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Gloria FACCANONI[a], Grégoire ALLAIRE[b], Samuel KOKH[c]

[a]Équipe de Sismologie, Institut de Physique du Globe de Paris, 4 place Jussieu, 75252 Paris, France
[b]CMAP, École Polytechnique, CNRS, 91128 Palaiseau, France
[c]DEN/DANS/DM2S/SFME/LETR, Commissariat à l'Énergie Atomique, Saclay, 91191
Gif-sur-Yvette Cedex, France

Summary

The present work is dedicated to the simulation of compressible two-phase flows with phase change for pool boiling type problems. The model we are concerned with involves scales that allow to distinguish the interface between both phases. The mass transfer is driven by assuming local and instantaneous equilibria with respect to phasic pressures, temperatures and chemical potentials, which enables dynamic generation of two-phase interfaces within a pure phase. We present a general numerical solver that allows to cope with any type of EOS and preliminary numerical results of nucleation with transition towards film boiling.

Keywords: Compressible Flow, Liquid-Vapor Phase Change, Hyperbolicity, Relaxation, Finite-Volume Method

1. Phenomenon

The simulation of liquid-vapor phase change in pool boiling type flows concerns various engineering fields such as the study of pressurized water reactors in the nuclear industry. Indeed, understanding the triggering of boiling crisis is a critical safety issue for the nuclear industry: when the transition occurs from nucleate boiling to film boiling in the vicinity of heating wall, the vapor acts as a thermal insulator and the wall temperature raises suddenly. If this phenomenon occurs, it may cause serious damages to the facility.

2. Two-Phase Model

We assume that we are far from the critical point, thus the vapor (resp. liquid) phase can be considered as a compressible fluid governed by an Equation of State (EOS) given by $(\tau_\alpha, \varepsilon_\alpha) \mapsto s_\alpha$, $\alpha = v$, (resp. $\alpha = l$), where τ_α, ε_α, s_α are respectively the specific volume, internal energy and entropy of the phase α. Let T_α, P_α and g_α denote respectively the temperature, the pressure and the chemical potential of phase α. The mass fraction of the vapor (resp. liquid) is noted $y_v = y$ (resp. $y_l = 1 - y$). We suppose that the specific volume τ and the internal energy ε of the medium are defined by $\tau = 1/\varrho = y_v\tau_v + y_l\tau_l$ and $\varepsilon = y_v\varepsilon_v + y_l\varepsilon_l$. We also assume that for $\alpha = v, l$ the Hessian matrix of $(\tau_\alpha, \varepsilon_\alpha) \mapsto s_\alpha$ is negative definite, which is a classic thermodynamical assumption [5].

Using the lines of [2, 3, 6–8, 10, 11] we equip the two-phase material with an EOS defined thanks to the following entropy function

$$(\tau, \varepsilon) \mapsto s^{\text{eq}}(\tau, \varepsilon) = \sup\left\{ ys_v(\tau_v, \varepsilon_v) + (1 - y)s_l(\tau_l, \varepsilon_l) \,\middle|\, (\tau, \varepsilon) = y(\tau_v, \varepsilon_v) + (1 - y)(\tau_l, \varepsilon_l) \right\}. \quad (1)$$

This equilibrium entropy postulate defines the equilibrium between both phases within the material [5, 6, 10]. Indeed, for regions where both phases are present, one can see that the definition of s^{eq} implies the triple

equilibrium relations

$$(\tau, \varepsilon) = y(\tau_v, \varepsilon_v) + (1 - y)(\tau_l, \varepsilon_l), \quad (P_v, g_v, T_v)(\tau_v, \varepsilon_v) = (P_l, g_l, T_l)(\tau_l, \varepsilon_l) = (P, T, g) \tag{2}$$

$$0 < y < 1. \tag{3}$$

Let us now recall that, according to standard thermodynamics [5], when one considers solution of (2)-(3), the phasic variables τ_l, ε_l, τ_v, ε_v, y are said to be "at saturation" and they can be parametrized by a single thermodynamical variable such as P or T. It is then common to define the coexistence curve $T \mapsto P^{\mathrm{sat}}(T)$ [5, 6].

