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A fluid mechanical model for two-phase flows

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A modified Allen–Cahn equation is combined with the compressible Navier–Stokes system. After a physically motivated modification of the stress tensor, for the resulting equations the second law of thermodynamics is valid. The model can be used to describe the forming of gas phases in a flowing liquid.

1. INTRODUCTION

In the present text, a modified Allen–Cahn equation [1] is combined with the Navier–Stokes system. The resulting model has some simplifications, but is a first step to describe the behaviour of gas phases in a flowing liquid. The model allows phases to grow or shrink due to changes of temperature and density in the fluid and incorporates their transport with the flow. For related works we refer to a combination of the Cahn–Hilliard model with the Navier–Stokes equations [2], the general variational approach of the energy [3], and to the models [4, 6].

2. NOTATIONS AND THERMODYNAMIC RELATIONSHIPS

Let $\Omega \subset \mathbb{R}^d$, $1 \le d \le 3$ be a bounded domain with Lipschitz boundary. For $0 < D \le \infty$ let $\Omega_D := \Omega \times (0, D)$ and $\varrho : \Omega_D \to \mathbb{R}^+$ denote the (averaged) density of the fluid, $e : \Omega_D \to \mathbb{R}^+$ the internal energy, $v : \Omega_D \to \mathbb{R}^d$ the velocity field of the fluid. Governed by a phase parameter $\chi : \Omega_D \to [0, 1]$, two phases (e.g. a gas and a liquid phase) may exist in Ω. Let $\sqrt{\delta}$ denote the thickness of transition layers between two phases. Generally, we postulate the potential energy density E_{pot} of the system to be the convex combination of the corresponding values of the two phases, giving rise to the definition

$$E_{\text{pot}} = \chi E_{\text{pot},1} + (1-\chi) E_{\text{pot},2} \,. \tag{1}$$

Similar relationships will be assumed for the entropy density S and the Gibbs free energy density G. The internal energy density E is obtained after adding the kinetic energy:

$$E = E_{\text{pot}} + \frac{1}{2}\,|v|^2 .$$

Capital letters genericly denote densities, values corresponding to small letters include a factor ρ or ρ_i. Indices refer to the phase, values without index to the whole system. Hence,

$$\begin{aligned} e_{\text{pot}} &= e_{\text{pot},1} + e_{\text{pot},2} = \varrho_1 E_{\text{pot},1} + \varrho_2 E_{\text{pot},2} = \varrho\,[\chi E_{\text{pot},1} + (1-\chi) E_{\text{pot},2}] = \varrho E_{\text{pot}} \,, \\ e &= e_{\text{pot}} + \frac{\varrho}{2}\,|v|^2 . \end{aligned} \tag{2}$$

ϱ and χ are solutions of the system of partial differential equations (4)–(7) below and allow us to calculate the specific densities ϱ_1, ϱ_2 of the phases.

Consider the specific volume $V = \frac{1}{\varrho}$. Let V_i be the specific volume of phase i and $\tilde{V}_i$ be the volume phase i is actually occupying in V. Now we define

$$\psi_i := \frac{\tilde{V}_i}{V} \quad \text{– volume fraction of phase } i \text{ in } V,\ 0 \le \psi_i \le 1,$$

$$\varrho_i := \frac{\psi_i}{V_i} = \frac{\tilde{V}_i}{V_i}\frac{1}{V} \quad \text{– specific density of phase } i,\ 0 \le \rho_i \le \rho,$$

$$\chi_i := \frac{\varrho_i}{\varrho} = \frac{\tilde{V}_i}{V_i} \quad \text{– density quotient = mass of phase } i \text{ in } V,\ 0 \le \chi_i \le 1.$$

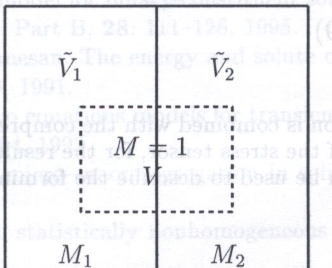


Fig. 1. Specific Volume V

In the following we write χ for χ_1 and $(1-\chi)$ for χ_2. Notice that ρ and χ are solutions of the systems of equations presented below and will allow us to calculate ρ_1, ρ_2 via

$$\rho_1 = \rho\chi, \qquad \rho_2 = \rho(1-\chi).$$

To guarantee the formation of phases, we subtract the mixing entropy density $\tilde{S}$,

$$\begin{aligned} \tilde{S} &:= W(\chi) + \frac{\delta}{2}\,|\nabla\chi|^2, \\ W(\chi) &:= \chi\ln\chi + (1-\chi)\ln(1-\chi) - \frac{1}{2}\chi^2, \end{aligned} \tag{3}$$

from S and set $\tilde{s} := \varrho\tilde{S}$. This represents the entropy density as

$$S = \chi S_1 + (1-\chi)S_2 - W(\chi) - \frac{\delta}{2}\,|\nabla\chi|^2$$

and consequently for the free energy density F and the Helmholtz free energy density G

$$F = \chi F_1 + (1-\chi)F_2 + T\tilde{S}, \qquad G = \chi G_1 + (1-\chi)G_2 + T\tilde{S}.$$

3. MATHEMATICAL FORMULATION

Beside the definitions above, the parameter $\varepsilon > 0$ scales the substantial derivative $d\chi := \partial_t\chi + v\cdot\nabla\chi$ of χ and is related to the time scale of the underlying physical problem. Furthermore, let $T : \Omega_D \to \mathbb{R}^+$ be the temperature and $p : \Omega_D \to \mathbb{R}^+$ the pressure of the fluid. For given velocity field v, let R_I denote the inlet, R_O the outlet of the domain Ω, where $\vec{n}$ is the unit outer normal vector to $\partial\Omega$. R_I, R_O and Ω are assumed not to depend on time t.

