

# Test-case number 7a: One-dimensional phase-change of a vapor phase in contact with a wall (PA)

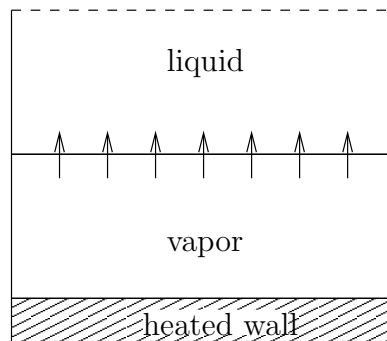
Didier Jamet, DER/SSTH/LMDL, CEA/Grenoble, 38054 Grenoble cedex 9, France  
Phone: +33 (0)4 38 78 45 42, Fax: +33 (0)4 38 78 50 36, E-Mail: [didier.jamet@cea.fr](mailto:didier.jamet@cea.fr)

Christophe Duquennoy, EDF-SEPTEN, 12-14 av. Dutrievoz,  
69628 Villeurbanne cedex, France, E-Mail: [christophe.duquennoy@edf.fr](mailto:christophe.duquennoy@edf.fr)

## 1 Practical significance and interest of the test-case

In numerical methods dedicated to two-phase flows and for which interfaces are well defined in space (local instantaneous models rather than averaged models), phase-change phenomena are particularly difficult to simulate. The main reason is that the velocity field is discontinuous at an interface, which speed of displacement is different from the fluid velocities. Another difficulty comes from the local thermodynamic equilibrium condition which must be satisfied at an interface and which governs mass and energy transfer and therefore the local speed of displacement of the interface.

In this paper, analytical solutions of one-dimensional liquid-vapor phase-change problems are provided. The general problem is that of a phase in contact with a heated wall, as sketched in figure 1. Due to this heating, the temperature of the fluid in contact with the wall rises up and the temperature at the interface, located at the upper boundary of this phase, also tends to increase. However, the interface tends to keep at local thermodynamic equilibrium. Therefore, if the pressure of the system is given, for instance if the upper boundary of the upper phase is maintained at a constant pressure, say  $P_0$ , the pressure at the interface is approximately  $P_0$  and, due to the local thermodynamic equilibrium condition, the interface temperature  $T^i$  is equal to the saturation temperature corresponding to the pressure  $P_0$ :  $T^i = T^{sat}(P_0)$ . Thus, the interface temperature remains constant. Since the heating of the lower phase tends to increase the interface temperature, heat must be absorbed at the interface to keep the interface temperature constant, which is achieved through *vaporization*. The rate of phase-change is related to the energy supplied by the heated wall through the phase in contact with the latter.



**Figure 1:** Sketch of a one-dimensional phase-change problem.

The proposed test-case gives analytical solutions in one dimension which can be compared to numerical results and therefore tests the ability of a numerical method to

account for interfacial liquid-vapor phase-change dominated by thermal effects. Indeed, in the physical situation described above, it is clear that the interfacial phase-change is due to a thermal equilibrium condition and not to a pressure equilibrium condition.

Two different solutions are provided. The first one is a steady state solution in the frame of reference linked to the interface. As will be discussed in section 3, this solution corresponds to a physical problem in which heat transfer is dominated by heat conduction. This first test-case aims at testing the ability of a numerical method to account for interfacial mass and energy balance equations accurately. The second solution corresponds to an unsteady problem for which the initial temperature of one of the phases is uniformly superheated (its temperature is larger than the saturation temperature) or subcooled (its temperature is lower than the saturation temperature). This test-case aims at testing the ability of a numerical method to accurately solve highly unsteady phase-change problems dominated by thermal effects. Indeed, in this test-case, the two key issues are the development of the thermal boundary layers close to the interface and the interfacial mass and energy balance equations. In both cases, the pressure of the system is assumed to be imposed and not to vary much in time, which is relevant essentially if the phases can be approximated as incompressible.

## 2 General definitions and model description

Let us consider a *plane interface* and assume that all the physical variables are functions of the *only space coordinate normal to the interface*, say  $z$ .

### 2.1 Bulk balance equations

Let us assume that both the liquid and vapor phases can be modeled as *incompressible* fluids. If gravity forces are neglected, the general equations of motions of the bulk phases are the following:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho V)}{\partial z} = 0 \quad (1)$$

$$\rho \left( \frac{\partial V}{\partial t} + V \frac{\partial V}{\partial z} \right) = -\frac{\partial P}{\partial z} + \frac{\partial}{\partial z} \left( \frac{4}{3} \mu \frac{\partial V}{\partial z} \right) \quad (2)$$

$$\rho C_p \left( \frac{\partial T}{\partial t} + V \frac{\partial T}{\partial z} \right) = \frac{\partial}{\partial z} \left( k \frac{\partial T}{\partial z} \right) + T \kappa_T \frac{dP}{dt} + \frac{4}{3} \mu \left( \frac{\partial V}{\partial z} \right)^2 \quad (3)$$

where  $\rho$  is the density,  $V$  is the velocity,  $P$  is the pressure,  $\mu$  is the viscosity,  $T$  is the temperature,  $C_p$  is the heat capacity at constant pressure,  $k$  is the thermal conductivity and  $\kappa_T$  is the coefficient of thermal expansion at constant pressure.