We now suppose that both phases have the same velocity u. If we neglect the dissipative effects, capillarity and gravity, the two-phase medium is governed by the compressible Euler equations with an equilibrium pressure law given by $P^{\mathrm{eq}} = (\partial s^{\mathrm{eq}}/\partial \tau)_{\varepsilon}/(\partial s^{\mathrm{eq}}/\partial \varepsilon)_{\tau}$. For a one-dimensional problem we thus have

$$\mathbf{W}_t + \mathbf{F}(\mathbf{W})_x = \mathbf{0} \tag{4}$$

with $\mathbf{W} = [\varrho, \varrho u, \varrho \varepsilon + \varrho u^2/2]^{\mathsf{T}}$ and $\mathbf{F}(\mathbf{W}) = [\varrho u, \varrho u^2 + P^{\mathrm{eq}}, (\varrho \varepsilon + \varrho u^2/2 + P^{\mathrm{eq}})u]^{\mathsf{T}}$. Mathematical properties of this model have been examined in [2, 6, 12, 14, 15]. In particular, the system (4) is strictly hyperbolic [2], provided that $(\tau_\alpha, \varepsilon_\alpha) \mapsto s_\alpha$, $\alpha = v, l$ verifies standard concavity properties [2, 5].

3. A Relaxation Numerical Solver

In order to discretize the system (4), we implement a two-step relaxation approach [9] following the lines of [8, 11]. This method allows to decouple the computation of the convection from the computation of the equilibrium for the thermodynamical parameters by confining it within the projection step. We consider an augmented system based on the five-equation system of [1] that is an off-equilibrium version of (4). For one-dimensional problems the system reads

$$\begin{cases} \mathbf{W}_t + \mathbf{G}(\mathbf{W}, y, z)_x = \mathbf{0}, \\ (\varrho y)_t + (\varrho y u)_x = \lambda Q(\mathbf{W}, y, z), \\ z_t + u z_x = \mu R(\mathbf{W}, y, z), \end{cases} \tag{5}$$

with $\mathbf{G}(\mathbf{W}, y, z) = [\varrho u, \varrho u^2 + \pi, (\varrho \varepsilon + \varrho u^2/2 + \pi)]^{\mathsf{T}}$, $Q(\mathbf{W}, y, z) = \frac{g_l - g_v}{T}$, $R(\mathbf{W}, y, z) = \frac{P_v - P_l}{T}$, where the volume fraction z verifies $z = \tau_v \varrho y$, the pressure π verifies $\pi = z P_v + (1 - z) P_l$ and the temperature T is obtained through the closure relation $T = T_l = T_v$. We see that the assumptions of equilibrium with respect to the partial pressures and the chemical potentials of system (4) are relaxed in (5). However, these equilibria are formally restored when $\mu, \lambda \to +\infty$ as it implies that $R(\mathbf{W}, y, z) = Q(\mathbf{W}, y, z) = 0$. Another consequence is that the entropy of the augmented system defined by $y s_v + (1 - y s_l)$ tends to the equilibrium entropy s^{eq} (see [11]) as $\mu, \lambda \to +\infty$

Let $(\mathbf{W}, \varrho y, z)^n$ be the discretized augmented variable at instant n. The discretization strategy reads:
Step I Update $(\mathbf{W}, \varrho y, z)^n$ to $(\mathbf{W}, \varrho y, z)^{n+1/2}$ by solving (5) without source terms, *i.e.* with $R = Q = 0$.
Step II Perform an approximate projection of $(\mathbf{W}, \varrho y, z)^{n+1/2}$ onto the equilibrium defined by $\mu, \lambda \to +\infty$ by approaching the solution of $R(\mathbf{W}, y, z) = Q(\mathbf{W}, y, z) = 0$. This task is achieved by seeking the equilibrium value $\widehat{T}$ of the temperature as the solution of the non-linear equation (8) (specified in section 4.) with a dichotomy algorithm. Then update $(\mathbf{W}, \varrho y, z)$ by setting

$$\mathbf{W}^{n+1} = \mathbf{W}^{n+1/2}, \quad T^{n+1} = \widehat{T}, \quad y^{n+1} = Y(\widehat{T}), \quad z^{n+1} = \begin{cases} 0 & \text{if } y^{n+1} = 0 \\ \tau_v^{n+1} \varrho^{n+1} y^{n+1} & \text{if } 0 < y^{n+1} < 1 \\ 1 & \text{if } y^{n+1} = 1 \end{cases}. \tag{6}$$

