A GENERALIZATION OF THE NAVIER-STOKES EQUATIONS TO TWO-PHASE FLOWS

Thomas Blesgen

Fakultät für Mathematik u. Inf., Universität Leipzig, Augustusplatz 10/11, D-04109 Leipzig, Germany

<u>Summary</u> 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.

INTRODUCTION

In the present text, a modified Allen-Cahn equation¹, 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 current. For related works we refer to a combination of the Cahn-Hilliard model with the Navier-Stokes equations², the general variational approach of the energy³, and to the models^{4,5}.

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 $\varrho : \Omega_D \to \mathbb{R}^+$ 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

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

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

 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

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

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

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

from S and set $\tilde{s} := \rho \tilde{S}$. 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

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

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 , $T : \Omega_D \to \mathbb{R}^+$ 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 and Ω are assumed not to depend on time t.

We modify the stress tensor and set $(\delta_{ij}$ be the Kronecker delta)

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

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 $-\delta\rho T\partial_i\chi\partial_j\chi$ is a consequence of adding $\frac{\delta\rho}{2} |\nabla\chi|^2$ to the system entropy.

The thermodynamic 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, χ_r) and ϱ_I find the solution $U = (\varrho, \varrho v, e, \chi)^t$ of

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

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

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

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

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

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

and

$$\varrho = \varrho_I \quad on \ R_I.$$

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 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).

The above approach has some simplifications, e.g. that both phases move with the same velocity vector, that no chemical reactions take place, that the temperature of two neighbouring phases is the same, that there is no buoyancy, and that no heat is generated by shearing of boundary layers.

One can show that the entropy of the system obeys the formula

$$\int_{\Omega} \partial_t s + \int_{\partial\Omega} sv \cdot \vec{n} = \int_{\Omega} \left[L \frac{|\nabla T|^2}{T^2} + \frac{\tau}{T} : \nabla v + \varepsilon \rho \left(\partial_t \chi + v \cdot \nabla \chi \right)^2 \right] \\ - \int_{\partial\Omega} \rho (\partial_t \chi + v \cdot \nabla \chi) \, \delta \nabla \chi \cdot \vec{n} + \int_{\partial\Omega} \frac{L \, \nabla T}{T} \cdot \vec{n}.$$
(8)

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 (8) vanish. $L\frac{|\nabla T|^2}{T^2}$ is a production term due to heat diffusion, $\frac{\tau}{T}$: ∇v is the dissipated motion energy that is positive for $\nu \geq -\frac{2}{3}\mu$ (d = 3) or for $\nu \geq -\mu$ (d = 2), as can be shown by principal axis transformation. Hence the second law of thermodynamics is valid. Notice that $\int \varepsilon \varrho \ (\partial_t \chi + v \cdot \nabla \chi)^2$ corresponds to the Lyapunov functional of the unmodified Allen-Cahn equation.

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 conserved order parameter. It still needs generalizations to be applicable to practical problems. Numerical sample calculations underline the physical meaningness of the approach.

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