

A Generalization of the Navier-Stokes equations to Two-Phase-Flows

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Abstract. A modified Allen-Cahn equation is combined with the compressible Navier-Stokes system. We show that after a modification of the stress-tensor, for the resulting equations the second law of thermodynamics is valid. We give a physical motivation for this altered stress tensor and compare the new equations with the well known phase field approach. The model can be used to describe cavitation in a flowing liquid.

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1. Introduction

During the last 40 years, remarkable advances have been made to describe the behaviour of materials undergoing phase changes, see the well known works [1], [3] and [2]. Unfortunately, most approaches consider inert systems, only a few, like [4], [5], [6] and [7], incorporate convection. From the theoretical point of view as well as for a certain class of applications, it is desirable to overcome this restriction. In this article, a modified Allen-Cahn equation is combined with the Navier-Stokes system. The resulting model, due to some assumptions that generally need not be fulfilled, requires further generalization, 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 current. In a forthcoming paper an adapted numerical scheme and sample solutions will be presented to underline the physical importance of the model.

As a main result of this work, it is shown that, compared to the Navier-Stokes equations, the stress tensor contains an additional term $-\delta\rho T\nabla\chi\otimes\nabla\chi$.

2. Notations and Thermodynamic Relationships

Let $\Omega \subset \mathbb{R}^d$, $1 \leq d \leq 3$ be a bounded domain with Lipschitz boundary. For $0 < D \leq \infty$ let $\Omega_D := \Omega \times (0, D)$ and $\varrho : \Omega_D \rightarrow \mathbb{R}^+$ denote the (averaged) density of the fluid, $e : \Omega_D \rightarrow \mathbb{R}^+$ the internal energy, $v : \Omega_D \rightarrow \mathbb{R}^d$ the velocity field of the fluid. Governed by a phase parameter $\chi : \Omega_D \rightarrow [0, 1]$, 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

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

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 generically 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. For instance, we have

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

ϱ and χ are solutions of the system of partial differential equations (5) – (8) below and allow us to calculate the specific densities ϱ_1, ϱ_2 of the phases.

To make the definitions precise, consider the specific volume $V = \frac{1}{\varrho}$. Let V_i be the specific volume of phase i (phase i has mass 1 in V_i) and \tilde{V}_i be the volume phase i is actually occupying in V . Now we define

$$\begin{aligned} \psi_i &:= \frac{\tilde{V}_i}{V} && \text{volume fraction of phase } i \text{ in } V, \quad 0 \leq \psi_i \leq 1, \\ \varrho_i &:= \frac{\psi_i}{V_i} = \frac{\tilde{V}_i}{V_i} \frac{1}{V} && \text{specific density of phase } i, \quad 0 \leq \rho_i \leq \rho, \\ \chi_i &:= \frac{\varrho_i}{\varrho} = \frac{\tilde{V}_i}{V_i} && \text{density quotient} = \text{mass of phase } i \text{ in } V, \quad 0 \leq \chi_i \leq 1. \end{aligned}$$

Direct from the definition follows $\sum_i \varrho_i V_i = \sum_i \psi_i = 1$.

We synonymously use $\chi_1 = \chi$, $\chi_2 = 1 - \chi$. Let (for the moment) M_i denote the mass of phase i in V . If we assume $M_i V_i = \tilde{V}_i$, that is both phases shall be incompressible, then

$$\chi_i = \frac{\varrho_i}{\varrho} = \frac{M_i}{V} \frac{1}{\varrho} = M_i.$$

The specific densities ϱ_i are therefore obtained by

$$\varrho_1 = \varrho\chi, \quad \varrho_2 = \varrho(1 - \chi),$$

thereby explaining the third equation in (2).

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

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

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

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

Let $T : \Omega_D \rightarrow \mathbb{R}^+$ be the temperature and $p : \Omega_D \rightarrow \mathbb{R}^+$ the pressure of the fluid. Since $f/T = e_{\text{pot}}/T - s$ and $(\partial_T f)_V = -s$, we have

$$T \left[\partial_T \left(\frac{f}{T} \right) \right]_V = -\frac{e_{\text{pot}}}{T}.$$

Therefore, the mixing entropy is not present in e_{pot} , but with a factor $-T$ in the Helmholtz free energy f and the Gibbs energy g . This leads to the representation of e above and the definitions for the densities F and G by

$$F = \chi F_1 + (1 - \chi)F_2 + T\tilde{S}, \quad G = \chi G_1 + (1 - \chi)G_2 + T\tilde{S}. \quad (4)$$

3. Mathematical Formulation

Beside the definitions above, let $\varepsilon > 0$ be a scaling constant for the substantial derivative $d\chi := \partial_t \chi + v \cdot \nabla \chi$ of χ . For given velocity field v , let $R_I := \{x \in \partial\Omega \mid v(x) \cdot \vec{n}(x) < 0\}$ denote the inlet, $R_O := \{x \in \partial\Omega \mid v(x) \cdot \vec{n}(x) > 0\}$ the outlet of the domain Ω , where \vec{n} is the unit outer normal vector to $\partial\Omega$.

