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A model for two phase flow with evaporation

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Abstract

The dynamic behavior of a free gas–liquid phase boundary is often influenced by evaporation or condensation to an extend that may not be neglected. In this paper, we derive a general model for the dynamics of a two phase flow with evaporation, starting from the balance of mass, energy, and momentum. The model takes into account that the gas phase might consist of a mixture of vapor and inert gas. It is based on the incompressible Navier–Stokes equations in the bulk of the liquid and the gas phase, convection–diffusion equations for heat and vapor, and appropriate conditions for the transfer of mass, momentum, and energy through the phase boundary.

As a simplification, the flow field in the liquid and gaseous phase can be decoupled, if the stress from the gas phase on the free surface is neglected. The special case of a gas phase containing only pure vapor is considered, which allows one to neglect the gas phase completely, leading to a single phase flow problem with a free boundary.

1 Introduction

Mass transport by evaporation or condensation through the phase boundary of a gas–liquid system is of importance in many applications. Let us just mention the case of evaporation in falling films, see [1, 5, 8, 9] or the evaporation of cryogenic propellants, see [6].

To fix the setting, denote by $\Omega \subset \mathbf{R}^d$, $d \in \{2,3\}$ the volume occupied by the fluids. We assume the system to consist of two distinguished *phases*, a liquid and a gaseous phase, denoted by Ω_l and Ω_g, respectively. The two phases are assumed to be separated by a sharp, smooth interface Γ_S. Note that a priori Ω_l and Ω_g (or equivalently Γ_S) are unknown and part of the problem, thus giving rise to a *free boundary problem.*

The goal of this article is to derive a mathematical model describing such a system. The model takes into account that the gas phase might consist of a mixture of vapor and inert gas. It is based on the incompressible Navier–Stokes equations in the bulk of the liquid and the gas phase, convection–diffusion equations for heat and vapor, and appropriate conditions for the transfer of mass, momentum, and energy through the phase boundary. Note that hereafter, we use the term evaporation also for the case of condensation, since the latter one may be considered as an evaporation with negative mass flux.

The rest of this paper is organized as follows. In Section 2 we briefly recall the derivation of balance equations for mass, momentum, and energy including balance laws at the phase boundary. The analysis uses a standard continuum approach.

In Section 3 we deal with a continuum model to describe evaporation. As a special case, the flow field in the liquid and gaseous phase respectively can be decoupled, if the stress from the gas phase acting on the free surface is neglected. The same approach have also been used by Burelbach et al. in [2]. This case is treated in Section 3.2. Further simplifications are made in Section 3.3, where the case of a gas phase containing only pure vapor is considered. This allows one to neglect the vapor phase completely, leading to a single phase flow problem with a free boundary.

2 Balance equations

In this section we briefly recall the derivation of balance equations for mass, momentum, and energy. Since the mathematics behind these balance equations is basicly the same for any quantity, we start by considering balance equations for an arbitrary generic quantity in Sections 2.1, 2.2 and consider the special cases for mass, momentum, energy in Sections 2.3 – 2.5. For a similar approach see e.g. [3, 7].

As the derivations below do not depend on the specific structure of the fluid, we assume the system to consist of two different general phases, say phase A and phase B, separated by a sharp, smooth boundary Γ_S that might move with time. Later we will specify these phases to be the liquid and gaseous part of the fluid, respectively.

To simplify notation, hereafter vector– as well as tensor-valued quantities will be denoted by bold characters, whereas plain characters indicate scalars.

2.1 Generic balance in a control volume

It is very common to consider balance equations either in Eulerian or in Lagrangian coordinates, see e.g. [7]. We apply a slightly generalized approach by considering balance equations in an arbitrarily moving control volume $V(t)$: consider some initial test volume $V_0 \subset \mathbf{R}^d$ and a coordinate function $\boldsymbol{\xi}(\mathbf{x}, t) \subset \mathbf{R}^d$ describing the motion of the control volume, i.e. $V(t) = \boldsymbol{\xi}(V_0, t)$. We assume $\boldsymbol{\xi}$ to be sufficiently smooth in time and for every time instant t, the mapping $\boldsymbol{\xi}(\cdot, 0) \to \boldsymbol{\xi}(\cdot, t)$ to be a homeomorphism. Let $\mathbf{w}$ denote the velocity of the motion of the control volume that is $\mathbf{w} = \partial_t \boldsymbol{\xi}$. Let $S(t)$ denote the surface of $V(t)$ and $\mathbf{n}_S$ the outward pointing normal vector at any point of $S(t)$.

Now consider the balance of some generic quantity b in $V(t)$:

$$\frac{d}{dt} \int_{V(t)} b \, dV = \int_{S(t)} -\boldsymbol{\Phi} \cdot \mathbf{n}_S \, dS + \int_{V(t)} \Psi \, dV. \tag{2.1}$$

Here, $\boldsymbol{\Phi}$ denotes the flux density of b relative to $\mathbf{w}$. Thus $-\boldsymbol{\Phi} \cdot \mathbf{n}_S$ is the net inflow rate of b into $V(t)$ at any point of its surface $S(t)$. Ψ denotes the net production rate of b in the control volume.