We modify the stress tensor and set (δ_{ij} be the Kronecker delta)

$$\begin{aligned} \Gamma_{ij} &:= \tau_{ij} - p\delta_{ij} - \delta\varrho T\,\partial_i\chi\,\partial_j\chi\,, \\ \tau_{ij} &:= \mu(\partial_i v_j + \partial_j v_i) + \nu(\operatorname{div} v)\delta_{ij} \end{aligned}$$

with viscosity coefficients ν, μ, where $\nu \geq -\frac{2}{3}\mu$ for $d = 3$ and $\nu \geq -\mu$ for $d = 2$.

One can show that the new term $-\delta\varrho T\, \partial_i\chi\, \partial_j\chi$ is a consequence of adding $\frac{\delta\varrho}{2}|\nabla\chi|^2$ to the system entropy.

The thermodynamical driving force of the Allen–Cahn type equation is defined by

$$J(\varrho, T, \chi) := W(\chi) + \frac{1}{T}[\chi G_1(\varrho, T) + (1-\chi)G_2(\varrho, T)].$$

With these definitions, we introduce the following system of equations corresponding to conservation of mass (4), momentum (5) and energy (6):

For given $(\varrho_0\,, v_0\,, e_0\,, \chi_0)$, $(v_r\,, T_r\,, \chi_r)$ *and* ϱ_I *find the solution* $U = (\varrho, \varrho v, e, \chi)^t$ *of*

$$\partial_t\varrho \quad = -\mathrm{div}(\varrho v), \tag{4}$$

$$\partial_t(\varrho v) = -\mathrm{div}(\varrho v \otimes v + \delta\varrho T\, \nabla\chi \otimes \nabla\chi) + \mathrm{div}(\tau) - \nabla p, \tag{5}$$

$$\partial_t e \quad = \mathrm{div}(L\nabla T - (e - \Gamma)v), \tag{6}$$

$$\varepsilon\, \partial_t\chi \quad = -\partial_\chi J + \frac{\delta}{\varrho}\mathrm{div}(\varrho\nabla\chi) - \varepsilon v \cdot \nabla\chi, \tag{7}$$

in Ω *with the initial values*

$$(\varrho, \varrho v, e, \chi)(\cdot, 0) = (\varrho_0\,, \varrho_0 v_0\,, e_0\,, \chi_0) \qquad \text{in } \Omega$$

and the boundary values

$$\chi = \chi_r\,, \qquad v = v_r\,, \qquad T = T_r \qquad \text{on } \partial\Omega$$

and

$$\varrho = \varrho_I \qquad \text{on } R_I\,.$$

As a consequence of a parabolic maximum principle for (7), the logarithmic form of W in (3) guarantees $0 < \chi < 1$ in Ω_∞, if the same is true for the initial datum χ_0.

All extrema β of the phase parameter χ satisfy

$$\partial_\chi J(\varrho, T, \beta) = \ln\left(\frac{\beta}{1-\beta}\right) - \beta + \frac{1}{T}(G_1(\varrho, T) - G_2(\varrho, T)) = 0.$$

This equation explains how ρ and T determine β and hence which phase (gas or liquid) forms. The dependency is illustrated in Table 1.

The principle is the same as the temperature dependence of the phase value in the phase field model and is explained in [5].

Table 1. Predicted extrema β of χ

$\frac{G_1-G_2}{T}$	β
0	0.65905
−1	0.86599
−2	0.95028
−3	0.98169
−5	0.99752

$\frac{G_1-G_2}{T}$	β
−8	0.99988
+1	0.34095
+2	0.13401
+3	0.04972
+5	0.00674

4. ASSUMPTIONS

It follows a list of all physical assumptions that were implicitly made in the approach above.

- The domain Ω as well as the inlet and outlet do not depend on time t.
- All phases are assumed to be moving with identical velocity vector v.
- For E_{pot}, Eq. (1) is assumed. Similar relationships are assumed to hold for S, F and G as explained above.
- The volume of a mixture consisting of 2 phases is supposed to obey the formula

$$V = \chi V_1 + (1-\chi) V_2 \,. \tag{8}$$

- The viscosities ν_i and μ_i, the heat coefficients L_i and the adiabatic coefficients γ_i are assumed to be constants and shall have one value for both phases.
- Chemical reactions don't take place. Magnetic and electric forces are neglected.
- Both phases are assumed to be incompressible.
- $T_1 = T_2$: Two neighbouring phases shall have the same temperature (instantaneous equalization of entropy).
- $p_1 = p_2$: The partial pressures of two phases are identical (instantaneous equalization of volume).
- The heat generated by shearing of boundary layers is not taken into account.
- The buoyancy of gas phases is not incorporated.