If the density is assumed to be constant, which means that the *density does not depend on the temperature*, these equations are simplified as follows:

$$\frac{\partial V}{\partial z} = 0 \quad (4)$$

$$\rho \left( \frac{\partial V}{\partial t} + V \frac{\partial V}{\partial z} \right) = -\frac{\partial P}{\partial z} \quad (5)$$

$$\rho C_p \left( \frac{\partial T}{\partial t} + V \frac{\partial T}{\partial z} \right) = \frac{\partial}{\partial z} \left( k \frac{\partial T}{\partial z} \right) \quad (6)$$

Equation (4) shows that *the velocity is uniform within each bulk phase.*

## 2.2 Interfacial balance equations

The interfacial balance equations are the following (Delhaye *et al.*, 1981):

$$\rho_v (V_v - V^i) = \rho_l (V_l - V^i) = \dot{m} \quad (7)$$

$$P_l^i - P_v^i = \dot{m}^2 \left( \frac{1}{\rho_v} - \frac{1}{\rho_l} \right) \quad (8)$$

$$\left( -k \frac{\partial T}{\partial z} \right)_l^i - \left( -k \frac{\partial T}{\partial z} \right)_v^i = \dot{m} \left[ \mathcal{L} + \frac{\dot{m}^2}{2} \left( \frac{1}{\rho_v^2} - \frac{1}{\rho_l^2} \right) \right] \quad (9)$$

where the subscripts  $l$  and  $v$  denote the liquid and vapor phases respectively, the superscript  $i$  denotes the interface,  $V^i$  is the speed of displacement of the interface,  $\dot{m}$  is the interfacial mass flux,  $\mathcal{L}$  is the latent heat of vaporization.

Note that the term in  $\dot{m}^2$  in equation (9) accounts for kinetic energy effects and is generally negligible compared to  $\mathcal{L}$ .

## 2.3 Interface thermodynamic equilibrium

The unknowns of the problem are, the two bulk velocities, the two bulk pressure fields, the two bulk temperature fields and the speed of displacement of the interface. Therefore, an equation must be added to the system (4)-(9). This equation is a condition of local thermodynamic equilibrium of the interface, which reads:

$$T^i = T^{sat}(P^i) \quad (10)$$

where  $P^i$  is the pressure at the interface given by (Ishii, 1975)

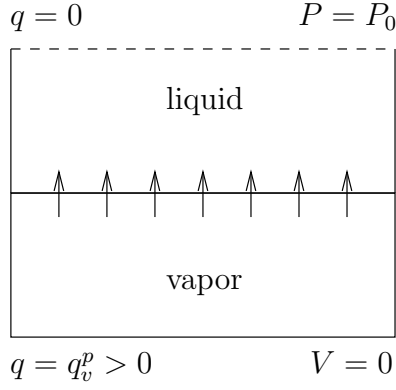
$$P^i = \frac{P_v^i + P_l^i}{2} \quad (11)$$

Of course, boundary and initial conditions must be added to the above system of PDEs. In the models considered here, different thermal boundary conditions are considered. However, it is generally considered that the *pressure at the upper boundary is imposed*, say  $P_0$ .

# 3 Steady state model

## 3.1 Model

Let us consider that the system sketched in figure 2 is initially at rest and at a uniform temperature equal to the saturation temperature corresponding to the pressure  $P_0$ :  $T(z, t = 0) = T^{sat}(P_0)$ . Let us then impose a heat flux on the lower boundary, which leads to a phase-change at the interface as described in section 1. It can be shown that, in certain conditions (see hereafter), the interface reaches a constant speed. In this case,



**Figure 2:** One-dimensional phase-change problem with imposed boundary heat fluxes.

in the *frame of reference linked to the interface*, the problem is *stationary*. The equations of motion of the bulk phases (4)-(6) then read:

$$\frac{dV}{dz} = 0 \quad (12)$$

$$\frac{dP}{dz} = 0 \quad (13)$$

$$\dot{m} C_p \frac{dT}{dz} = \frac{d}{dz} \left( k \frac{dT}{dz} \right) \quad (14)$$

Since the pressure of the liquid phase is imposed at the upper boundary, equation (13) can be integrated and one gets:

$$P_l(z) = P_0 \quad (15)$$

$$P_v(z) = P_0 - \dot{m}^2 \left( \frac{1}{\rho_v} - \frac{1}{\rho_l} \right) \quad (16)$$

If  $C_p$  and  $k$  are assumed to be constant, equation (14) can be integrated to get

$$T(z) = A \exp\left(\frac{\dot{m} C_p}{k} z\right) + \frac{B}{\dot{m} C_p}$$

where  $A$  and  $B$  are two constants of integration.

Let us denote  $z^p$  the position of the phase boundaries and  $z^i$  the position of the interface; since the system is supposed to be in a steady state, these are constant. If we assume that the conductive heat flux is imposed for  $z = z^p$  and is denoted  $q^p$ , and since the interface temperature is known, the two constants of integration can be determined and one gets:

$$T(z) = T^i + \frac{q^p}{\dot{m} C_p} \left[ \exp\left(-\frac{\dot{m} C_p}{k} (z^p - z^i)\right) - \exp\left(-\frac{\dot{m} C_p}{k} (z^p - z)\right) \right] \quad (17)$$

where the interface temperature  $T^i$  is determined by equations (10) and (11)

$$T^i = T^{sat} \left( P_0 - \frac{\dot{m}^2}{2} \left( \frac{1}{\rho_v} - \frac{1}{\rho_l} \right) \right) \quad (18)$$

The temperature profile (17) is valid for each phase.