Let us denote by $\mathbf{u}$ the flow field in the fluid, i.e. the averaged velocity of all fluid particles in every point. With this notation, we may split $\boldsymbol{\Phi} = b\mathbf{u} - b\mathbf{w} + \mathbf{f}$ into its contributions given by the advection of b by the flow field, by the motion of the control

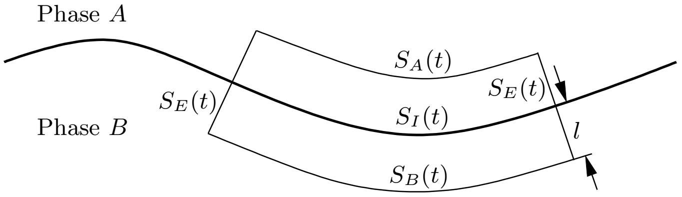

Figure 1: Control volume at the phase boundary.

volume, and by diffusive fluxes $\mathbf{f}$, respectively. This gives

$$\frac{d}{dt}\int_{V(t)} b\,dV = \int_{S(t)} -(b\,(\mathbf{u}-\mathbf{w}) + \mathbf{f})\cdot\mathbf{n}_S\,dS + \int_{V(t)} \Psi\,dV. \tag{2.2}$$

Note that from (2.2) we may recover the Eulerian approach, e.g. the motion of mass in a fixed coordinate system, by setting $\mathbf{w}=0$, as well as the Lagrangian approach, e.g. a coordinate system that follows the motion of the mass particles, by setting $\mathbf{w}=\mathbf{u}$.

If $V(t)$ lies entirely in one of the two phases, we may assume sufficient spatial smoothness so that we can apply the divergence theorem to get

$$\frac{d}{dt}\int_{V(t)} b\,dV = \int_{V(t)} -\nabla\cdot(b\,(\mathbf{u}-\mathbf{w})) - \nabla\cdot\mathbf{f} + \Psi\,dV. \tag{2.3}$$

To derive a partial differential equation, we set $\mathbf{w}=0$, interchange differentiation and integration for the time derivative and observe that the above identity holds for arbitrary (smooth) test volumes to arrive at the pointwise identity

$$\partial_t b + \nabla\cdot(b\,\mathbf{u}+\mathbf{f}) = \partial_t b + \mathbf{u}\cdot\nabla b + b\,\nabla\cdot\mathbf{u} + \nabla\cdot\mathbf{f} = \Psi. \tag{2.4}$$

Note that (2.4) does not hold across phase boundaries in general but only in the bulk, since the above derivation relies on the smoothness of the quantities involved.

2.2 Generic balance at a phase boundary

In order to establish the balance equations at the phase boundary, we consider a particular control volume that follows the motion of the boundary as depicted for the two dimensional case in Figure 1: for some segment $S_I(t)\subset\Gamma_S(t)$ of the phase boundary the control volume $V(t)$ is a layer of thickness l at both sides of $S_I(t)$. We denote by $S_A(t)$ and $S_B(t)$ the parts of the control volume's surface parallel to $S_I(t)$ that lie in phase A and in phase B, respectively, and we denote by $S_E(t)$ the parts of the control volume's surface normal to the phase boundary.

Using this notation, (2.2) yields

$$\begin{aligned}\frac{d}{dt}\int_{V(t)} b\,dV = &-\int_{S_A(t)} (b\,(\mathbf{u}-\mathbf{w})+\mathbf{f})\cdot\mathbf{n}_{S_A}\,dS \\ &-\int_{S_B(t)} (b\,(\mathbf{u}-\mathbf{w})+\mathbf{f})\cdot\mathbf{n}_{S_B}\,dS \\ &-\int_{S_E(t)} (b\,(\mathbf{u}-\mathbf{w})+\mathbf{f})\cdot\mathbf{n}_{S_E}\,dS \\ &+\int_{V(t)} \Psi\,dV.\end{aligned} \tag{2.5}$$

Letting l tend to zero, the control volume's surface parts $S_A(t)$ and $S_B(t)$ tend to $S_I(t)$ from either sides. The left hand side of (2.5) and the integral over $S_E(t)$ vanish in the limit. The integral of the production rate Ψ also vanishes unless there is production *on* the surface.

