Modeling and Simulation of Nucleate Boiling

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

Abstract

This work investigates the modelization and simulation of liquid-vapor phase change in compressible flows. Each phase is modeled as a compressible fluid equipped with its own Equation of State (EOS). We suppose that inter-phase equilibrium processes in the medium operate at a short time-scale compared to the other physical phenomena such as convection or thermal diffusion. This assumption provides an implicit definition of an equilibrium EOS for the two-phase medium. Within this framework, mass transfer is the result of local and instantaneous equilibria between both phases. The overall model is strictly hyperbolic. We examine properties of the equilibrium EOS and we propose a discretization strategy based on a Finite-Volume relaxation method. This method allows to cope with the implicit definition of the equilibrium EOS, even when the model involves complex EOSs for the pure phases, including tabulated ones. We present two-dimensional numerical simulations that shows that the model is able to reproduce mechanism such as nucleation.

1 Phenomenon.

In this talk we propose an approximation method for using general equations of state (EOS), including tabulated ones, in the numerical simulation of dynamical liquid-vapor phase change in pool boiling type flows. This phenomenon 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 Model.

We suppose that the medium is far from the critical point. Therefore both phases are modeled by compressible fluids equipped with an EOS given by a function $(\tau_\alpha, \varepsilon_\alpha) \mapsto s_\alpha$, where $\tau_\alpha > 0$, $\varepsilon_\alpha > 0$ and s_α denote respectively the specific volume, the specific internal energy and the specific entropy of

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the liquid phase $\alpha = l$ (resp. vapor phase $\alpha = v$). The Hessian matrix of s_α is always negative definite and we define classically the temperature $T_\alpha = 1/(\partial s_\alpha/\partial \varepsilon_\alpha)_{\tau_\alpha} > 0$, the pressure $P_\alpha = (\partial s_\alpha/\partial \tau_\alpha)_{\varepsilon_\alpha} T_\alpha > 0$ and the chemical potential $g_\alpha = \varepsilon_\alpha + P_\alpha \tau_\alpha - T_\alpha s_\alpha$ of the phase $\alpha = l, v$. The mass fraction of the phase $\alpha = v$ (resp. $\alpha = l$) is noted $y_v = y$ (resp. $y_l = 1 - y$) and we suppose $y \in [0, 1]$. The total density and specific internal energy are classically defined respectively by $\varrho^{-1} = \tau = y\tau_v + (1-y)\tau_l$ and $\varepsilon = y\varepsilon_v + (1-y)\varepsilon_l$.

The model of mass transfer relies on the classical assumption that there is an instantaneous equilibrium at each point of the domain with respect to pressure, temperature and chemical potential between both phases. Under classical thermodynamical assumptions, this hypothesis boils down to provide the two-phase material with an equilibrium EOS defined thanks to the equilibrium entropy denoted by $(\tau, \varepsilon) \mapsto s^{\text{eq}}$ and given by (see [2, 4, 5, 6, 7, 8])

$$s^{\text{eq}}(\tau,\varepsilon) = \sup \Big\{ \quad y s_v(\tau_v,\varepsilon_v) + (1-y) s_l(\tau_l,\varepsilon_l) \quad \Big| \\ \tau = y\tau_v + (1-y)\tau_l,\ \varepsilon = y\varepsilon_v + (1-y)\varepsilon_l,\ 0 < y < 1 \quad \Big\}. \quad (1)$$

The pressure $(\tau, \varepsilon) \mapsto P^{\text{eq}}$ for the two-phase medium can then be defined by $P^{\text{eq}} = (\partial s^{\text{eq}}/\partial \tau)_\varepsilon / (\partial s^{\text{eq}}/\partial \varepsilon)_\tau$. Finally, if we suppose that both phases have the same velocity $\mathbf{u}$ in the two-phase medium and if we neglect all dissipative phenomena and local effects such as surface tension, gravity or heat diffusion, the two-phase system that governs the phase change phenomena consists of the compressible Euler equations with the equilibrium pressure law $(\tau, \varepsilon) \mapsto P^{\text{eq}}(\tau, \varepsilon)$, namely:

$$\begin{cases} \partial_t \varrho + \operatorname{div}(\varrho \mathbf{u}) = 0, \\ \partial_t(\varrho \mathbf{u}) + \operatorname{div}(\varrho \mathbf{u} \otimes \mathbf{u} + P^{\text{eq}} \operatorname{Id}) = \mathbf{0}, \\ \partial_t(\varrho\varepsilon + \varrho |\mathbf{u}|^2/2) + \operatorname{div}[(\varrho\varepsilon + \varrho |\mathbf{u}|^2/2 + P^{\text{eq}})\mathbf{u}] = 0. \end{cases} \quad (2)$$