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

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

with viscosity coefficients ν, μ , where $\nu \geq -\frac{2}{3}\mu$ for $d = 3$ and $\nu \geq -\mu$ for $d = 2$, see (15). Notice that the correct form of the stress tensor and the restrictions on ν and μ are assumed here, but will be a consequence of the entropy estimate in section 5.

The thermodynamic driving force of the Allen-Cahn like 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 (5), momentum (6) and energy (7):

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

$$\partial_t \varrho = -\operatorname{div}(\varrho v), \quad (5)$$

$$\partial_t(\varrho v) = -\operatorname{div}(\varrho v \otimes v + \delta \varrho T \nabla \chi \otimes \nabla \chi) + \operatorname{div}(\tau) - \nabla p, \quad (6)$$

$$\partial_t e = \operatorname{div}(L \nabla T - (e - \Gamma)v), \quad (7)$$

$$\varepsilon \partial_t \chi = -\partial_\chi J + \frac{\delta}{\varrho} \operatorname{div}(\varrho \nabla \chi) - \varepsilon v \cdot \nabla \chi \quad (8)$$

in Ω with the initial values

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

and the boundary values

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

and

$$\varrho = \varrho_I \quad \text{on } R_I.$$

As a consequence of a parabolic maximum principle for (8), the logarithmic form of W in (3) guarantees $0 < \chi < 1$ in Ω_∞ , if the same is true for the initial data 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 identity explains how ρ and T determine over $T^{-1}(G_1 - G_2)(\rho, T)$ the preferred phase (gas or liquid).

4. Assumptions

We list up 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} , equation (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

$$V = \chi V_1 + (1 - \chi) V_2. \quad (9)$$

- 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).
- $p_1 = p_2$: Two neighbouring phases shall possess the same pressure on the boundary (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 (5) – (8), 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

$$ds_i = d(\varrho_i S_i) = S_i d\varrho_i + \varrho_i dS_i.$$

Because of the Gibbs equation $dS_i = \frac{1}{T} dE_i + \frac{p}{T} dV_i$ it follows:

$$\begin{aligned} ds_i &= S_i d\varrho_i + \frac{\varrho_i}{T} dE_i + \frac{\varrho_i p}{T} dV_i \\ &= \left(S_i - \frac{pV_i}{T} \right) d\varrho_i + \frac{\varrho_i}{T} dE_i + \frac{p}{T} d(\varrho_i V_i) \\ &= \left(S_i - \frac{pV_i}{T} - \frac{E_i}{T} \right) d\varrho_i + \frac{1}{T} d(\varrho_i E_i) + \frac{p}{T} d\psi_i \\ &= -\frac{1}{T} G_i d\varrho_i + \frac{1}{T} de_i + \frac{p}{T} d\psi_i. \end{aligned}$$

And after summing up over all phases:

$$ds + d\tilde{s} = \sum_i ds_i = -\frac{1}{T} \sum_i G_i d\varrho_i + \frac{1}{T} de + \frac{p}{T} \underbrace{d\left(\sum_i \psi_i\right)}_{=0}.$$

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

$$ds + d\tilde{s} = -\frac{1}{T} \sum_i \chi_i G_i d\varrho + \frac{1}{T} de - \frac{\varrho}{T} (G_1 - G_2) d\chi. \quad (10)$$

Now we assume that the internal energy available for thermodynamic processes does not depend on v . For $v = 0$ the differential de in (10) is de_{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:

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

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

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

exploiting the conservation equations (5), (6) and (7) yields

$$\begin{aligned} \int_{\Omega} \frac{1}{T} \partial_t e_{\text{pot}} &= \int_{\Omega} \left[-\frac{v}{T} \cdot \partial_t(\rho v) + \frac{|v|^2}{2T} \partial_t \rho + \frac{1}{T} \operatorname{div}(L \nabla T - (e - \Gamma)v) \right] \\ &= \int_{\Omega} \left[-\frac{v}{T} \cdot \operatorname{div}(-\rho v \otimes v + \Gamma) - \frac{|v|^2}{2T} \operatorname{div}(\rho v) \right. \\ &\quad \left. + \frac{1}{T} \operatorname{div}(L \nabla T - (e_{\text{pot}} + \frac{\rho}{2} |v|^2 - \Gamma)v) \right]. \end{aligned}$$