We introduce subscripts $._A$ and $._B$ to denote the values on the phase boundary from phase A and B, respectively. Moreover, let us denote by $\mathbf{n}$ the normal vector on the phase boundary pointing in the direction of, say, phase A and by u_Γ the normal velocity of the phase boundary in direction of $\mathbf{n}$. With this notation we get

$$\begin{aligned}0 = \int_{S_I(t)} \big(&\Psi - (b_A\,(\mathbf{u}_A\cdot\mathbf{n}-u_\Gamma)) - \mathbf{f}_A\cdot\mathbf{n} \\ &+ (b_B\,(\mathbf{u}_B\cdot\mathbf{n}-u_\Gamma)) + \mathbf{f}_B\cdot\mathbf{n}\big)\,dS.\end{aligned} \tag{2.6}$$

Since this identity holds for any segment $S_I(t)$ of the phase boundary, the integrand must vanish pointwise. If we denote by $[\cdot] = ._B - ._A$ the jump of a quantity across the phase boundary, we finally deduce

$$[b\,(\mathbf{u}\cdot\mathbf{n}-u_\Gamma)+\mathbf{f}\cdot\mathbf{n}] = -\Psi. \tag{2.7}$$

Remark 1

i) The above derivation implicitly used the fact that there exists a well defined velocity $\mathbf{w}$ *describing the motion of the control volume* $V(t)$ *independently of* $l \to 0$*. This assumption is always true for sufficiently small* l*, as long as the phase boundary does not self-intersect nor that there are topological changes. In particular we exclude the formation of gas bubbles and liquid droplets from our model.*

ii) The choice of the direction of the normal $\mathbf{n}$*, pointing in the direction of phase* A*, is somewhat arbitrary. However, by the definition of the jump operator* $[\cdot]$*, equation* (2.7) *is in fact independent of this choice.*

2.3 Conservation of mass

Here, we apply (2.4) to the conservation of mass, in other word be take $b := \rho$. Since by definition of the flow field $\mathbf{u}$ there is no diffusive flux for the density, we have $\mathbf{f} = 0$. Furthermore, we assume that there are no sources or sinks for the density, which is equivalent to $\Psi = 0$. Thus (2.4) yields

$$\partial_t \rho + \mathbf{u} \cdot \nabla \rho + \rho \nabla \cdot \mathbf{u} = 0. \tag{2.8}$$

We furthermore assume all fluids to be incompressible:

Assumption 1 (Incompressibility) *The mass density is assumed to be piecewise constant in time and space for each of the phases (except for the case treated in Assumption 3).*

Using this assumption, the mass balance simplifies to

$$\nabla \cdot \mathbf{u} = 0 \tag{2.9}$$

in the bulk of the fluid phases.

On the phase boundary (2.7) now reads

$$[\rho\,(\mathbf{u} \cdot \mathbf{n} - u_\Gamma)] = 0. \tag{2.10}$$

2.4 Conservation of momentum

The vector of momentum is given by $\rho\mathbf{u}$. Thus the equations from Sections 2.1 and 2.2 have to be understood component wise for this vector valued quantity. Terms like $b\mathbf{u}$ and $\mathbf{f}$ as in (2.4) now become tensors.

The momentum forces acting on the surface S of some volume in the fluid are commonly called *stresses*. By virtue of Cauchy's Theorem, see [4, chap. V], stresses can be represented by a *stress tensor* $\mathbf{T}$: if $\mathbf{n}_S$ is the outer normal vector to S, then the stress acting on this surface is given by $\mathbf{T}\mathbf{n}_S$. Thus in the balance of momentum $-\mathbf{T}$ is what we denoted by $\mathbf{f}$ in the generic case in Sections 2.1 and 2.2.

The stress tensor may be decomposed into two parts

$$\mathbf{T} = -p\mathbf{I} + \boldsymbol{\tau} \tag{2.11}$$

with the isotropic part of $\mathbf{T}$ given by the scalar *pressure* p and the *viscous stress* $\boldsymbol{\tau}$. We make the usual convention that a positive pressure describes inward directed forces.

In the present article we are only interested in incompressible *Newtonian* fluids, which are by definition given by:

Assumption 2 (Newtonian) *The viscous stress is assumed to be proportional to the rate of strain tensor:*

$$\boldsymbol{\tau} = \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^t), \tag{2.12}$$

where μ denotes the dynamic viscosity, which is assumed to be a scalar valued quantity, piecewise constant with respect to the phases.

Note that using (2.9), we get

$$\begin{aligned}
-\nabla\cdot\mathbf{T} &= -\nabla\cdot(\mu(\nabla\mathbf{u}+(\nabla\mathbf{u})^t))+\nabla p\\
&= -\mu(\nabla\cdot\nabla\mathbf{u}+\nabla\nabla\cdot\mathbf{u})+\nabla p\\
&= -\mu\Delta\mathbf{u}+\nabla p.
\end{aligned}\tag{2.13}$$

Regarding the external body forces Ψ in the momentum balance, we restrict ourselves to an acceleration force $\mathbf{g}$ acting uniformly in space (e.g. gravitation) for convenience. However, we still allow this force to vary with time. As acceleration acts on the mass, the momentum exerted by acceleration is

$$\Psi = \rho\mathbf{g}. \tag{2.14}$$

In Section 2.3 we assumed ρ to be constant (Assumption 1). This is somewhat too simple here, as this would exclude buoyancy, which is the momentum given by the variation of ρ in (2.14) due to differences in temperature. In order to also incorporate this effect but still keep the assumption of incompressibility in the conservation of mass, we use the *Boussinesq* approximation to model buoyancy:

Assumption 3 (Boussinesq) *The variation in density may be neglected except for the external forces in the balance of momentum, where it is assumed to be a linear function of temperature:*

$$\rho = \rho_0 - \rho_0\beta_T(\vartheta-\vartheta_0), \tag{2.15}$$

where ϑ denotes the temperature, ϑ_0 some reference temperature, ρ_0 the reference density of the material at ϑ_0, and β_T the thermal expansion coefficient of the material. We set $\rho=\rho_0$ everywhere else.