3 Approximation of the Equilibrium: Phase Change Equation.

While the equilibrium EOS $(\tau, \varepsilon) \mapsto s^{\text{eq}}$ is unambiguously defined, computing its value in practice is a difficult task. Let us denote by $(\tau_v^*, \varepsilon_v^*, \tau_l^*, \varepsilon_l^*, y^*)$ the maximizer of the mixture entropy $y s_v + (1-y) s_l$ under the constraints set by definition (1). Let $\mathcal{C} = \{\tau > 0, \varepsilon > 0\}$. When $0 < y^* < 1$, both phases are present at equilibrium and they are said to be "at saturation". In this case, for a given couple $(\tau, \varepsilon) \in \mathcal{C}$, the saturated state $(\tau_v^*, \varepsilon_v^*, \tau_l^*, \varepsilon_l^*, y^*)$ is also the unique solution of the following optimality system (3)-(4) for the maximization (1) (see *e.g.* [2, 4, 5, 6, 7, 8]):

$$\begin{cases} \tau = y\tau_v + (1-y)\tau_l, & \text{(3a)} \\ \varepsilon = y\varepsilon_v + (1-y)\varepsilon_l, & \text{(3b)} \\ P_v(\tau_v, \varepsilon_v) = P_l(\tau_l, \varepsilon_l), & \text{(3c)} \\ T_v(\tau_v, \varepsilon_v) = T_l(\tau_l, \varepsilon_l), & \text{(3d)} \\ g_v(\tau_v, \varepsilon_v) = g_l(\tau_l, \varepsilon_l), & \text{(3e)} \end{cases}$$

$$y \in (0,1). \tag{4}$$

Considering the solution of (3)-(4), if we note $P = P_v = P_l$ and $T = T_v = T_l$, then saturated states $(\tau_v^*, \varepsilon_v^*, \tau_l^*, \varepsilon_l^*, y^*)$ can be parametrized by a single thermodynamical variable such as P or T. This classical result provides the definition of the coexistence curve $T \mapsto P = P^{\text{sat}}(T)$. Far from the critical point, we can reasonably assume that $\tau_v(P,T) > \tau_l(P,T)$, for any $P > 0$ and $T > 0$, without breaking the thermodynamical coherence. Now the overall procedure for computing the equilibrium EOS lies in the following alternative:

1. if $(\tau_v^*, \varepsilon_v^*, \tau_l^*, \varepsilon_l^*, y^*)$ verifies both (3) and (4) then $y^* = \frac{\tau - \tau_l^*}{\tau_v^* - \tau_l^*}$ and we set $P^{\text{eq}}(\tau,\varepsilon) = P_v(\tau_v^*, \varepsilon_v^*) = P_l(\tau_l^*, \varepsilon_l^*)$, $T^{\text{eq}}(\tau,\varepsilon) = T_v(\tau_v^*, \varepsilon_v^*) = T_l(\tau_l^*, \varepsilon_l^*)$, $y^{\text{eq}} = y^*$;

2. otherwise, if $s_v(\tau,\varepsilon) > s_l(\tau,\varepsilon)$ (resp. $s_v(\tau,\varepsilon) < s_l(\tau,\varepsilon)$) then we set $y^{\text{eq}} = 1$ and $P^{\text{eq}}(\tau,\varepsilon) = P_v(\tau,\varepsilon)$, $T^{\text{eq}}(\tau,\varepsilon) = T_v(\tau,\varepsilon)$ (resp. $y^{\text{eq}} = 0$ and $P^{\text{eq}}(\tau,\varepsilon) = P_l(\tau,\varepsilon)$, $T^{\text{eq}}(\tau,\varepsilon) = T_l(\tau,\varepsilon)$).

The case (2) corresponds to a pure phase $\alpha = l$ or $\alpha = v$ state which means that either system (3) has no solution either the condition (4) fails. However, we can then see that settling between the case (1) and the case (2) requires first to solve the non-linear system (3) which is a difficult step, especially when one deals with general thermodynamical functions, *a fortiori* with tabulated laws. Let us mention that even for general stiffened gas laws, there is no explicit solution for (3) (see [4]). Below we propose a general method that allows to approximating the possible solution of (3) using experimental data.