After partial integration, this means

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

We get

$$\begin{aligned} \int_{\Omega} \partial_t s &= \int_{\Omega} \left[L \frac{|\nabla T|^2}{T^2} + \frac{\Gamma}{T} : \nabla v + e_{\text{pot}} v \cdot \nabla \left(\frac{1}{T} \right) - \frac{\rho}{T} (G_1 - G_2) \partial_t \chi \right. \\ &\quad \left. - \frac{1}{T} \sum_i \chi_i G_i \partial_t \rho - \partial_t \tilde{s} \right] + \int_{\partial \Omega} \left[-e_{\text{pot}} \frac{v}{T} + L \frac{\nabla T}{T} \right] \cdot \vec{n}. \end{aligned} \quad (11)$$

Now we transform the term $-\frac{1}{T} \sum_i \chi_i G_i \partial_t \rho$ in (11).

$$\begin{aligned} \int_{\Omega} -\frac{1}{T} \sum_i \chi_i G_i \partial_t \rho &= \int_{\Omega} \frac{1}{T} \sum_i \chi_i G_i \operatorname{div}(\rho v) \\ &= \int_{\Omega} -\nabla \left(\frac{1}{T} \sum_i \chi_i G_i \right) \cdot (\rho v) + \int_{\partial \Omega} \frac{1}{T} \sum_i \rho_i G_i v \cdot \vec{n} \\ &= \int_{\Omega} \left[-\sum_i \rho_i G_i v \cdot \nabla \left(\frac{1}{T} \right) - \frac{\rho}{T} \sum_i G_i \nabla \chi_i \cdot v - \frac{v}{T} \cdot \sum_i \rho_i dG_i \right] \\ &\quad + \int_{\partial \Omega} \frac{1}{T} \sum_i \rho_i G_i v \cdot \vec{n}. \end{aligned} \quad (12)$$

We simplify this further. The first and third integrand in (12) are

$$\begin{aligned} \int_{\Omega} -\sum_i \rho_i G_i v \cdot \nabla \left(\frac{1}{T} \right) &= \int_{\Omega} \left[-e_{\text{pot}} v \cdot \nabla \left(\frac{1}{T} \right) - \frac{v}{T} (s + \tilde{s}) \cdot \nabla T - p v \cdot \nabla \left(\frac{1}{T} \right) \right], \\ \int_{\Omega} -\frac{v}{T} \cdot \sum_i \rho_i dG_i &= \int_{\Omega} -\frac{v}{T} \cdot (\nabla p - (s + \tilde{s}) \nabla T). \end{aligned}$$

The last equality is a consequence of $dG_i = -S_i dT + V_i dp$ and $\sum_i \varrho_i V_i = 1$. Therefore

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

By inserting this in (11), we obtain

$$\begin{aligned} \int_{\Omega} \partial_t s &= \int_{\Omega} \left[L \frac{|\nabla T|^2}{T^2} + \frac{\tau}{T} : \nabla v - p \operatorname{div} v - p v \cdot \nabla \left(\frac{1}{T} \right) - \frac{v}{T} \cdot \nabla p - \partial_t \tilde{s} \right] \\ &\quad - \int_{\Omega} \delta \varrho \nabla \chi \otimes \nabla \chi : \nabla v - \int_{\Omega} \frac{\varrho}{T} (G_1 - G_2) (v \cdot \nabla \chi + \partial_t \chi) \\ &\quad + \int_{\partial\Omega} \left[\sum_i \varrho_i G_i - e_{\text{pot}} \right] \frac{v}{T} \cdot \vec{n} + \int_{\partial\Omega} \frac{L \nabla T}{T} \cdot \vec{n}. \end{aligned} \quad (13)$$

In (13) we remark at once, that

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

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

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

Inserting in (13) yields:

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

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

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

and for the transport term after partial integration

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

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

Thus we get

$$\begin{aligned} \int_{\Omega} \partial_t s &= \int_{\Omega} L \frac{|\nabla T|^2}{T^2} + \frac{\tau}{T} : \nabla v + \varepsilon \varrho (\partial_t \chi + v \cdot \nabla \chi)^2 + \nabla \tilde{s} \cdot v - \tilde{S} \partial_t \varrho - \tilde{S} \nabla \varrho \cdot v \\ &\quad - \int_{\partial \Omega} \tilde{s} v \cdot \vec{n} - \int_{\partial \Omega} s v \cdot \vec{n} + \int_{\partial \Omega} L \frac{\nabla T}{T} \cdot \vec{n} - \int_{\partial \Omega} \delta \varrho (\partial_t \chi + v \cdot \nabla \chi) \nabla \chi \cdot \vec{n}. \end{aligned}$$

Finally we use

$$\begin{aligned} \int_{\partial \Omega} -\tilde{s} v \cdot \vec{n} &= \int_{\Omega} -\operatorname{div}(\tilde{s} v) = \int_{\Omega} -v \cdot \nabla \tilde{s} - \tilde{s} \operatorname{div} v, \\ \int_{\Omega} [-\tilde{S} \partial_t \varrho - \tilde{s} \operatorname{div} v - \tilde{S} \nabla \varrho \cdot v] &= 0, \end{aligned}$$

to get the result:

$$\begin{aligned} \int_{\Omega} \partial_t s + \int_{\partial \Omega} s v \cdot \vec{n} &= \int_{\Omega} \left[L \frac{|\nabla T|^2}{T^2} + \frac{\tau}{T} : \nabla v + \varepsilon \varrho (\partial_t \chi + v \cdot \nabla \chi)^2 \right] \\ &\quad - \int_{\partial \Omega} \varrho (\partial_t \chi + v \cdot \nabla \chi) \delta \nabla \chi \cdot \vec{n} + \int_{\partial \Omega} \frac{L \nabla T}{T} \cdot \vec{n}. \end{aligned} \quad (14)$$

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 $\chi \equiv \text{const}$ on $\partial \Omega$, all boundary integrals in (14) 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 $\tau : \nabla v \geq 0$:

$$\begin{aligned} \tau : \nabla v &= \mu \sum_{i,j} (\partial_i v_j + \partial_j v_i) \partial_j v_i + \nu (\operatorname{div} v) \sum_{i,j} \partial_j v_i \delta_{ij} \\ &= \mu \sum_{i,j} 2(f_{ij})^2 + \nu \sum_k f_{kk} \sum_{i,j} f_{ij} \delta_{ij} \\ &= 2\mu \sum_{i,j} (f_{ij})^2 + \nu (\sum_i f_{ii})^2. \end{aligned} \quad (15)$$

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. Interpretation of the New Stress Tensor

As we have seen above, in comparison to the Navier-Stokes equations, the tensor Γ has been changed in our model. Beside the motivation by the second law of thermodynamics,

there exists another physical reason for this modification. To see this, we look at the Navier-Stokes equations and remember the identity

$$p = \frac{d}{dV}[-F_{\text{NST}}(V, T)]. \quad (16)$$

So $p\delta_{ij}$ is the part of the stress tensor that responds to changes of volume and that we therefore shall call the elastic component of Γ . Now we split Γ and set

$$\Gamma = \Gamma_{\text{el}} + \Gamma_{\text{inel}}, \quad \Gamma_{\text{el}} = -p \delta_{ij}. \quad (17)$$

For our equations consider the functional (the specific density fulfils $V = \varrho^{-1}$)

$$\mathcal{F}(V, T, \chi) := \int_{\Omega} \varrho(x) F\left(\frac{1}{\varrho(x)}, T(x), \chi(x)\right) + \varrho(x) T(x) \frac{\delta}{2} |\nabla \chi(x)|^2 d\mathcal{L}^n(x). \quad (18)$$

Let $\Phi : \Omega_0 \rightarrow \Omega$ be the transformation from Lagrange- to Euler-coordinates, ϱ_0 be the density in Ω_0 . For a C^1 -vectorfield ξ , let $\psi : \mathbb{R}^d \times [0, 1] \rightarrow \mathbb{R}^d$ be a deformation in the direction of ξ , that is $\psi(x, 0) = x$ and $\partial_s \psi = \xi \circ \psi$, $0 \leq s \leq 1$. To explain the method we start with the second term in (18), map it to Ω_0 and rewrite it in the form

$$\mathcal{F}_2 := \int_{\Omega_0} \left[\tilde{\varrho}_0 \tilde{T}_0 \frac{\delta}{2} |\nabla \tilde{\chi}|^2 \right] \circ \tilde{\Phi},$$