In view of the above considerations and Assumption 1 through Assumption 3 equation (2.4) yields the momentum equation of the Navier-Stokes equations:

$$\rho_0\,(\partial_t\mathbf{u}+\mathbf{u}\cdot\nabla\mathbf{u})-\mu\Delta\mathbf{u}+\nabla p = \rho_0\,\mathbf{g}-\rho_0\,\beta_T(\vartheta-\vartheta_0)\mathbf{g} \tag{2.16}$$

in the bulk of either phase.

On the phase boundary, we have to take into account surface tension. Surface tension exerts a stress in normal direction to the phase boundary proportional to its mean curvature. The mean curvature is given by the (surface) divergence of the normal vector $\nabla_S\cdot\mathbf{n}$ (up to a factor of $1/d$). In tangential direction we have a force proportional to the (surface) gradient of the surface tension on the boundary, which is called *Marangoni* stress. We restrict ourselves to variations of surface tension due to temperature and assume this dependency to be linear. That is, we assume

$$\nabla_S\,\sigma = -\sigma_T\nabla_S\,\vartheta, \tag{2.17}$$

where σ denotes the surface tension and $\sigma_T = -\frac{\partial\sigma}{\partial\vartheta}$.

Inserting (2.17) into (2.7) gives

$$[\rho_0\mathbf{u}\,(\mathbf{u}\cdot\mathbf{n}-u_\Gamma)-\mathbf{T}\mathbf{n}] = -(\sigma(\nabla_S\cdot\mathbf{n})\mathbf{n}-\sigma_T\nabla_S\,\vartheta). \tag{2.18}$$

2.5 Conservation of energy

The energy density in the system is given by the sum of the internal energy density ρE_U and the kinetic energy density $\rho\frac{\mathbf{u}\cdot\mathbf{u}}{2}$. The rate of work acting on the surface of some control volume by its surroundings is $\mathbf{Tu}$. Thus, $-\mathbf{Tu}$ is the diffusive flux of kinetic energy in terms of the generic case in Sections 2.1 and 2.2. We denote by $\mathbf{q}$ the diffusive flux of internal energy. Following the considerations from Section 2.4, we have an external source of kinetic energy, given by $\rho\mathbf{u}\cdot\mathbf{g}$. We assume to have no sources or sinks of internal energy. Inserting this in (2.4) and using (2.9) yields

$$\begin{aligned}\partial_t\left(\rho E_U+\rho\frac{\mathbf{u}\cdot\mathbf{u}}{2}\right)+\mathbf{u}\cdot\nabla\left(\rho E_U+\rho\frac{\mathbf{u}\cdot\mathbf{u}}{2}\right)&\\ +\nabla\cdot(-\mathbf{Tu}+\mathbf{q})&=\rho\mathbf{u}\cdot\mathbf{g}.\end{aligned}\tag{2.19}$$

Following Assumption 3, we replace ρ by ρ_0 on the left hand side and arrange the equation a little bit differently to get

$$\begin{aligned}\rho_0(\partial_t E_U+\mathbf{u}\cdot\nabla E_U)+\nabla\cdot\mathbf{q}-\mathbf{T}:(\nabla\mathbf{u})&\\ +\mathbf{u}\cdot\underbrace{\left(\rho_0(\partial_t\mathbf{u}+\mathbf{u}\cdot\nabla\mathbf{u})-\nabla\cdot\mathbf{T}-\rho\mathbf{g}\right)}_{=0}&=0,\end{aligned}\tag{2.20}$$

where for matrices A, B the inner product $A:B$ is defined by $A:B=\sum_{i,j}A_{ij}B_{ij}$. The last term on the left hand side of (2.20) vanishes according to the conservation of momentum in (2.16). Using (2.11) and (2.9) we have

$$\mathbf{T}:(\nabla\mathbf{u})=-p\,\nabla\cdot\mathbf{u}+\boldsymbol{\tau}:(\nabla\mathbf{u})=\boldsymbol{\tau}:(\nabla\mathbf{u}).\tag{2.21}$$

The internal energy density can be decomposed as $E_U=c_p\vartheta+E_P$ with c_p the specific heat capacity and E_P the potential energy related to the aggregate state. Assuming Fourier's law for the flux $\mathbf{q}$ we get $\mathbf{q}=-\lambda\nabla\vartheta$ in each phase, where λ denotes the heat conductivity. We assume c_p, λ and E_P to be constant in each phase. With this setting we get

$$\rho_0 c_p(\partial_t\vartheta+\mathbf{u}\cdot\nabla\vartheta)-\lambda\Delta\vartheta=\boldsymbol{\tau}:(\nabla\mathbf{u})\tag{2.22}$$

in the bulk of each phase.