Let us note $\tau_\alpha^{\text{sat}}(T) = \tau_\alpha(T, P^{\text{sat}}(T))$ and $\varepsilon_\alpha^{\text{sat}}(T) = \varepsilon_\alpha(T, P^{\text{sat}}(T))$, $\alpha = l, v$, whose values are commonly available in experiment measurements tables [9]. Given a fixed couple $(\tau,\varepsilon) \in \mathcal{C}$, we observe that solving (3) is equivalent to seeking T as the solution of

$$\frac{\tau A(T) - 1}{B(T) - 1} = \frac{\varepsilon C(T) - 1}{D(T) - 1}, \tag{5}$$

where $(A,B,C,D)(T) = (1/\tau_v^{\text{sat}}, \tau_l^{\text{sat}}/\tau_v^{\text{sat}}, 1/\varepsilon_v^{\text{sat}}, \varepsilon_l^{\text{sat}}/\varepsilon_v^{\text{sat}})(T)$. The equation (5) is referred to the Phase Change Equation. For a fixed $(\tau,\varepsilon) \in \mathcal{C}$, instead of solving (5) we propose to seek T as the solution of the alternative equation

$$\frac{\tau \widehat{A}(T) - 1}{\widehat{B}(T) - 1} = \frac{\varepsilon \widehat{C}(T) - 1}{\widehat{D}(T) - 1}, \tag{6}$$

where $T \mapsto (\widehat{A}, \widehat{B}, \widehat{C}, \widehat{D})(T)$ are proper approximations of the tabulated laws $T \mapsto (A,B,C,D)(T)$. The equation (6) is referred to the Approximate Phase Change Equation. For the water and the dodecane, see [4, 6] for an example of the Approximate Phase Change Equation with stiffened gas laws and [4, 5] with tabulated data.

4 Numerical Solver.

In order to discretize the system (2), we implement a relaxation approach (see [4, 8]). 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 the augmented system (7) that is a relaxed version of (2):

$$\begin{cases} \partial_t \mathbf{W} + \mathrm{div}\mathbf{F}(\mathbf{W}, z) = \mathbf{R}(\mathbf{W}, z) \\ \partial_t z + \mathbf{u} \cdot \mathbf{grad} z = Q(\mathbf{W}, z) \end{cases} \tag{7}$$

where

$$\begin{aligned} \mathbf{W} &= \Big(z\varrho_v, (1-z)\varrho_l, \varrho\mathbf{u}, \varrho\big(\varepsilon + \tfrac{|\mathbf{u}|^2}{2}\big) \Big), \\ \mathbf{F}(\mathbf{W}, z) &= \Big(z\varrho_v\mathbf{u}, (1-z)\varrho_l\mathbf{u}, \varrho\mathbf{u}\otimes\mathbf{u} + \pi\mathrm{Id}, \big(\varrho\big(\varepsilon + \tfrac{|\mathbf{u}|^2}{2}\big) + \pi\big)\mathbf{u} \Big), \\ \mathbf{R}(\mathbf{W}, z) &= (\mu(g_l - g_v)/\vartheta, -\mu(g_l - g_v)/\vartheta, 0, 0)\,, \\ Q(\mathbf{W}, z) &= \nu\,(P_v - P_l)\,/\vartheta, \end{aligned}$$

with the volume fraction z such that $\varrho = z\varrho_v + (1-z)\varrho_l$, the pressure π such that $\pi = zP_v + (1-z)P_l$ and the closure $T_v = T_l = \vartheta$. Formally the equilibrium $\mu, \nu \to +\infty$ implies that $\mathbf{R}(\mathbf{W}, z) = \mathbf{0}$, $Q(\mathbf{W}, z) = 0$ which matches equilibrium.

The numerical strategy to solve the system (2) (that involves additional physical effects as gravity, surface tension and thermal diffusion) consists in the following fractional step approach:

Step 1. solve the off-equilibrium hydrodynamics system (7) with $\mathbf{R}(\mathbf{W}, z) = \mathbf{0}$, $Q(\mathbf{W}, z) = 0$ 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 [3];

Step 4. compute thermal diffusion related terms thanks to a classic implicit Finite-Volume scheme;

Step 5. project onto the approximate equilibrium thanks to the Approximate Phase Change Equation (6).

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

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