5. ENTROPY ESTIMATE

We prove the validity of the second law of thermodynamics for system (4)–(7), corresponding directly to the existence of a Lyapunov functional. We start by calculating ds_i, the total differential of phase i, $i = 1, 2$. By definition, we have

$$\mathrm{d}s_i = \mathrm{d}(\varrho_i S_i) = S_i\,\mathrm{d}\varrho_i + \varrho_i\,\mathrm{d}S_i \,.$$

Because of the Gibbs equation $\mathrm{d}S_i = \frac{1}{T}\,\mathrm{d}E_i + \frac{p}{T}\,\mathrm{d}V_i$ it follows:

$$\mathrm{d}s_i = S_i\,\mathrm{d}\varrho_i + \frac{\varrho_i}{T}\,\mathrm{d}E_i + \frac{\varrho_i p}{T}\,\mathrm{d}V_i = \left(S_i - \frac{pV_i}{T}\right)\mathrm{d}\varrho_i + \frac{\varrho_i}{T}\,\mathrm{d}E_i + \frac{p}{T}\,\mathrm{d}(\varrho_i V_i)$$

$$= \left(S_i - \frac{pV_i}{T} - \frac{E_i}{T}\right)\mathrm{d}\varrho_i + \frac{1}{T}\,\mathrm{d}(\varrho_i E_i) + \frac{p}{T}\,\mathrm{d}\psi_i = -\frac{1}{T} G_i\,\mathrm{d}\varrho_i + \frac{1}{T}\,\mathrm{d}e_i + \frac{p}{T}\,\mathrm{d}\psi_i \,.$$

And after summing up over all phases

$$\mathrm{d}s + \mathrm{d}\tilde{s} = \sum_i \mathrm{d}s_i = -\frac{1}{T}\sum_i G_i\,\mathrm{d}\varrho_i + \frac{1}{T}\,\mathrm{d}e + \frac{p}{T}\,\mathrm{d}\Big(\underbrace{\sum_i \psi_i}_{=0}\Big) \,.$$

Here we use the relationship $\mathrm{d}\varrho_i = \chi_i\,\mathrm{d}\varrho + \varrho\,\mathrm{d}\chi_i$ and observe $\mathrm{d}\chi_1 = -\mathrm{d}\chi_2$. It follows

$$\mathrm{d}s + \mathrm{d}\tilde{s} = -\frac{1}{T}\sum_i \chi_i G_i\,\mathrm{d}\varrho + \frac{1}{T}\,\mathrm{d}e - \frac{\varrho}{T}(G_1 - G_2)\,\mathrm{d}\chi . \tag{9}$$

Now we assume that the internal energy available for thermodynamic processes does not depend on v. For $v = 0$ the differential $\mathrm{d}e$ in (9) is $\mathrm{d}e_{\mathrm{pot}}$. If we consider the arising equation as a relation in phase space, so that we can compare the ∂_t-terms separately, we get after integration

$$\int\limits_\Omega \partial_t s = \int\limits_\Omega \left[\frac{1}{T}\,\partial_t e_{\mathrm{pot}} - \frac{1}{T}\sum_i \chi_i G_i\,\partial_t\varrho - \frac{\varrho}{T}(G_1 - G_2)\,\partial_t\chi - \partial_t\tilde{s}\right].$$

Now we need a representation of $\frac{1}{T}\,\partial_t e_{\mathrm{pot}}$. Because of

$$\partial_t e = \partial_t\left(e_{\mathrm{pot}} + \frac{\varrho}{2}|v|^2\right) = \partial_t e_{\mathrm{pot}} + v\cdot\partial_t(\varrho v) - \frac{|v|^2}{2}\,\partial_t\varrho,$$

exploiting the conservation equations (4), (5) and (6) yields

$$\begin{aligned}\int\limits_\Omega \frac{1}{T}\,\partial_t e_{\mathrm{pot}} &= \int\limits_\Omega \left[-\frac{v}{T}\cdot\partial_t(\varrho v) + \frac{|v|^2}{2T}\,\partial_t\varrho + \frac{1}{T}\,\mathrm{div}(L\nabla T - (e-\Gamma)v)\right]\\ &= \int\limits_\Omega \left[-\frac{v}{T}\cdot\mathrm{div}(-\varrho v\otimes v + \Gamma) - \frac{|v|^2}{2T}\,\mathrm{div}(\varrho v) + \frac{1}{T}\,\mathrm{div}\left[L\nabla T - \left(e_{\mathrm{pot}} + \frac{\varrho}{2}|v|^2 - \Gamma\right)v\right]\right].\end{aligned}$$