One can see in the lines above that the mass fraction is updated by the projection step (6). This means that the mass transfer is driven by the two-phase equilibrium. Moreover, the model intrinsically accounts for phase appearance and phase disappearance.

4. Approximation of the Equilibrium: Phase Change Equation

While the equilibrium EOS $(\tau, \varepsilon) \mapsto s^{\mathrm{eq}}$ is unambiguously defined, computing its value in practice is a difficult task. Indeed, for a given couple (τ, ε) this computation requires to seek the values $y^*, \tau_v^*, \tau_l^*, \varepsilon_v^*$ and ε_l^* that maximize $y s_v(\tau_v, \varepsilon_v) + (1-y)s_l(\tau_l, \varepsilon_l)$ under the constraint $(\tau, \varepsilon) = y(\tau_v, \varepsilon_v) + (1-y)(\tau_l, \varepsilon_l)$. Nevertheless, this procedure boils down to the following alternative:

(a) Two-Phase Equilibrium: if $y^*, \tau_v^*, \tau_l^*, \varepsilon_v^*, \varepsilon_l^*$ verify both (2) and (3) then
$\tau_l^* < \tau < \tau_v^*, y^* = (\tau - \tau_l^*)(\tau_v - \tau_l^*)^{-1}$, and we set $P^{\mathrm{eq}} = P_v(\tau_v^*, \varepsilon_v^*) = P_l(\tau_l^*, \varepsilon_l^*)$,

(b) Pure Phase: otherwise, if $s_v(\tau, \varepsilon) > s_l(\tau, \varepsilon)$ (resp. $s_v(\tau, \varepsilon) < s_l(\tau, \varepsilon)$) then
we set $y^* = 1$ (resp. $y^* = 0$) and $P^{\mathrm{eq}} = P_v(\tau, \varepsilon)$ (resp. $P^{\mathrm{eq}} = P_l(\tau, \varepsilon)$).

However, we can then see that settling between the case (a) and the case (b) requires first to solve the non-linear system (2) which is a difficult step, especially when one deals with tabulated or complex thermodynamical laws. Let us mention that even for general stiffened gas laws, there is no explicit solution for (2). We propose a method that allows to bypass this difficulty. We note $T \mapsto (\tau_\alpha^{\mathrm{sat}}, \varepsilon_\alpha^{\mathrm{sat}})(T) = (\tau_\alpha, \varepsilon_\alpha)(T, P^{\mathrm{sat}}(T))$, which are functions that are commonly available for a wide range of material in thermodynamical tables (see e.g. `http://webbook.nist.gov`). Given a fixed couple (τ, ε), we remark that solving the system (2) is equivalent to determine T as the solution of the non-linear "Phase Change Equation"

$$[\tau A(T) - 1][B(T) - 1]^{-1} = [\varepsilon C(T) - 1][D(T) - 1]^{-1}, \tag{7}$$

where $(A, B, C, D)(T) = (1/\tau_v^{\mathrm{sat}}, \tau_l^{\mathrm{sat}}/\tau_v^{\mathrm{sat}}, 1/\varepsilon_v^{\mathrm{sat}}, \varepsilon_l^{\mathrm{sat}}/\varepsilon_v^{\mathrm{sat}})(T)$ [6, 8]. The corresponding value of the mass fraction y for the two-phase saturation state at temperature T then reads $y = 1 - [\tau A(T) - 1)][(B(T) - 1]^{-1}$. Instead of solving the phase change equation (7), we propose to solve for T an approximate phase change equation