Equation (2.22) describes the balance of internal energy. The diffusive flux is given by $-\lambda\nabla\vartheta$ and the production in the volume is given by $\boldsymbol{\tau}:(\nabla\mathbf{u})$, which describes the transformation of kinetic energy into heat by friction.

Applying (2.7) to the balance of internal energy, we get

$$[\rho_0(c_p\vartheta+E_P)(\mathbf{u}\cdot\mathbf{n}-u_\Gamma)-\lambda\partial_{\mathbf{n}}\vartheta]=0\tag{2.23}$$

at the phase boundary. Let us denote $j=\rho_0(\mathbf{u}\cdot\mathbf{n}-u_\Gamma)$. From (2.10) we have $[j]=0$. This allows us to write (2.23) as

$$[\rho_0 c_p\vartheta(\mathbf{u}\cdot\mathbf{n}-u_\Gamma)-\lambda\partial_{\mathbf{n}}\vartheta]=-j[E_P].\tag{2.24}$$

Since hereafter we are only using ρ_0 and there is no danger of confusion, we replace ρ_0 by ρ for the ease of presentation.

3 Model of evaporation

In this section we derive a mathematical model of evaporation. We consider two different situations: first, in Section 3.1 we treat a general, non-homogeneous case, where the gaseous phase consists of the mixture of vapor and some inert gas. This model will then be simplified in Section 3.2, allowing for the decoupling of the computation of the flows in both phases. Finally, in Section 3.3, we consider a special case, where the gaseous phase consists of pure vapor only.

Throughout this section we use subscripts $\cdot_l$ and $\cdot_g$ to denote liquid and the gaseous phase, respectively. Let j denote the rate of evaporation, e.g. the mass flux through the phase boundary, at each point of the free surface. From the conservation of mass in (2.10) we have

$$j = \rho_l(\mathbf{u}_l \cdot \mathbf{n} - u_\Gamma), \tag{3.1a}$$

$$j = \rho_g(\mathbf{u}_g \cdot \mathbf{n} - u_\Gamma). \tag{3.1b}$$

We assume a no slip condition for the velocity on the phase boundary in tangential direction:

Assumption 4 (No slip) *The tangential component of the velocity is continuous on the phase boundary:*

$$[\mathbf{u}] = \mathbf{u}_l - \mathbf{u}_g = (\mathbf{u}_l \cdot \mathbf{n} - \mathbf{u}_g \cdot \mathbf{n})\mathbf{n} \qquad \text{on } \Gamma_S. \tag{3.2}$$

The combination of (3.1) and (3.2) yields a jump condition for the velocity as a function of the mass flux:

$$[\mathbf{u}] = -\frac{\rho_l - \rho_g}{\rho_l \rho_g} j \mathbf{n}. \tag{3.3}$$

Now we can write (2.18) a little bit nicer:

$$\begin{aligned} \sigma(\nabla_S \cdot \mathbf{n})\mathbf{n} - \sigma_T \nabla_S \vartheta &= [\mathbf{T}\mathbf{n} - \rho \mathbf{u}\,(\mathbf{u} \cdot \mathbf{n} - u_\Gamma)] \\ &= [\mathbf{T}\mathbf{n}] - j[\mathbf{u}] \\ &= [\mathbf{T}\mathbf{n}] + \frac{\rho_l - \rho_g}{\rho_l \rho_g} j^2 \mathbf{n}. \end{aligned} \tag{3.4}$$

To proceed we need a further assumption.

Assumption 5 (Continuity of temperature) *We assume the temperature to be continuous on the phase boundary:*

$$[\vartheta] = 0. \tag{3.5}$$

We denote by $\Lambda = -[E_P]$ the *latent heat* of vaporization. Using (3.5) and the mass balance in (3.1), we can simplify the balance of internal energy on the phase boundary in (2.24) to read as

$$[-\lambda \partial_{\mathbf{n}} \vartheta] = (\Lambda - [c_p]\vartheta) j. \tag{3.6}$$

The rate of evaporation j is determined by the temperature and the partial pressure of vapor in the gas. The latter can be computed in the simplest case by using the ideal gas law:

$$\psi = \frac{\rho_v}{m} k_B \vartheta \tag{3.7}$$

with ρ_v the mass density of vapor, m the mass of a vapor particle, and $k_B = 1.381 \cdot 10^{-23}$ $\mathrm{J\,K^{-1}}$ the Boltzmann constant.