After partial integration, this means

$$\int\limits_\Omega \frac{1}{T}\,\partial_t e_{\mathrm{pot}} = \int\limits_\Omega \left[L\frac{|\nabla T|^2}{T^2} + \frac{\Gamma}{T} : \nabla v + e_{\mathrm{pot}} v\cdot\nabla\left(\frac{1}{T}\right)\right] + \int\limits_{\partial\Omega}\left[-e_{\mathrm{pot}}\frac{v}{T} + L\frac{\nabla T}{T}\right]\cdot\vec{n}.$$

We get

$$\begin{aligned}\int\limits_\Omega \partial_t s = \int\limits_\Omega &\left[L\frac{|\nabla T|^2}{T^2} + \frac{\Gamma}{T}:\nabla v + e_{\mathrm{pot}} v\cdot\nabla\left(\frac{1}{T}\right) - \frac{\varrho}{T}(G_1 - G_2)\,\partial_t\chi - \frac{1}{T}\sum_i \chi_i G_i\,\partial_t\varrho - \partial_t\tilde{s}\right]\\ &+ \int\limits_{\partial\Omega}\left[-e_{\mathrm{pot}}\frac{v}{T} + L\frac{\nabla T}{T}\right]\cdot\vec{n}.\end{aligned} \tag{10}$$

Now we transform the term $-\frac{1}{T}\sum_i \chi_i G_i \partial_t\varrho$ in (10).

$$\begin{aligned}\int\limits_\Omega -\frac{1}{T}\sum_i \chi_i G_i\,\partial_t\varrho &= \int\limits_\Omega \frac{1}{T}\sum_i \chi_i G_i\,\mathrm{div}(\varrho v)\\ &= \int\limits_\Omega -\nabla\left(\frac{1}{T}\sum_i \chi_i G_i\right)\cdot(\varrho v) + \int\limits_{\partial\Omega}\frac{1}{T}\sum_i \varrho_i G_i v\cdot\vec{n}\\ &= \int\limits_\Omega \left[-\sum_i \varrho_i G_i v\cdot\nabla\left(\frac{1}{T}\right) - \frac{\varrho}{T}\sum_i G_i\nabla\chi_i\cdot v - \frac{v}{T}\cdot\sum_i \varrho_i\,\mathrm{d}G_i\right]\\ &\quad + \int\limits_{\partial\Omega}\frac{1}{T}\sum_i \varrho_i G_i v\cdot\vec{n}.\end{aligned} \tag{11}$$

We simplify this further. The first and third integrand in (11) are

$$\begin{aligned}\int\limits_\Omega -\sum_i \varrho_i G_i v\cdot\nabla\left(\frac{1}{T}\right) &= \int\limits_\Omega \left[-e_{\mathrm{pot}} v\cdot\nabla\left(\frac{1}{T}\right) - \frac{v}{T}(s+\tilde{s})\cdot\nabla T - pv\cdot\nabla\left(\frac{1}{T}\right)\right],\\ \int\limits_\Omega -\frac{v}{T}\cdot\sum_i \varrho_i\,\mathrm{d}G_i &= \int\limits_\Omega -\frac{v}{T}\cdot[\nabla p - (s+\tilde{s})\nabla T].\end{aligned}$$

The last equality is a consequence of $\mathrm{d}G_i = -S_i\,\mathrm{d}T + V_i\,\mathrm{d}p$ and $\sum_i \varrho_i V_i = 1$. Therefore

$$\int_\Omega -\frac{1}{T}\sum_i \chi_i G_i\,\partial_t\varrho = \int_\Omega \left[-e_{\text{pot}}v\cdot\nabla\left(\frac{1}{T}\right) - \frac{1}{T}(\varrho v)\cdot\sum_i G_i\nabla\chi_i\right] - \int_\Omega\left[pv\cdot\nabla\left(\frac{1}{T}\right) + \frac{v}{T}\cdot\nabla p\right] + \int_{\partial\Omega}\frac{1}{T}\sum_i \varrho_i G_i v\cdot\vec{n}\,.$$

By inserting this in (10), we obtain

$$\begin{aligned}\int_\Omega \partial_t s = &\int_\Omega\left[L\frac{|\nabla T|^2}{T^2} + \frac{\tau}{T}:\nabla v - p\,\mathrm{div}v - pv\cdot\nabla\left(\frac{1}{T}\right) - \frac{v}{T}\cdot\nabla p - \partial_t\tilde{s}\right]\\ &- \int_\Omega \delta\varrho\nabla\chi\otimes\nabla\chi:\nabla v - \int_\Omega\frac{\varrho}{T}(G_1-G_2)(v\cdot\nabla\chi + \partial_t\chi)\\ &+ \int_{\partial\Omega}\left[\sum_i\varrho_i G_i - e_{\text{pot}}\right]\frac{v}{T}\cdot\vec{n} + \int_{\partial\Omega}\frac{L\nabla T}{T}\cdot\vec{n}\,. \end{aligned} \tag{12}$$