It can be shown, using the Clapeyron relation, that the interface temperature given by (18) can be approximated by

$$T^i \simeq T^{sat}(P_0) \quad (19)$$

if the following condition is satisfied

$$\mathcal{L} \gg \frac{\dot{m}^2}{2} \left( \frac{1}{\rho_v} - \frac{1}{\rho_l} \right)^2 \quad (20)$$

It is worth noting that this condition is generally satisfied.

From the temperature profiles (17), the interfacial energy equation (9) implies

$$q_l^p \exp \left( -\frac{\dot{m} C_{pl}}{k_l} (z_l^p - z^i) \right) - q_v^p \exp \left( -\frac{\dot{m} C_{pv}}{k_v} (z_v^p - z^i) \right) = \dot{m} \left[ \mathcal{L} + \frac{\dot{m}^2}{2} \left( \frac{1}{\rho_v^2} - \frac{1}{\rho_l^2} \right) \right] \quad (21)$$

Since the position of the boundaries  $z_l^p$  and  $z_v^p$  are given, this equation can be seen as a relation between the heat fluxes  $q_l^p$  and  $q_v^p$ , the position of the interface  $z^i$  (which is an unknown of the problem) and the interfacial mass flux  $\dot{m}$ . For instance, if the heat fluxes are imposed as well as the position of the interface (in the middle of the domain for instance  $z^i = (z_l^p + z_v^p)/2$ ), this relation gives the interfacial mass flux  $\dot{m}$ .

Let us introduce the bulk Peclet numbers

$$Pe = \frac{\dot{m} C_p L^p}{k} \quad (22)$$

where  $L^p$  is the length of the considered phase.

If  $Pe \ll 1$ , the general temperature profile (17) is greatly simplified:

$$T(z) \simeq T^i + \frac{q^p}{k} (z^p - z) \quad (23)$$

This equation shows that, when the convective heat flux can be neglected compared to the conductive heat flux (*i.e.*  $Pe \ll 1$ ), the temperature profile within each phase is linear. This means that the information concerning the temperature  $T^{sat}$  at the interface has the time to diffuse within the phases without being perturbed by convection effects. In this case, the interfacial energy balance equation (21) simplifies as follows:

$$q_l^p - q_v^p = \dot{m} \left[ \mathcal{L} + \frac{\dot{m}^2}{2} \left( \frac{1}{\rho_v^2} - \frac{1}{\rho_l^2} \right) \right] \quad (24)$$

Note that this relation is different from the general condition (9) since the fluxes are those imposed on the boundaries and not those at the interface, which is a great simplification. This is because the condition  $Pe \ll 1$  implies, as shown by equation (14),

that the conductive heat flux is constant within each phase.

Note also that equation (24) can generally be simplified by neglecting the kinetic energy compared to the latent heat:

$$\mathcal{L} \gg \frac{\dot{m}^2}{2} \left( \frac{1}{\rho_v^2} - \frac{1}{\rho_l^2} \right) \quad (25)$$

Note that, since  $\rho_v < \rho_l$ , this condition is more restrictive than the condition (20).

If the condition (25) is satisfied, one can return very easily to the absolute frame of reference and one finds that the position of the interface is given by:

$$z^i(t) = z^i(0) + V^i t$$

where

$$V^i = V_l - \frac{q_l^p - q_v^p}{\rho_l \mathcal{L}}$$

or

$$V^i = V_v - \frac{q_l^p - q_v^p}{\rho_v \mathcal{L}}$$

and the corresponding interfacial mass flux is given by

$$\dot{m} = \frac{q_l^p - q_v^p}{\mathcal{L}}$$

For instance, for the system sketched in figure 2,  $V_v = 0$ ,  $q_l^p = 0$  and  $q_v^p > 0$ , one gets

$$\dot{m} = -\frac{q_v^p}{\mathcal{L}} \quad (26)$$

and the corresponding speed of displacement of the interface is given by

$$V^i = -\frac{\dot{m}}{\rho_v} \quad (27)$$

The speed of the liquid phase is therefore given by

$$V_l = -\dot{m} \left( \frac{1}{\rho_v} - \frac{1}{\rho_l} \right) \quad (28)$$

### 3.2 Comments

The model described in section 3.1 shows that the speed of displacement of the interface, *i.e.* a macroscopic characteristic of the system, depends on the interfacial mass and energy balance equations (27) and (26). Therefore, this model can be used as a test-case to verify *how well a numerical method accounts for the interfacial mass and energy balance equations*. In the general interfacial energy balance equation (9), which is valid even for an unsteady motion of the interface, only the conductive heat fluxes at the interface appear; the convective fluxes appear as a correction of the latent heat and can generally be neglected, which can be checked through the condition (25). The reason why the energy balance equation (9) gives rise to the relatively complex equation (21) is because the conductive

heat fluxes at the interface are different from the imposed heat fluxes at the boundaries because of convection effects *within the bulk phases*, which have been integrated. The general difficulty of two-phase systems, and in particular when phase-change exists, comes from interfacial characteristics and not from bulk phase characteristics. Therefore, it is fair to assume that the issue concerning the ability of a method to accurately account for the competition between the conductive and convective heat fluxes within the bulk phases can be seen as secondary compared to the issue of knowing how accurately the interfacial mass and energy balance equations are accounted for by a numerical method. That's the reason why it is proposed that the simplified model corresponding to the condition  $Pe \ll 1$  should be used as a first test-case.