Assumption 6 (Saturation temperature) *The temperature on the free surface is given by the saturation temperature (which in turn depends on the partial pressure of vapor and material properties):*

$$\vartheta = \vartheta_{eq}(\psi(\rho_v, \vartheta)) \qquad \text{on } \Gamma_S. \tag{3.8}$$

Note that since the saturation temperature depends on the partial pressure, which in turn depends on the temperature, the temperature on the phase boundary is implicitly determined by the algebraic fixed point equation (3.8).

Assumption 6 provides a Dirichlet boundary condition that allows one to solve the heat transport problem in both phases. The heat flow equation (3.6) may then be used to determine the mass flux. This approach to model evaporation have also been used in [6].

Remark 2

i) The pressure p obtained from equations (2.16), (2.9) *cannot be used to compute the partial pressure of vapor, because Assumption 1 on the incompressibility of the fluid introduces an error, causing p to be inconsistent in a thermodynamic meaning.*

ii) In a precise physical sense Assumption 6 is contradictory to a non-vanishing evaporation rate, since it is the statement of equilibrium. However, the difference $\vartheta - \vartheta_{eq}$ is negligible in many practical cases.

3.1 The non-homogeneous case

In the non-homogeneous case, we assume the gaseous phase to be a mixture of inert gas and vapor. In order to determine the mass density and thus the partial pressure of vapor on the phase boundary, we have to consider vapor transport in the gas. We model this by an advection-diffusion equation for ρ_v:

$$\partial_t \rho_v + \mathbf{u} \cdot \nabla \rho_v - \varsigma \Delta \rho_v = 0 \tag{3.9}$$

in Ω_g, with some diffusion coefficient ς.

In addition to the mass balance (3.1), we can express the mass flow of vapor through the phase boundary also in terms of the vapor transport given by (3.9):

$$j = -\varsigma \nabla \rho_v \cdot \mathbf{n} + \rho_v (\mathbf{u}_g \cdot \mathbf{n} - u_\Gamma). \tag{3.10}$$

The combination of (3.1b) and (3.10) yields a Robin-type boundary condition for the vapor transport on Γ_S:

$$\varsigma \partial_{-\mathbf{n}} \rho_v = \Big(1 - \frac{\rho_v}{\rho_g}\Big) j. \tag{3.11}$$

Now, we are in a state to formulate the fully coupled model.

In the bulk of both phases $\Omega_l \cup \Omega_g$ the following equations hold:

$$\begin{aligned} \rho(\partial_t \mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u}) - \mu\Delta\mathbf{u} + \nabla p &= \rho\mathbf{g} - \rho\beta_T(\vartheta - \vartheta_0)\mathbf{g}, && \text{(3.12a)}\\ \nabla\cdot\mathbf{u} &= 0, && \text{(3.12b)}\\ \rho c_p(\partial_t\vartheta + \mathbf{u}\cdot\nabla\vartheta) - \lambda\Delta\vartheta &= \boldsymbol{\tau} : (\nabla\mathbf{u}). && \text{(3.12c)} \end{aligned}$$

In Ω_g the vapor density ρ_v fulfills

$$\partial_t\rho_v + \mathbf{u}\cdot\nabla\rho_v - \varsigma\Delta\rho_v = 0. \tag{3.12d}$$

The boundary conditions on Γ_S are

$$\begin{aligned} \frac{\rho_l - \rho_g}{\rho_l\rho_g} j^2\mathbf{n} + [\mathbf{T}\mathbf{n}] &= \sigma(\nabla_S\cdot\mathbf{n})\mathbf{n} - \sigma_T\nabla_S\vartheta, && \text{(3.12e)}\\ [\mathbf{u}] &= -\frac{\rho_l - \rho_g}{\rho_l\rho_g} j\mathbf{n}, && \text{(3.12f)}\\ \mathbf{u}_l\cdot\mathbf{n} - \frac{1}{\rho_l} j &= u_\Gamma, && \text{(3.12g)}\\ \vartheta &= \vartheta_{eq}(\psi(\rho_v, \vartheta)), && \text{(3.12h)}\\ \varsigma\partial_{-\mathbf{n}}\rho_v &= \Big(1 - \frac{\rho_v}{\rho_g}\Big) j, && \text{(3.12i)}\\ j &= \frac{[-\lambda\partial_{\mathbf{n}}\vartheta]}{\Lambda - [c_p]\vartheta}. && \text{(3.12j)} \end{aligned}$$

Remark 3

i) Note that $\mathbf{n}$ *is the normal on the phase boundary pointing from the liquid to the gaseous phase. Thus,* $-\mathbf{n}$ *is the outer normal to the gaseous phase and* $\partial_{-\mathbf{n}}\rho_v$ *the usual (outer) normal derivative of* ρ_v*.*

ii) The equation for u_Γ *yields a kinematic condition for the phase boundary* $\Gamma_S = \Gamma_S(t)$ *and thus in turn for the a priori unknown phases* Ω_g*,* Ω_l*.*

iii) The pressure p *appears in this model only as a gradient* ∇p *and in the jump term* $[\mathbf{T}\mathbf{n}]$*. It is therefore only determined up to an additive constant.*

The model needs to be closed by appropriate conditions on the outer boundary of Ω and by initial conditions. This of course strongly depends on the settings of the actual experiment or simulation and will not be discussed here.