In (12) we remark at once, that

$$\int_\Omega\left[-\frac{p}{T}\,\mathrm{div}v - pv\cdot\nabla\left(\frac{1}{T}\right) - \frac{v}{T}\cdot\nabla p\right] = \int_\Omega -\mathrm{div}(p\frac{v}{T}) = \int_{\partial\Omega} -p\frac{v}{T}\cdot\vec{n}\,,$$

enabling us to reformulate the boundary integrals

$$\int_{\partial\Omega}\left[\sum_i\varrho_i G_i - e_{\text{pot}}\right]\frac{v}{T}\cdot\vec{n} - \int_{\partial\Omega}p\frac{v}{T}\cdot\vec{n} = -\int_{\partial\Omega}(s+\tilde{s})v\cdot\vec{n}\,.$$

Now we write the modified Allen–Cahn equation in the form

$$-\frac{1}{T}(G_1 - G_2) = \varepsilon(\partial_t\chi + v\cdot\nabla\chi) + W'(\chi) - \frac{\delta}{\varrho}\,\mathrm{div}(\varrho\nabla\chi).$$

Inserting in (12) yields

$$\begin{aligned}\int_\Omega\partial_t s = &\int_\Omega\left[L\frac{|\nabla T|^2}{T^2} + \frac{\tau}{T}:\nabla v - \delta\varrho\nabla\chi\otimes\nabla\chi:\nabla v + \varepsilon\varrho\,(\partial_t\chi + v\cdot\nabla\chi)^2 - \partial_t\tilde{s}\right]\\ &+ \int_\Omega(\varrho W'(\chi) - \delta\mathrm{div}(\varrho\nabla\chi))(\partial_t\chi + v\cdot\nabla\chi) - \int_{\partial\Omega}(s+\tilde{s})v\cdot\vec{n} + \int_{\partial\Omega}\frac{L\nabla T}{T}\cdot\vec{n}\,.\end{aligned}$$

Next we systematically remodel $[\varrho W'(\chi) - \delta\mathrm{div}(\varrho\nabla\chi)]\,(\partial_t\chi + v\cdot\nabla\chi)$. Firstly,

$$\begin{aligned}\int_\Omega[\varrho W'(\chi) - \delta\mathrm{div}(\varrho\nabla\chi)]\,\partial_t\chi = &\int_\Omega\left[-\left(W(\chi) + \frac{\delta}{2}\,|\nabla\chi|^2\right)\partial_t\varrho + \partial_t\left(\varrho W(\chi) + \frac{\delta\varrho}{2}|\nabla\chi|^2\right)\right]\\ &- \int_{\partial\Omega}\delta\varrho\,\partial_t\chi\nabla\chi\cdot\vec{n}\,,\end{aligned}$$

and for the transport term after partial integration

$$\int_\Omega [\varrho W'(\chi) - \delta \operatorname{div}(\varrho \nabla\chi)]\, v\cdot\nabla\chi = \int_\Omega \nabla\left(\varrho W(\chi) + \frac{\delta\varrho}{2}|\nabla\chi|^2\right)\cdot v - \int_\Omega \left(W(\chi) + \frac{\delta}{2}|\nabla\chi|^2\right)\nabla\varrho\cdot v$$

$$+ \int_\Omega \delta\varrho\nabla\chi\otimes\nabla\chi : \nabla v - \int_{\partial\Omega} \delta\varrho(v\cdot\nabla\chi)\nabla\chi\cdot\vec{n}\,.$$

Thus we get

$$\int_\Omega \partial_t s = \int_\Omega L\frac{|\nabla T|^2}{T^2} + \frac{\tau}{T} : \nabla v + \varepsilon\varrho\,(\partial_t\chi + v\cdot\nabla\chi)^2 + \nabla\tilde{s}\cdot v - \tilde{S}\partial_t\varrho - \tilde{S}\nabla\varrho\cdot v$$

$$- \int_{\partial\Omega} \tilde{s}v\cdot\vec{n} - \int_{\partial\Omega} sv\cdot\vec{n} + \int_{\partial\Omega} L\frac{\nabla T}{T}\cdot\vec{n} - \int_{\partial\Omega} \delta\varrho(\partial_t\chi + v\cdot\nabla\chi)\nabla\chi\cdot\vec{n}\,.$$

Finally we use

$$\int_{\partial\Omega} -\tilde{s}v\cdot\vec{n} = \int_\Omega -\operatorname{div}(\tilde{s}v) = \int_\Omega -v\cdot\nabla\tilde{s} - \tilde{s}\operatorname{div} v\,,$$

$$\int_\Omega \left[-\tilde{S}\,\partial_t\varrho - \tilde{s}\operatorname{div} v - \tilde{S}\,\nabla\varrho\cdot v\right] = 0\,,$$

to get the result

$$\int_\Omega \partial_t s + \int_{\partial\Omega} sv\cdot\vec{n} = \int_\Omega \left[L\frac{|\nabla T|^2}{T^2} + \frac{\tau}{T} : \nabla v + \varepsilon\varrho\,(\partial_t\chi + v\cdot\nabla\chi)^2\right]$$

$$- \int_{\partial\Omega} \varrho(\partial_t\chi + v\cdot\nabla\chi)\,\delta\nabla\chi\cdot\vec{n} + \int_{\partial\Omega} \frac{L\,\nabla T}{T}\cdot\vec{n}\,. \tag{13}$$