### 3.3 Test-case description

In this section, we describe how the previous analytical results should be used as a numerical test to verify how well a numerical method accounts for the interfacial mass and energy balance equations. The physical problem considered is that sketched in figure 2, on which the boundary conditions imposed are indicated, and one seeks for a state in which the interface moves at a constant speed.

The main physical parameters are

- the densities  $\rho_l$  and  $\rho_v$ ;
- the specific heat capacities  $Cp_l$  and  $Cp_v$ ;
- the thermal conductivities  $k_l$  and  $k_v$ ;
- the corresponding thermal diffusivities  $\alpha_l$  and  $\alpha_v$ ;
- the pressure  $P_0$  and the corresponding saturation temperature  $T^{sat}$  and latent heat of vaporization  $\mathcal{L}$ ;
- the heat flux  $q_v^p$ ;
- the length  $L$  of the system.

Their values should be provided.

The stationary speed of displacement of the interface  $V^i$  and interfacial mass flux  $\dot{m}$  can be approximated by equations (27) and (26) respectively. It should be verified that the Peclet numbers of the phases defined by (22) are always small compared to one, so that the approximation (24) is valid. Note that the Peclet numbers calculated using the total length of the system  $L$  instead of the larger length of one phase during the calculation  $L^p$  is an upper bound for the validity of the approximation. It should also be checked that the condition (25) is satisfied so that the simplified solution (26) can be used. Note that if the condition (25) is not satisfied, equation (26) can still be used but  $\mathcal{L}$  must be replaced by  $[\mathcal{L} + \dot{m}^2/2(1/\rho_v^2 - 1/\rho_l^2)]$ , in which case equation (26) is a *non-linear* equation in  $\dot{m}$ .

No particular initial state is imposed since only the stationary state is of interest for this test-case. However, it is highly recommended that the initial length of the vapor phase should be as small as possible to shorten the unsteady stage of the simulation (in the frame linked to the interface). Moreover, it is recommended that the initial

temperature profile should be that given by equation (23) (where it is recalled that the position of the interface is taken as the origin  $z^i = 0$ ).

The main physical parameter which must be compared to the analytical solution is the speed of displacement of the interface  $V^i$ . It is recommended that  $V^i(t)$  should be provided and compared to its theoretical value given by equation (27) through the  $L^1$  norm of the error. Likewise, the speed of the liquid velocity should be compared to its theoretical value given by equation (28). Moreover, the pressure within the phases should also be compared to their theoretical values given by equation (15) and (16).

## 4 Unsteady model for a phase initially uniformly superheated or undercooled

### 4.1 Model

In this section, we consider the same system as the one considered in section 3, which is governed by the general system of equations (4)-(11). The difference between the case considered in this section and that treated in section 3 comes essentially from the initial conditions. Indeed, in section 3, the system was supposed to be stationary in the frame of reference linked to the interface; if the Peclet number in each phase is small enough, the initial conditions are not important because the temperature field within each phase reaches a quasi-steady state. On the contrary, in the case considered in this section, the initial conditions are essential. Indeed, the initial state is such that both phases are at rest and the temperature of one of the phases is uniform and equal to the saturation temperature corresponding to the imposed pressure, whereas the temperature of the other phase is *uniform but different from the saturation temperature*. This system has been studied analytically and numerically by Welch & Wilson (2000) and the developments given here are inspired by this work. However, a fully analytical solution is provided here whereas Welch & Wilson (2000) provided only a semi-analytical solution. This fully analytical solution was initially proposed by Duquennoy (2000) in the particular case for which the liquid phase is initially superheated.

In the following, we consider the system sketched in figure 3 for which the vapor is in contact with a fixed wall, whereas the liquid is free to flow through the upper boundary. Note that equation (4) implies that the vapor phase is always at rest:

$$V_v = 0 \quad (29)$$

In section 4.1.1 and 4.1.2 we consider the cases for which the vapor and the liquid temperature respectively is initially different from the saturation temperature.

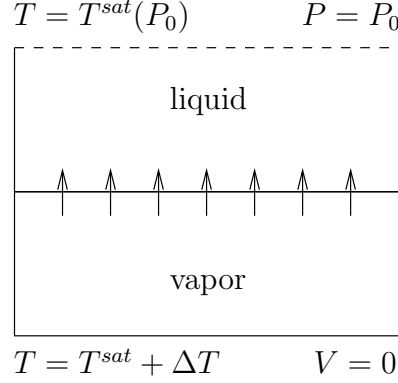
#### 4.1.1 Vapor initially not at thermodynamic equilibrium

In this section we consider the case for which the initial temperature of the liquid phase is the saturation whereas the initial temperature of the vapor phase is uniform but different from the saturation temperature:

$$T_l(z, 0) = T^{sat}(P_0) \quad (30)$$

$$T_v(z, 0) = T^{sat}(P_0) + \Delta T \quad (31)$$





**Figure 3:** One-dimensional phase-change problem for a vapor initially superheated ( $\Delta T > 0$ ).

If  $\Delta T > 0$ , the phase is said to be superheated and if  $\Delta T < 0$ , the phase is said to be subcooled.

