r \varphi = 0, \quad \partial_r T = 0.$$

On $\partial\Omega_T$:

$$\partial_z u_r = 0, \quad \partial_z u_z = 0, \quad p = 0, \quad \partial_z \varphi = 0, \quad T = 373.$$

5.2 Physical constants considered

ρ_ℓ, ρ_g the densities of liquid and gaz under atmospheric pressure: $\rho_\ell = 1000 \text{ kg/m}^3$, $\rho_g = 1.3 \text{ kg/m}^3$.

μ the dynamical viscosity, $\mu_\ell = 0.28 \times 10^{-3} \text{ pa.s}$ (pa.s=kg/m.s) for water at 100°C and $\mu_g = 0.015 \times 10^{-3}$ for vapor.

χ the surface tension coefficient between water and vapor, $\chi = 0.06 \text{ N/m}$ (N=kg.m/s²) at temperature 100°C .

k the thermal conductivity, $k_\ell \approx 0.3 \text{ J.m}^{-1}.\text{K}^{-1}.\text{s}^{-1}$ for water at temperature 100°C , and $k_g = 0.016$ for vapor.

c_V the specific heat capacity, $c_{V\ell} = 4186 \text{ J.kg}^{-1}.\text{K}$ for water, and $c_{Vg} = 1850$ for vapor.

\mathcal{L} the latent heat of vaporization, $\mathcal{L} = 2258 \times 10^3 \text{ J.kg}^{-1}$.

We use the smearing function H_ϵ based on the values of φ in order to smooth discontinuous quantities across interface. Following Patankar suggestion (see [12, p.45]) based on the stationary case, we use a harmonic mean for the conductivity and the viscosity, the arithmetic mean otherwise:

$$\begin{aligned} \mu &= 10^{-3} \left(\frac{1}{0.015} H_\epsilon(\varphi) + \frac{1}{0.28} (1 - H_\epsilon(\varphi)) \right)^{-1}, \quad \chi = 0.06 \delta_\epsilon(\varphi) \\ k &= \left(\frac{1}{0.016} H_\epsilon(\varphi) + \frac{1}{0.3} (1 - H_\epsilon(\varphi)) \right)^{-1}, \quad c_V = 1850 H_\epsilon(\varphi) + 4186 (1 - H_\epsilon(\varphi)). \end{aligned}$$