$$[\tau \widehat{A}(T) - 1][\widehat{B}(T) - 1]^{-1} = [\varepsilon \widehat{C}(T) - 1][\widehat{D}(T) - 1]^{-1}, \tag{8}$$

where $T \mapsto (\widehat{A}, \widehat{B}, \widehat{C}, \widehat{D})$ are convenient approximations of the laws $T \mapsto (A, B, C, D)$. Example of such approximations obtained by means of least square approximation techniques for water and dodecane can be found in [6]. This then leads to define the following function $Y(\widehat{T}) = 1 - [\tau \widehat{A}(\widehat{T}) - 1][\widehat{B}(\widehat{T}) - 1]^{-1}$, that provides the approximate value of the mass fraction as a function of the temperature for a two-phase saturated state.

5. Numerical Results

We present thereafter preliminary simulation results of nucleation phenomena for pool boiling type conditions. This test involves additional physical effects: gravity, surface tension and thermal diffusion. The overall numerical strategy consists in the following fractional step approach:

Step 1. Solve the off-equilibrium hydrodynamics system (5) using the Roe-type solver proposed in [1],

Step 2. Compute gravity related terms by means of a centered discretization,

Step 3. Compute surface tension related terms using the classic CSF approach of [4] with the z variable,

Step 4. Project onto the approximate equilibrium thanks to (8),

Step 5. Compute thermal diffusion related terms thanks to a classic implicit Finite-Volume scheme.

For the sake of computational time we used in this test two fictitious EOS that mimic the liquid-vapor water properties. At the initial instant the domain is filled with liquid at saturation. The boundary condition for the temperature at the bottom is a fixed sinusoidal temperature profile. We can see in figure 1 that vapor bubbles appear at the boundary located where the temperature reaches its local maxima. Then the bubbles depart from the bottom towards lower temperature regions. The bubbles recondensate as their temperature decreases. The nucleation sites quickly start to form a film that covers the bottom of the domain.

An implementation of our algorithm for the case of two stiffened gas fitted together with the properties of liquid-vapor water following the lines of [13] was proposed in [8] for phase change phenomenon induced by
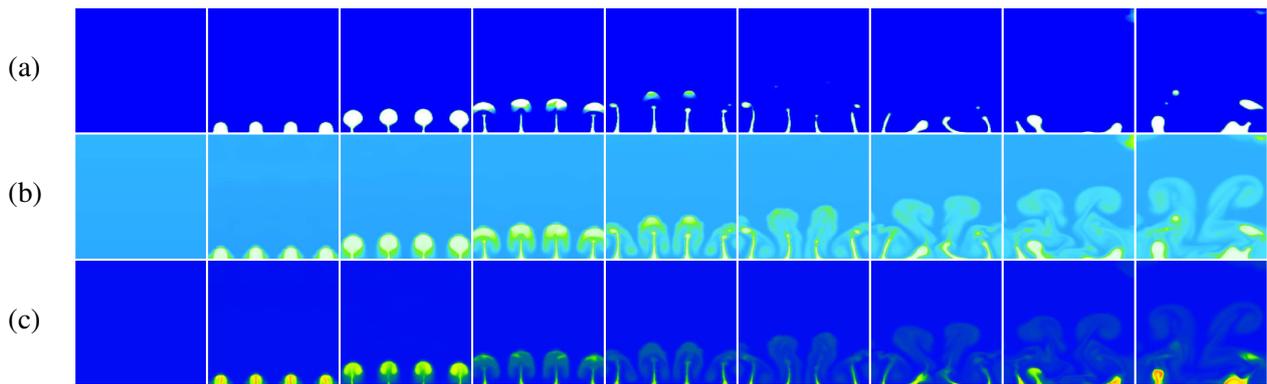
Figure 1: Profiles of the (a) mass fraction, (b) density and (c) temperature for the nucleation test.

pressure waves. An extension for general tabulated thermodynamical laws is proposed in [6, 7]. Future work will involve the use of more realistic thermodynamical laws and boundary conditions.

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