Since the liquid is initially at thermodynamic equilibrium at the interface and if the condition (20) is satisfied, no temperature gradient will appear in the liquid phase; equation (6) then shows that the temperature of the liquid phase does not evolve in time. Therefore, *the temperature of the liquid phase is constant and uniform and equal to the saturation temperature  $T^{sat}$ .*

The situation is different for the vapor since this phase is initially not at thermodynamic equilibrium at the interface. Since the temperature of each phase is supposed to be always equal to the saturation temperature at the interface, the initial temperature field in the vapor at the interface varies from  $T^{sat}$  to  $(T^{sat} + \Delta T)$  on a zero distance which creates an infinite temperature gradient which tends to diffuse in time. In the following, the vapor temperature field  $T(z, t)$  is determined analytically.

Let us first make the following change of variable:

$$\zeta = z - \int_0^t V^i(\tau) d\tau$$

The energy balance equation (6) then reads

$$\rho_v C p_v \left[ \frac{\partial T_v}{\partial t} + (V_v - V^i) \frac{\partial T_v}{\partial \zeta} \right] = \frac{\partial}{\partial \zeta} \left( k_v \frac{\partial T_v}{\partial \zeta} \right) \quad (32)$$

The initial conditions (31) therefore reads:

$$T_v(\zeta, 0) = T^{sat} + \Delta T \quad (33)$$

The boundary condition at the interface (10) reads:

$$T_v(\zeta = 0, t) = T^{sat} \quad (34)$$

To simplify the analysis, it is assumed that the vapor phase is infinite so that the boundary condition on the wall is transformed as follows:

$$T_v(\zeta \rightarrow -\infty, t) = T^{sat} + \Delta T \quad (35)$$

This approximation is valid as long as the initial perturbation of the temperature field has a small influence on the temperature on the real boundary, which is measured by the Fourier number  $Fo = k/(\rho C p) \tau/L^2$  where  $L$  is a characteristic length and  $\tau$  is a characteristic time. The above approximation is therefore valid for times  $t < \tau$  with  $\tau$  such that  $Fo \ll 1$ . This issue is analyzed in detail in section 4.2.1.

Since the liquid phase is at a constant temperature, equation (9) implies

$$\left( k \frac{\partial T}{\partial \zeta} \right)_v (\zeta = 0, t) = \dot{m} \mathcal{L} \quad (36)$$

in which kinetic energy effects have been neglected for the sake of simplicity.

Since the vapor phase is always at rest, equation (7) implies

$$\dot{m} = -\rho_v V^i \quad (37)$$

Equations (36) and (37) show that the speed of displacement of the interface is given by

$$V^i(t) = -\frac{k_v}{\rho_v \mathcal{L}} \left( \frac{\partial T}{\partial \zeta} \right)_v (\zeta = 0, t) \quad (38)$$

The energy balance equation (32) then reads

$$\frac{\partial T_v}{\partial t} - V^i \frac{\partial T_v}{\partial \zeta} = \frac{1}{\rho_v C p_v} \frac{\partial}{\partial \zeta} \left( k_v \frac{\partial T_v}{\partial \zeta} \right) \quad (39)$$

If the thermal conductivity  $k_v$  is assumed to be constant, we can introduce the following variables:

$$\eta = \sqrt{\frac{1}{2 \alpha_v}} \frac{\zeta}{\sqrt{t}} \quad (40)$$

$$\theta(\eta) = \frac{C p_v}{\mathcal{L}} T_v(\zeta, t) \quad (41)$$

where

$$\alpha_v = \frac{k_v}{\rho_v C p_v} \quad (42)$$

Equation (39) can then be transformed, to get the following ordinary differential equation on  $\theta(\eta)$ :

$$\theta'' + (\eta - \theta'(0)) \theta' = 0 \quad (43)$$

where  $\theta' \equiv d\theta/d\eta$ .

The boundary conditions (34) and (35) imply the following boundary conditions for  $\theta(\eta)$ :

$$\theta(0) = \frac{Cp_v}{\mathcal{L}} T^{sat} \quad (44)$$

$$\theta(\eta \rightarrow -\infty) = \frac{Cp_v}{\mathcal{L}} (T^{sat} + \Delta T) \quad (45)$$

Equation (43) can be integrated once to get

$$\theta' = \theta'(0) \exp \left[ -\frac{\eta^2}{2} + \eta \theta'(0) \right] \quad (46)$$

From (38) and (46), the speed of displacement of the interface is then given by

$$V^i = -\sqrt{\frac{\alpha_v}{2}} \frac{\theta'(0)}{\sqrt{t}} \quad (47)$$

Since  $\theta'(0)$  is constant (which is still to be determined), equation (47) shows that the speed of displacement of the interface  $V^i$  varies as  $1/\sqrt{t}$ . This means that the initial infinite temperature gradient at the interface leads to an initial infinite value for  $V^i$  and that, as thermal diffusion develops, the temperature gradient at the interface decreases as well as  $V^i$ .