where $\tilde{\chi} = \chi \circ \psi^{-1}$, $\tilde{\varrho}_0 = \varrho_0 \circ \psi^{-1}$, $\tilde{T}_0 = T_0 \circ \psi^{-1}$ and $\tilde{\Phi} = \psi \circ \Phi$. Because of $\partial_j \tilde{\chi} = \sum_{i=1}^d (\partial_i \chi) \circ \psi^{-1} \partial_j (\psi^{-1})_i$, we have

$$\begin{aligned} \mathcal{F}_2 &= \int_{\Omega_0} \left[\tilde{\varrho}_0 \tilde{T}_0 \frac{\delta}{2} \sum_{i,j,k} \partial_i \chi \circ \psi^{-1} \partial_j (\psi^{-1})_i \partial_k \chi \circ \psi^{-1} \partial_j (\psi^{-1})_k \right] \circ \tilde{\Phi} \\ &= \int_{\Omega_0} \left[\varrho_0 T_0 \frac{\delta}{2} \sum_{i,j,k} \partial_i \chi \partial_j (\psi^{-1})_i \circ \psi \partial_j (\psi^{-1})_k \circ \psi \partial_k \chi \right] \circ \Phi. \end{aligned}$$

From this result, as an application of the product rule, we obtain

$$\begin{aligned} \partial_s \mathcal{F}_2 \Big|_{s=0} &= \int_{\Omega_0} \left\{ \varrho_0 T_0 \frac{\delta}{2} \sum_{i,j,k} \partial_i \chi \partial_k \chi \left[\partial_s (\partial_j (\psi^{-1})_i \circ \psi) \partial_j (\psi^{-1})_k \circ \psi \right. \right. \\ &\quad \left. \left. + \partial_j (\psi^{-1})_i \circ \psi \partial_s (\partial_j (\psi^{-1})_k \circ \psi) \right] \right\} \circ \Phi. \end{aligned}$$

A short calculation gives $\partial_s [\partial_j (\psi^{-1})_i \circ \psi] \partial_j (\psi^{-1})_k \circ \psi = -\partial_i \xi_k$ and we get:

$$\begin{aligned} \partial_s \mathcal{F}_2 \Big|_{s=0} &= - \int_{\Omega_0} \left[\varrho_0 T_0 \frac{\delta}{2} \sum_{i,k} \partial_i \chi (\partial_i \xi_k + \partial_k \xi_i) \right] \circ \Phi \\ &= - \int_{\Omega_0} \varrho_0 T_0 \delta \nabla \chi \otimes \nabla \chi : \nabla \xi \circ \Phi. \end{aligned}$$

In the same manner, the first part of (18) is treated. Because of (16) and (17) it follows ($\text{div} \xi$ comes from $\partial_s \det(D\psi)$):

$$\partial_s \mathcal{F}_1 \Big|_{s=0} = - \int_{\Omega_0} \varrho_0 p \text{div} \xi \circ \Phi = \int_{\Omega_0} \varrho_0 \Gamma_{\text{el}} : \nabla \xi \circ \Phi.$$

Combining the results, we obtain ($\text{Id}_{ij} = \delta_{ij}$)

$$\partial_s \mathcal{F} \Big|_{s=0} = - \int_{\Omega_0} \varrho_0 [p \text{Id} + \delta T_0 \nabla \chi \otimes \nabla \chi] : \nabla \xi \circ \Phi.$$

So we understand the change of the stress tensor as a consequence of subtracting $\frac{\delta}{2} |\nabla \chi|^2$ from the entropy density S .

7. Comparison with the Phase Field equation

For $v \equiv 0$, the entropy estimate is fulfilled 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 $L = \text{const}$, equations (5) – (8) can be rewritten as

$$\begin{aligned} \nabla p &= 0, \\ \partial_t e &= L\Delta T, \\ \partial_t \chi &= -\partial_\chi J + \delta\Delta\chi. \end{aligned} \tag{19}$$

Now, by setting

$$E_{\text{pot},1} := T + 1, \quad E_{\text{pot},2} := T, \tag{20}$$

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

$$\begin{aligned} \partial_t(T + \chi) &= L\Delta T, \\ \partial_t \chi &= -\partial_\chi J + \delta\Delta\chi, \end{aligned}$$

where due to (19) a physical situation with constant pressure is considered. Apparently, due to (20), 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.

8. Conclusion

The model presented here is a first step to incorporate transport mechanisms in the description of phase formation processes where the mass of the phases is no order parameter. It still needs generalizations to be applicable to practical problems. The approach was made as general as possible to simplify further improvements, this is why the system is compressible while single phases are regarded as incompressible.

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