However, let us just remark that the total volumes of the fluids grow with evaporation at a rate of $\int_{\Gamma_S} \frac{\rho_l - \rho_g}{\rho_l \rho_g} j \, dS$. Therefore one cannot use only no slip (e.g. homogeneous Dirichlet) condition for the flow, but one has to compensate for the growing volume by allowing some outflow condition at some part of the boundary of Ω.

3.2 The decoupled model

Typically, viscosities in gas are much smaller than those in liquids. Therefore we may neglect shear stresses in gas in comparison to liquid. Assume that $\mathbf{T}_g\mathbf{n} \ll \mathbf{T}_l\mathbf{n}$ (see [2]):

Assumption 7

$$[\mathbf{Tn}] = \mathbf{T}_l\mathbf{n} \qquad \text{on } \Gamma_S. \tag{3.13}$$

Using this assumption, the flow in the gaseous phase does not have any direct influence on the shape of the free surface. The flow in both phases is only weekly coupled by the temperature and the mass flux.

The decoupled model in the liquid phase reads:

In the bulk Ω_l the equations

$$\rho(\partial_t \mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u}) - \mu\Delta\mathbf{u} + \nabla p = \rho\mathbf{g} - \rho\beta_T(\vartheta - \vartheta_0)\mathbf{g}, \tag{3.14a}$$

$$\nabla \cdot \mathbf{u} = 0, \tag{3.14b}$$

$$\rho c_p(\partial_t \vartheta + \mathbf{u}\cdot\nabla\vartheta) - \lambda\Delta\vartheta = \boldsymbol{\tau} : (\nabla\mathbf{u}). \tag{3.14c}$$

are fulfilled. The boundary conditions on Γ_S are

$$\frac{\rho_l - \rho_g}{\rho_l \rho_g} j^2 \mathbf{n} + \mathbf{Tn} = \sigma(\nabla_S \cdot \mathbf{n})\mathbf{n} - \sigma_T \nabla_S \vartheta, \tag{3.14d}$$

$$\mathbf{u}\cdot\mathbf{n} - \frac{1}{\rho} j = u_\Gamma, \tag{3.14e}$$

$$\vartheta = \vartheta_{eq}(\psi(\rho_v, \vartheta)). \tag{3.14f}$$

As the free surface Γ_S is determined by the flow in the liquid phase only, we get a flow problem in a predetermined, moving domain for the gaseous phase, with Dirichlet condition for the flow on the phase boundary:

In the bulk Ω_g we have

$$\rho(\partial_t \mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u}) - \mu\Delta\mathbf{u} + \nabla p = \rho\mathbf{g} - \rho\beta_T(\vartheta - \vartheta_0)\mathbf{g}, \tag{3.15a}$$

$$\nabla \cdot \mathbf{u} = 0, \tag{3.15b}$$

$$\rho c_p(\partial_t \vartheta + \mathbf{u}\cdot\nabla\vartheta) - \lambda\Delta\vartheta = \boldsymbol{\tau} : (\nabla\mathbf{u}), \tag{3.15c}$$

$$\partial_t \rho_v + \mathbf{u}\cdot\nabla\rho_v - \varsigma\Delta\rho_v = 0. \tag{3.15d}$$

The boundary conditions on Γ_S are

$$\mathbf{u} = \mathbf{u}_l + \frac{\rho_l - \rho_g}{\rho_l \rho_g} j\mathbf{n}, \tag{3.15e}$$

$$\vartheta = \vartheta_{eq}(\psi(\rho_v, \vartheta)), \tag{3.15f}$$

$$\varsigma \partial_{-\mathbf{n}} \rho_v = \Big(1 - \frac{\rho_v}{\rho_g}\Big) j. \tag{3.15g}$$

The equation for the mass flux remains the same as in the fully coupled model:

$$j = \frac{[-\lambda \partial_{\mathbf{n}} \vartheta]}{\Lambda - [c_p]\vartheta} \quad \text{on } \Gamma_S. \tag{3.16}$$

It might be sensible to neglect the quadratic order terms j^2 and $\boldsymbol{\tau} : (\nabla \mathbf{u})$ also. But this would not affect the structure of the model, so this decision need not to be taken here.