Let

$$\Theta_0 = \theta'(0) \exp \left[ \frac{\theta'(0)^2}{2} \right] \quad (48)$$

$$\Lambda = \frac{\eta - \theta'(0)}{\sqrt{2}} \quad (49)$$

Integrating (46) and accounting for (48) and (49), one gets

$$\theta(\Lambda) = \Theta_0 \frac{\sqrt{\pi}}{2} [\operatorname{erf}(\Lambda) - \operatorname{erf}(\Lambda_0)] + \frac{Cp_v}{\mathcal{L}} T^{sat} \quad (50)$$

where

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt \quad (51)$$

Equation (50) gives the temperature field. However, two constants  $\Theta_0$  and  $\Lambda_0$  appear in the expression for  $\theta$  which still have to be determined. The definitions (48) and (49) show that these two constants depend only on  $\theta'(0)$ , which is therefore the only constant to be determined. The value of  $\theta'(0)$  is determined thanks to the boundary condition (35). Indeed, given the expression (50) for  $\theta$ , the boundary condition (35) implies:

$$\frac{Cp_v}{\mathcal{L}} \Delta T + \theta'(0) \exp \left[ \frac{\theta'(0)^2}{2} \right] \frac{\sqrt{\pi}}{2} \left[ 1 - \operatorname{erf} \left( \frac{\theta'(0)}{\sqrt{2}} \right) \right] = 0 \quad (52)$$

Equation (52) is a non-linear equation in  $\theta'(0)$ .

Equations (52) and (50) therefore fully determine the temperature field in the vapor phase.

Turning back to the dimensional variables, one gets the following temperature field in the frame of reference linked to the interface:

$$T_v(\zeta, t) = T^{sat} + \Delta T \frac{\operatorname{erf}(\lambda_v) - \operatorname{erf}\left(\lambda_v + \sqrt{\frac{1}{\alpha_v}} \frac{\zeta}{2\sqrt{t}}\right)}{1 + \operatorname{erf}(\lambda_v)} \quad (53)$$

where  $\lambda_v = -\theta'(0)/\sqrt{2}$  satisfies the following non-linear equation

$$\frac{Cp_v}{\mathcal{L}} \Delta T = \sqrt{\frac{\pi}{2}} \lambda_v e^{\lambda_v^2} (1 + \operatorname{erf}(\lambda_v)) \quad (54)$$

Note that, for “small” values of  $\Delta T$ , the following approximation for  $\lambda_v$  can be used

$$\lambda_v \simeq \sqrt{\frac{2}{\pi}} \frac{Cp_v}{\mathcal{L}} \Delta T$$

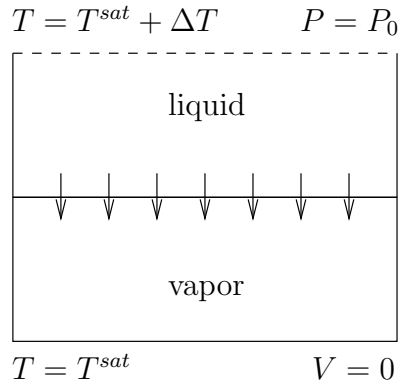
From equation (47), one gets the following expression for the speed of displacement of the interface:

$$V^i(t) = \sqrt{\alpha_v} \frac{\lambda_v}{\sqrt{t}} \quad (55)$$

Equation (7) allows to determine the liquid phase velocity:

$$V_l(t) = V^i(t) \left(1 - \frac{\rho_v}{\rho_l}\right) \quad (56)$$

#### 4.1.2 Liquid initially not at thermodynamic equilibrium



**Figure 4:** One-dimensional phase-change problem for a liquid initially undercooled ( $\Delta T < 0$ ).

If the temperature of the liquid phase is initially uniform at a value different from the saturation temperature, whereas the vapor phase is initially at equilibrium, a similar analysis to that developed in the previous section can be developed and one finds that the

temperature field within the liquid phase, in the frame of reference linked to the interface, is the following

$$T_l(\zeta, t) = T^{sat} + \Delta T \frac{\operatorname{erf}\left(\lambda_l + \sqrt{\frac{1}{\alpha_l}} \frac{\zeta}{2\sqrt{t}}\right) - \operatorname{erf}(\lambda_l)}{1 - \operatorname{erf}(\lambda_l)} \quad (57)$$

where

$$\frac{C_{pl}}{\mathcal{L}} \Delta T = \sqrt{\frac{\pi}{2}} \lambda_l e^{\lambda_l^2} (1 - \operatorname{erf}(\lambda_l)) \quad (58)$$

In this case, the speed of displacement of the interface is the following

$$V^i(t) = \frac{\rho_l}{\rho_v} \sqrt{\alpha_l} \frac{\lambda_l}{\sqrt{t}} \quad (59)$$

The expression for the liquid phase velocity is given by equation (56).

## 4.2 Test-case description

### 4.2.1 About the boundary conditions

One of the difficulties of this test-case comes from the fact that the analytical solution provided in section 4.1 is valid for an infinite length, which is impossible to achieve numerically. The solution recommended is to *impose a constant temperature on the boundaries* of the system as sketched in figures 3 and 4. The analytical solutions (53) and (57) are therefore only approximations of the exact solutions of the problems sketched in figures 3 and 4, which will be actually simulated numerically. In this section, we study the conditions under which the analytical solutions (53) and (57) are good approximations of the solutions of the problems actually simulated. In other words, we study the conditions under which the approximation of an infinite length of the phases approaches the solution for a finite length.