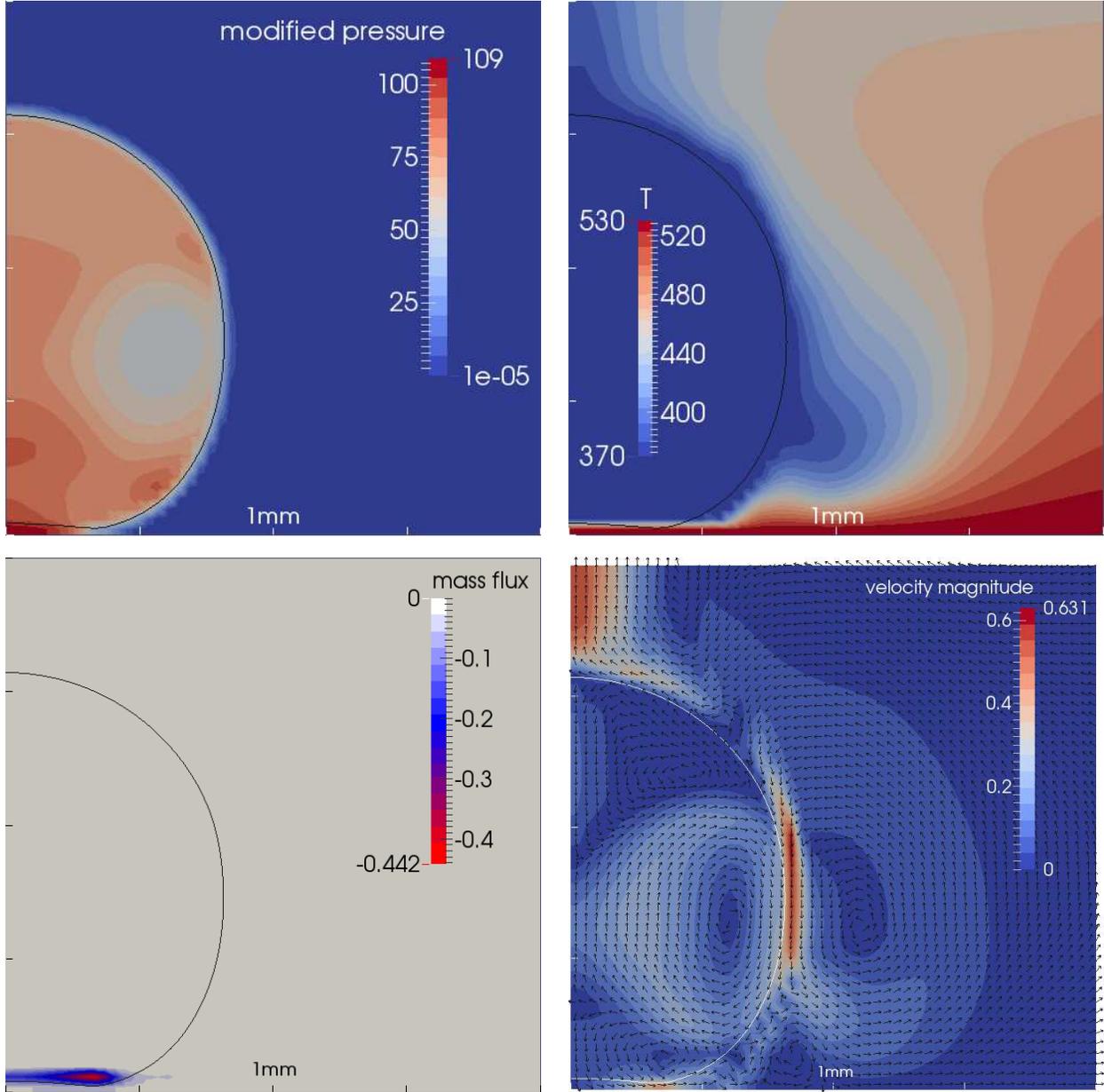


FIGURE 5: From top to bottom and from left to right: modified pressure \tilde{p} (defined in (28)), temperature, mass flux Φ_m , velocity field, during the evaporation of a droplet at time $t = 17.9s$.

5.3 Numerical validation

The computations were performed for a droplet of $4.2 \cdot 10^{-9} m^3$ on a square box of width about 5 radius. Figure 5 displays a cropped snapshot during the evaporation of this droplet following the model under consideration, which shows good qualitative behavior. As expected the phase change is localized under the droplet (see bottom-left image) and the pressure field is higher underneath the droplet. The temperature field shows a high gradient under the droplet, which corresponds to the fact that the heat flux coming from underneath is used for phase change instead of diffusion, in contrast

with the situation in the air. Finally the velocity field exhibits a toroidal vortex inside the droplet that has been already observed in physical experiments.

In order to perform a more quantitative test of our numerical algorithm, we compared on figure 6 the volume decrease of this evaporating droplet obtained from formulas (2), (3) and from our computations. Note that the theoretical curves were shifted to fit the numerical volume reached after the relaxation time of the droplet. The results show good agreement between our numerical computation and the corrected theoretical prediction.

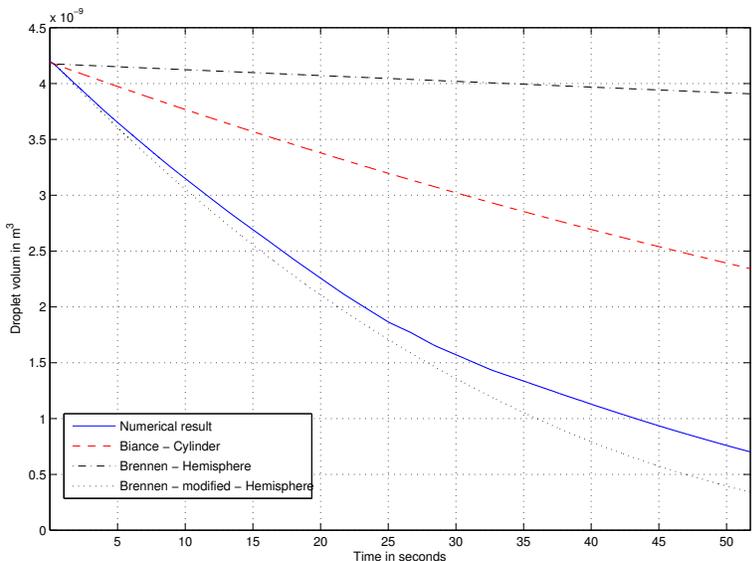


FIGURE 6: Comparison between our numerical code and some analytical formulas for volume decrease: the original formula from Brennen for the hemispherical shape, the modified formula (2) and the formula from Biance & al. for the cylindrical shape (3).

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