Now, for a thermodynamically closed system, there is no temperature and entropy flux at $\partial\Omega$. So, by choosing Neumann-boundary data for χ or $\chi \equiv$ const on $\partial\Omega$, all boundary integrals in (13) vanish. $L\frac{|\nabla T|^2}{T^2}$ is a production term due to heat diffusion, $\frac{\tau}{T} : \nabla v$ the dissipated motion energy. Defining the tensor $f_{ij} := \frac{1}{2}(\partial_i v_j + \partial_j v_i)$, we see $\tau : \nabla v \geq 0$:

$$\begin{aligned}\tau : \nabla v &= \mu\sum_{i,j}(\partial_i v_j + \partial_j v_i)\partial_j v_i + \nu(\operatorname{div} v)\sum_{i,j}\partial_j v_i\delta_{ij}\\ &= \mu\sum_{i,j}2(f_{ij})^2 + \nu\sum_k f_{kk}\sum_{i,j} f_{ij}\delta_{ij} = 2\mu\sum_{i,j}(f_{ij})^2 + \nu\Big(\sum_i f_{ii}\Big)^2.\end{aligned} \tag{14}$$

After diagonalizing f_{ij} by principal axis transformation and for $\nu \geq -\frac{2}{3}\mu$ for $d = 3$ we get $\tau : \nabla v \geq 0$ and therefore $\partial_t \int_\Omega s \geq 0$ as claimed. Notice also that $\int_\Omega \varepsilon\varrho\,(\partial_t\chi + v\cdot\nabla\chi)^2$ corresponds to the Lyapunov functional of the unmodified Allen–Cahn equation.

6. COMPARISON WITH THE PHASE FIELD EQUATION

For $v \equiv 0$, the entropy estimate is fulfiled with the original stress tensor $\tilde{\Gamma}_{ij} := \tau_{ij} - p\delta_{ij}$ of the Navier–Stokes equations. Since $\partial_t\varrho = 0$, we may set without loss of generality $\varrho \equiv 1$. For $\varepsilon = 1$ and $L =$ const, Eqs. (4)–(7) can be rewritten as

$$\begin{aligned}&\nabla p = 0,\\ &\partial_t e = L\Delta T,\\ &\partial_t\chi = -\partial_\chi J + \delta\Delta\chi\,.\end{aligned} \tag{15}$$

Now, by setting

$$E_{\text{pot},1} := T + 1\,, \qquad E_{\text{pot},2} := T\,, \tag{16}$$

such that $e = e_{\text{pot}} = T + \chi$, and convenient $\partial_\chi J$, one recovers the phase field equations

$$\partial_t(T+\chi) = L\Delta T, \qquad \partial_t \chi = -\partial_\chi J + \delta\Delta\chi\,,$$

where due to (15) a physical situation with constant pressure is considered. Apparently, due to (16), T jumps between two phases. So we see that our model is related to the phase field model, but does not account for temperature jumps across boundary layers.

7. NUMERICAL SIMULATIONS IN 2D

We use a flux vector splitting to approximately solve (4)–(7) for $\Omega = [-1,1] \times [0,1] \subset \mathbb{R}^2$. The following calculations resolve Ω with 1661 knots and 3200 triangles. The grid is not adapted during the computations. The calculation principally illustrate typical features of the presented system. The following images always render the non-conserved order parameter χ.

Ideal gas law for both phases
$G_1 = G_2\,,$ $\gamma_1 = \gamma_2 = 1.4,$ $c_{V,1} = c_{V,2} = 1,$ $Re = 1000,$ $Prandtl = 1,$
$\varepsilon = 1,$ $\delta = 10^{-4},$ $\mu = 1,$ $\nu = -2/3,$ $v_{xI} \equiv 0.4,$ $v_{yI} \equiv 0,$ $\rho_I \equiv 1,$
$\Delta t = 0.005,$ $\rho_0 \equiv 1,$ $v_{x0} \equiv 0.4,$ $v_{y0} \equiv 0,$ $e_0 \equiv 2.5,$ $(\rho\chi)_s \equiv 0,$ $T_s \equiv 2.5,$
$\chi_0(x,y) = 1$ for $(x,y) \in B_{0.2}(-0.5, 0.5),$ $\chi_0(x,y) = 0$ else.