First, we study the case for which the vapor is initially not at thermodynamic equilibrium. Integrating equation (55), one gets the position of the interface as a function of time:

$$z^i(t) = z_0^i + 2 \lambda_v \sqrt{\alpha_v t} \quad (60)$$

Let  $L_v$  be the length of the vapor phase. From (60), one gets

$$L_v(t) = L_{v0} + 2 \lambda_v \sqrt{\alpha_v t} \quad (61)$$

The lower boundary is therefore located at a distance  $L_v(t)$  from the interface. If the vapor phase had an infinite length, the temperature at this location  $T_{p_v}(t)$  would be given by equation (53) for which  $\zeta = -L_v(t)$ :

$$T_{p_v}(t) = T^{sat} + \Delta T \frac{\operatorname{erf}(\lambda_v) + \operatorname{erf}\left(\frac{L_{v0}}{2\sqrt{\alpha_v t}}\right)}{1 + \operatorname{erf}(\lambda_v)} \quad (62)$$

We seek for the conditions under which the approximation  $T_{p_v} \simeq T^{sat} + \Delta T$  is satisfactory. Let  $\varepsilon$  be an approximation considered as reasonable, for instance  $\varepsilon = 10^{-2}$ :

$$T_{p_v} = T^{sat} + \Delta T (1 - \varepsilon) \quad (63)$$

From equation (62), one gets:

$$\frac{L_{v0}}{\sqrt{\alpha_v \tau_v}} = 2 \operatorname{erf}^{-1} [1 - \varepsilon (1 + \operatorname{erf}(\lambda_v))] \quad (64)$$

where  $\operatorname{erf}^{-1}$  represents the inverse of the error function and  $\tau_v$  is the time at which the condition (63) is satisfied.

Note that the left-hand-side of equation (64) can be expressed with a Fourier number based on the initial length of the vapor phase:  $1/\sqrt{Fo_v}$ . This shows that the approximation of a infinite length for the vapor phase is valid only for a certain period of time: beyond  $t = \tau_v$  the analytical solution (53) is no longer an acceptable approximation of the problem for which the temperature on the lower boundary is kept constant.

From a computationally point of view, if one aims at comparing his numerical results to the analytical solution (53) with a precision  $\varepsilon$  up to a time  $\tau_v$ , the initial length of the vapor phase must be that given by the condition (64).

A similar analysis can be developed in the case for which the liquid is initially not at thermodynamic equilibrium and one finds that the condition which must be satisfied is the following:

$$\frac{L_{l0}}{\sqrt{\alpha_l \tau_l}} = -2 \lambda_l \left(1 - \frac{\rho_l}{\rho_v}\right) + 2 \operatorname{erf}^{-1} [1 - \varepsilon (1 + \operatorname{erf}(\lambda_l))] \quad (65)$$

#### 4.2.2 About the initial condition

In the analytical solutions developed in section 4.1, the initial temperature field is not continuous at the interface: it varies from  $T^{sat}$  to  $T^{sat} + \Delta T$  on a zero distance. This condition cannot be imposed numerically. This initial condition must therefore be modified. It is recommended to *use the analytical solution at a time  $t_0 > 0$  as the initial condition*. No particular value for  $t_0$  is recommended; however, it is recommended to justify the choice for  $t_0$  on physical or numerical arguments. For instance, the number of grid points within the initial thermal boundary layer is considered as a good indication.

#### 4.2.3 Test-case

The physical parameters used for the simulation should be provided. These are

- the densities  $\rho_l$  and  $\rho_v$ ;
- the specific heat capacities  $Cp_l$  and  $Cp_v$ ;
- the thermal conductivities  $k_l$  and  $k_v$ ;
- the corresponding thermal diffusivities  $\alpha_l$  and  $\alpha_v$ ;
- the pressure  $P_0$  and the corresponding saturation temperature  $T^{sat}$  and latent heat of vaporization  $\mathcal{L}$ ;
- the initial temperature difference  $\Delta T$ ;
- the length of the system and the initial lengths of the phases  $L_{l0}$  and  $L_{v0}$ .

The time  $t_0$  for which the analytical solutions are used to initialize the temperature, velocity and pressure field should be provided.

Since the parameters  $\lambda_l$  or  $\lambda_v$  are key parameters of the analytical solutions (53) and (57) respectively, their value, determined through the numerical resolution of the non-linear equations (54) and (58), should be provided.

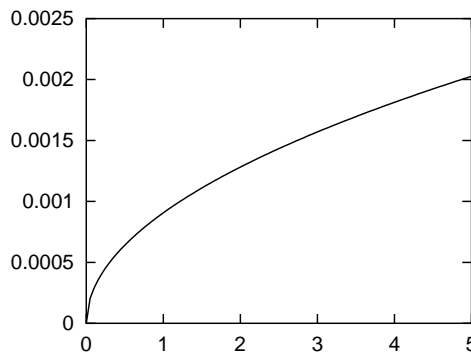
The precision  $\varepsilon$  at which the analytical solution is supposed to approach the solution of the finite length solution should be provided, as well as the times  $\tau_l$  or  $\tau_v$ , determined through the resolution of the non-linear equations (64) and (65) respectively, until which a reasonable comparison is still relevant.