3.3 The homogeneous case

In the homogeneous case, we assume the gaseous phase to consist of pure vapor. That is, here we assume

$$\rho_v = \rho_g. \tag{3.17}$$

As a consequence, since ρ_g was assumed to be constant, we get from (3.8) a constant saturation temperature all over the phase boundary. The Marangoni term $-\sigma_T \nabla_S \vartheta$ in (3.4) also vanishes, as the temperature (surface) gradient is zero. We furthermore assume the temperature also to be constant in the bulk of the gaseous phase:

Assumption 8 *The temperature in the gaseous phase is assumed to be constant, given by the solution of the fix point problem*

$$\vartheta = \vartheta_{eq}(\psi(\rho_v, \vartheta)). \tag{3.18}$$

If we apply these assumptions to the decoupled non-homogeneous model from Section 3.2, the gaseous phase does not have any influence on the liquid phase at all. We end up with the following one-phase flow problem in the liquid phase:

In the bulk Ω_l we have

$$\rho(\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u}) - \mu \Delta \mathbf{u} + \nabla p = \rho \mathbf{g} - \rho \beta_T (\vartheta - \vartheta_0) \mathbf{g}, \tag{3.19a}$$

$$\nabla \cdot \mathbf{u} = 0, \tag{3.19b}$$

$$\rho c_p (\partial_t \vartheta + \mathbf{u} \cdot \nabla \vartheta) - \lambda \Delta \vartheta = \boldsymbol{\tau} : (\nabla \mathbf{u}). \tag{3.19c}$$

The boundary conditions on Γ_S are

$$\frac{\rho_l - \rho_g}{\rho_l \rho_g} j^2 \mathbf{n} + \mathbf{T}\mathbf{n} = \sigma(\nabla_S \cdot \mathbf{n})\mathbf{n}, \tag{3.19d}$$

$$\mathbf{u}\cdot\mathbf{n} - \frac{1}{\rho} j = u_\Gamma, \tag{3.19e}$$

$$\vartheta = \vartheta_{eq}(\psi(\rho_v, \vartheta)), \tag{3.19f}$$

$$j = \frac{-\lambda \partial_{\mathbf{n}} \vartheta}{\Lambda - [c_p]\vartheta}. \tag{3.19g}$$

A Nomenclature

A.1 Latin characters

b	concentration of some quantity '.' per unit volume	$[./\mathrm{m}^3]$
c_p	specific heat capacity	$[\mathrm{J/(kg\,K)}]$
E_P	potential energy of aggregate state	$[\mathrm{J/kg}]$
E_U	internal energy	$[\mathrm{J/kg}]$
$\mathbf{f}$	diffusive flux vector of some quantity '.'	$[./(\mathrm{m}^2\,\mathrm{s})]$
$\mathbf{g}$	acceleration / gravity vector	$[\mathrm{m/s}^2]$
$\mathbf{I}$	identity tensor	[1]
j	mass flux through the phase boundary	$[\mathrm{kg/(m^2\,s)}]$
k_B	Boltzmann constant	$[\mathrm{J/K}]$
l	thickness of a layer	[m]
m	mass	[kg]
$\mathbf{n}$	normal vector	[1]
p	pressure	$[\mathrm{N/m}^2]$
$\mathbf{q}$	diffusive heat flux vector	$[\mathrm{W/m}^2]$
$\mathbf{R}$	real numbers	
S	surface	$[\mathrm{m}^2]$
t	time	[s]
$\mathbf{T}$	stress tensor	$[\mathrm{N/m}^2]$
$\mathbf{u}$	velocity vector	[m/s]
u_Γ	normal velocity at the interface	[m/s]
V	volume	$[\mathrm{m}^3]$
$\mathbf{w}$	velocity of the motion of the control volume	[m/s]

A.2 Greek characters

β_T	thermal expansion coefficient	[1/K]
Γ_S	free surface	
ϑ	temperature	[K]
λ	heat conductivity	[W/(K m)]
Λ	latent heat of evaporation	[J/kg]
μ	dynamic viscosity	[kg/(m s)]
$\boldsymbol{\xi}$	coordinate function	
ρ	density	[kg/m^3]
σ	surface tension	[N/m]
σ_T	temperature dependence of the surface tension	[N/(K m)]
ς	diffusion coefficient	[m^2/s]
$\boldsymbol{\tau}$	viscous stress vector	[N/m^2]
$\mathbf{\Phi}$	flux of some quantity ‘.’	[./(m^2 s)]
ψ	partial pressure of the gas	[Pa]
Ψ	production rate of some quantity ‘.’	[./m^3]
Ω	domain occupied by the fluid	
Ω_l	liquid part of Ω	
Ω_g	gaseous part of Ω	

A.3 Differential operators

∂_t	time derivative	[1/s]
$\partial_{\mathbf{n}}$	normal derivative	[1/m]
∇	gradient	[1/m]
Δ	laplace operator	[1/m^2]
∇_S	tangential gradient on Γ_S	[1/m]
$\nabla\cdot$	divergence operator	[1/m]
$\nabla_S\cdot$	tang. divergence operator on Γ_S	[1/m]

A.4 Subscripts

0	reference state
A	phase A
B	phase B
eq	equilibrium
g	gas
I	interface
l	liquid
T	dependence of the temperature
v	vapor

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