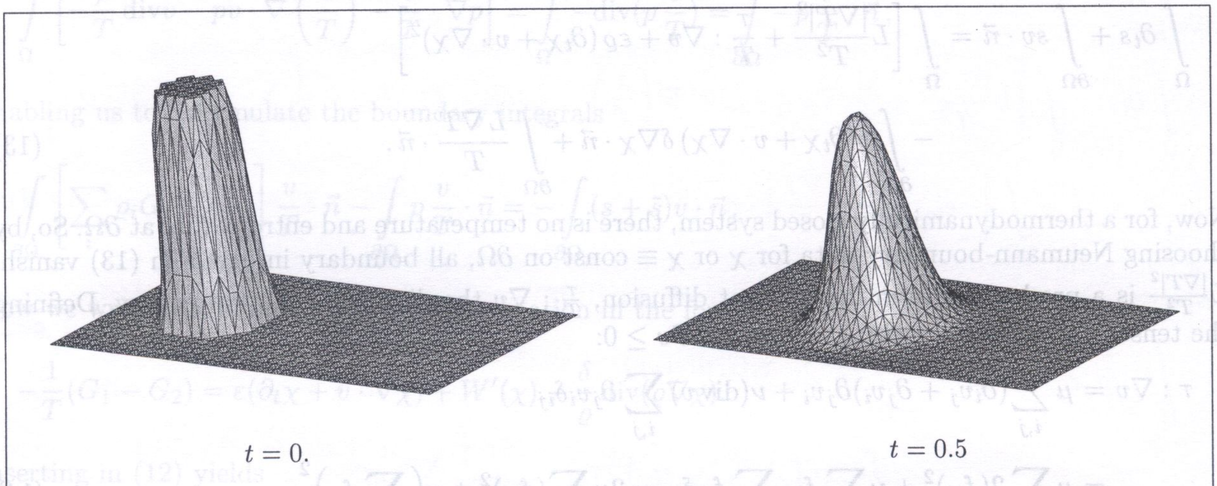

$t = 0.$ $t = 0.5$
$t = 1.0$ $t = 1.7$

Fig. 2. Decay and transport of a circular gas phase for $v = (0.2, 0)$

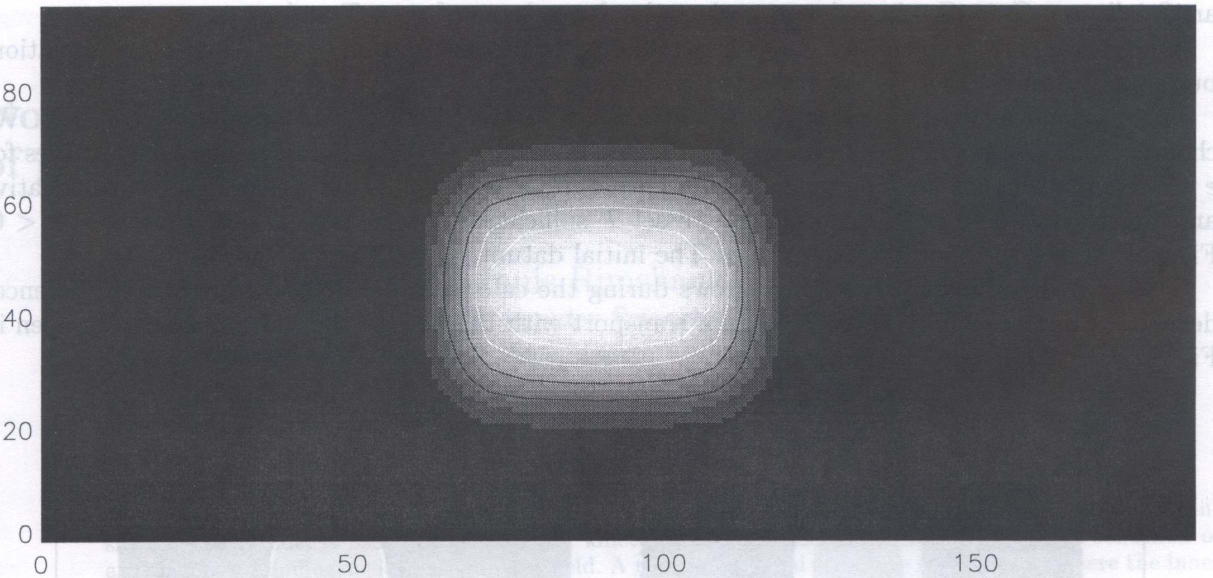


Fig. 3. Initial values for T (to Fig. 4)

Ideal gas law for both phases

$\gamma_1 = 1.4,$ $\gamma_2 = 1.00838,$ $c_{V,1} = 20.95,$ $c_{V,2} = 74.97,$ $Re = 1000,$ $Prandtl = \varepsilon = \mu = 1,$

$\nu = -2/3,$ $\delta = 10^{-4},$ $v_{xI} \equiv 1,$ $v_{yI} \equiv 0,$ $\Delta t = 0.001,$ $\rho_0 \equiv \rho_I \equiv 1,$

$v_{x0} \equiv 1,$ $v_{y0} \equiv 0,$ $\chi_0 \equiv 0.5,$ $(\rho\chi)_s \equiv 0.5,$ $T_s \equiv 2.53.$