It is recommended that numerical temperature fields should be compared to the analytical ones given by equations (53) or (57) at different times from  $t_0$  to  $\tau_v$  or  $\tau_l$ . At least one velocity and pressure field should be provided and compared to the corresponding analytical fields through the  $L^1$  norm of the error for instance. The position of the interface  $z^i(t)$  as well as its speed of displacement  $V^i(t)$  should also be provided and compared to the analytical solutions (55) or (59).

#### 4.2.4 Example

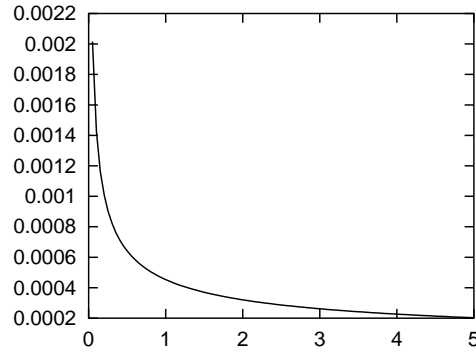
Let us consider water at a pressure  $P_0 = 160 \cdot 10^5$  Pa; the corresponding saturation temperature is  $T^{sat} = 620$  K. The physical characteristics of the bulk phases are the following:  $\rho_l = 586.5$  kg/m<sup>3</sup>,  $\rho_v = 106.4$  kg/m<sup>3</sup>,  $Cp_l = 9.35 \cdot 10^3$  J/kg K,  $Cp_v = 15.4 \cdot 10^3$  J/kg K,  $k_l = 0.444$  W/m K,  $k_v = 0.114$  W/m K,  $\alpha_l = 0.8096 \cdot 10^{-7}$  m<sup>2</sup>/s,  $\alpha_v = 0.6958 \cdot 10^{-7}$  m<sup>2</sup>/s and  $\mathcal{L} = 941$  J/kg; note that the latter value for  $\mathcal{L}$  is not the experimental value but is divided by a factor  $10^3$  so that the interface moves at a speed comparable to the speed at which the thermal boundary layer develops. Let us assume that the initial superheat of the vapor is  $\Delta T_v = 5$  K.

The solution of equation (54) is  $\lambda_v = 1.71814$ . The interface position  $z^i(t)$  is determined by equation (55), the speed of displacement of the interface  $V^i(t)$  is determined by equation (55) and the temperature profile within the vapor phase  $T_v(\zeta, t)$  is determined by equation (53); their graphical representations is given in figures 5, 6 and 7 respectively.

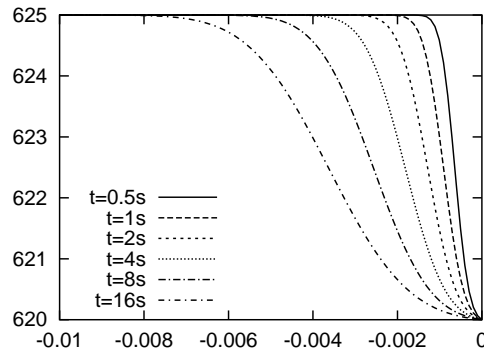


**Figure 5:** Time evolution of the interface position  $z^i(t)$  (position is in m and time is in s).

Note that, from equations (37) and (55) we can determine that the condition (25) is satisfied as long as  $t \gg 10^{-10}$  s, which is not a restrictive condition. Therefore, kinetic



**Figure 6:** Time evolution of the speed of displacement of the interface  $V^i(t)$  (velocity is in m/s and time is in s).



**Figure 7:** Time evolution of the temperature profile  $T_v(\zeta, t)$  (temperature is in K and distance is in m).

effects can be neglected compared the latent heat of vaporization.

If the initial length of the vapor phase is  $L_{v0} = 5$  mm and if the precision of the comparison between the numerical and the analytical temperature fields is  $\varepsilon = 10^{-2}$ , simulations can be run up to  $t = 33$  s; this time has been determined by solving equation (64).

Equation (61) shows that at this particular time, the length of the vapor phase is  $L_v = 10.216$  mm. This means if the simulation is run up to  $t = 33$  s, the initial length of the liquid phase should be such that  $L_{l0} > 5.2$  mm.

Note that if the value of  $\mathcal{L}$  were taken equal to its experimental value, at  $t \simeq 30$  s, the interface would be only about 0.1 mm away from its initial position, and the numerical and theoretical positions of the interface would be more difficult to compare.

## References

- Delhaye, J. M., Giot, M., & Riethmuller, M.L. 1981. *Thermohydraulics of two-phase systems for industrial design and nuclear engineering*. Hemisphere Publishing Corporation.
- Duquennoy, C. 2000. *Développement d'une approche de simulation numérique directe de l'ébullition en paroi*. Ph.D. thesis, Institut National Polytechnique de Toulouse.



Ishii, M. 1975. *Thermo-Fluid Dynamic Theory of Two-Phase Flow*. Eyrolles.

Welch, S.W.J., & Wilson, J. 2000. A volume of fluid based method for fluid flows with phase change. *J. Comp. Phys.*, **160**(2), 662–682. doi: 10.1006/jcph.2000.6481.