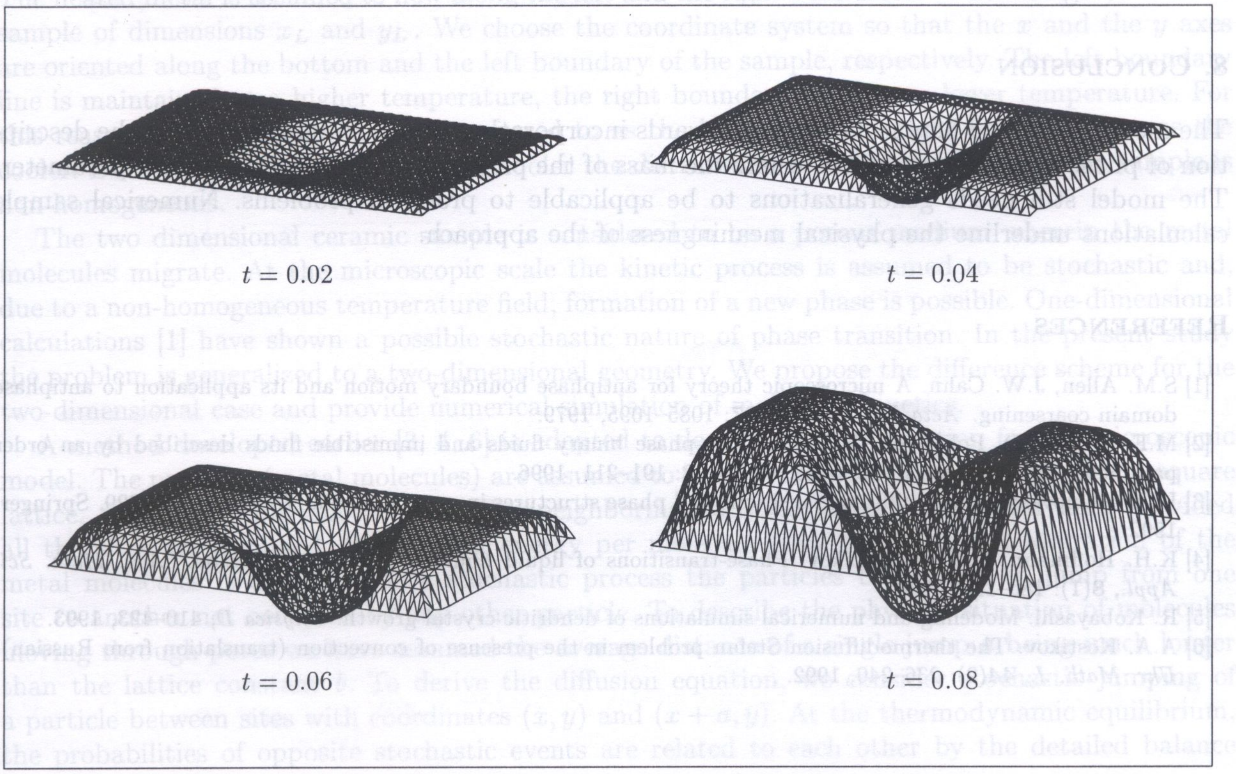


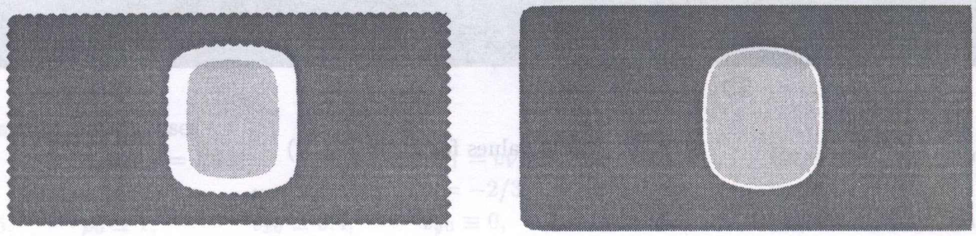
Fig. 4. Forming of two phases due to temperature effects and their convection

First we simulate a situation where $\rho \equiv 1$, $T \equiv 2.5$ and $v \equiv (0.2, 0)$ in $\Omega_T := \Omega \times (0, T)$. We artificially set $G_1 = G_2$, in order to neglect the dependence of χ on T and ρ.

One recovers the typical behaviour of a radially symmetric solution of the Allen–Cahn equation, but simultaneously there is the transport with the flow.

As a second example we simulate the creation of a gas phase due to temperature effects. We choose ideal gas laws for both phases. Hence, $\frac{G_1 - G_2}{T} = (c_{V,1} - c_{V,2})(1 - \ln T)$. The initial values for e are taken such that for a circular domain $\Omega_1 \subset\subset \Omega$, T is as large that $1 - \ln T$ becomes negative and therefore $\frac{G_1 - G_2}{T} > 0$. Accordingly, we set T sufficiently low in $\Omega \backslash \Omega_1$, such that $\frac{G_1 - G_2}{T} < 0$. Figure 4 shows the time behaviour of χ. The initial datum $\chi_0 \equiv 0.5$ is not shown.

Due to heat diffusion, Ω_1 slightly grows during the calculation and the temperature differences decrease. Simultaneously, there is again a transport with the flow to the right. This can be seen in Fig. 5.



$t = 0.02$ $t = 0.08$

Fig. 5. Diagram of the phases (to Fig. 4)

8. CONCLUSION

The model presented here is a first step towards incorporating transport mechanisms in the description of phase formation processes where the mass of the phases is a non-conserved order parameter. The model still needs generalizations to be applicable to practical problems. Numerical sample calculations underline the physical meaningness of the approach.

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