Models of phase segregation of Allen-Cahn type without and with temperature effects

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Abstract

We review two new models of phase segregation [3, 4], based on two balance equations for microforces and microenergy and on nonstandard thermodynamically compatible constitutive choices. The first model is akin to the well-known Allen-Cahn (for others, Ginzburg-Landau) equation for an order parameter, whose space-time evolution may lead to isothermal and diffusionless phase segregation by atomic rearrangement; the second model is a variation of the first that accounts for temperature effects. In both cases, we deal with a system of equations: for the order parameter and the chemical potential, in the first; for the order parameter, the chemical potential, and the temperature, in the second.

The study of these systems has been made the subject of an ongoing joint research program with G. Gilardi and J. Sprekels, whom we thank warmly for a pleasant and fruitful collaboration. Here we present a quick derivation of our models and delineate the peculiar features of their mathematical analysis.

1 Introduction

This note is an abridged exposition of the results contained in two articles, [3] and [4], where certain nonlinear evolution systems of the Allen-Cahn (A-C) type are studied, intended to provide a mathematical description of the phenomenology of diffusionless phase segregation by atom rearrangement in crystalline materials.

In the next section, we discuss the physics underlying A-C type models and their proposed generalizations, beginning with those isothermal, Fried and Gurtin's [7, 8] and the one analyzed in [3], and ending by the variant of the latter proposed in [4], where thermal effects are taken into account. In Section 3, we formulate the corresponding mathematical problems carefully, we delineate the solution strategies, and we list with some comments the main mathematical results, referring the reader to [3]and [4]for details.

The diffusionless isothermal model in [3]consists of a system of two nonlinear differential equations, the one ordinary the other partial, interpreted as balances of microforces and of microenergy. A well-posedness result is obtained, and the long-time behavior of solutions characterized. Crucial to success are the use of the maximal solution to the ODE and of an a priori uniform bound in the space-time domain for the time derivative of the order parameter.

As to the temperature-dependent phase segregation model in [4], a local-in-time existence theorem is proved for a fairly general initial-boundary value problem. The results obtained for the isothermal case serve as a starting point for such a local existence proof, which relies on a fixed-point argument involving the Tychonoff-Schauder theorem.

2 Phase segregation models of A-C type

The Allen-Cahn equation:

$$\kappa\,\partial_t\rho - \Delta\rho + f'(\rho) = 0 \tag{2.1}$$

is meant to describe evolutionary processes in a two-phase material body, including *phase segregation*. In (2.1),

- $\rho = \rho(x,t) \in [0,1]$ denotes an *order-parameter* field interpreted as the scaled volumetric density of one of the two phases;
- $\kappa > 0$ is a *mobility* coefficient;
- f' denotes the derivative of a double-well potential confined in $(0,1)$ and singular at the endpoints.

2.1 Fried and Gurtin's derivation of the A-C equation

The derivation of (2.1) proposed in [7] and [8] (see also [6] and [9] for similar derivations and discussions of related models) is based on a *balance of contact and distance microforces*:

$$\operatorname{div}\boldsymbol{\xi} + \pi + \gamma = 0 \tag{2.2}$$

and on a 'purely mechanical' dissipation inequality restricting the free-energy growth:

$$\partial_t\psi \le w, \quad w := -\pi\,\partial_t\rho + \boldsymbol{\xi}\cdot\nabla(\partial_t\rho), \tag{2.3}$$

where the distance microforce is split in an internal part π and an external part γ, the contact microforce is specified by the microscopic stress vector $\boldsymbol{\xi}$, and w is the internal microworking. The following constitutive choices:

$$\pi = \widehat{\pi}(\rho, \nabla\rho, \partial_t\rho), \;\; \boldsymbol{\xi} = \widehat{\boldsymbol{\xi}}(\rho, \nabla\rho, \partial_t\rho), \text{ and } \psi = \widehat{\psi}(\rho, \nabla\rho) = f(\rho) + \frac{1}{2}|\nabla\rho|^2, \quad (2.4)$$

turn out to be compatible with the dissipation inequality (2.3) in the sense of a classical paper by Coleman-Noll [1] if:

$$\widehat{\pi}(\rho, \nabla\rho, \partial_t\rho) = -f'(\rho) - \widehat{\kappa}(\rho, \nabla\rho, \partial_t\rho)\partial_t\rho \quad \text{and} \quad \widehat{\boldsymbol{\xi}}(\rho, \nabla\rho, \partial_t\rho) = \nabla\rho.$$

Under the further assumptions that $\widehat{\kappa}(\rho, \nabla\rho, \partial_t\rho) = \kappa$, a positive constant, and that $\gamma \equiv 0$, the microforce balance (2.2) yields the standard Allen-Cahn equation (2.1).

2.2 The A-C system in [3]

In [3], on adopting an approach put forward by one of us in [10], we deal with a substantially modified version of Fried and Gurtin's derivation, in which the dissipation inequality (2.3) is dropped and the microforce balance (2.2) is coupled with the *microenergy balance*:

$$\partial_t\varepsilon = e + w, \quad e := -\operatorname{div}\bar{\boldsymbol{h}} + \bar{\sigma}, \tag{2.5}$$

and with the *microentropy imbalance*:

$$\partial_t\eta \geq -\operatorname{div}\boldsymbol{h} + \sigma, \quad \boldsymbol{h} := \mu\bar{\boldsymbol{h}}, \quad \sigma := \mu\,\bar{\sigma} \tag{2.6}$$

(here $\bar{\sigma}$ is the external source of energy per unit volume). With a view toward modeling phase-segregation, we postulate that

- the microentropy inflow $(\boldsymbol{h}, \sigma)$ be proportional to the microenergy inflow $(\bar{\boldsymbol{h}}, \bar{\sigma})$ through the chemical potential μ, a positive field;

consistently, we define the free energy to be:

$$\boxed{\psi := \varepsilon - \mu^{-1}\eta,} \tag{2.7}$$

with

- the chemical potential playing the same role as the *coldness* ϑ^{-1} in the deduction of the heat equation.

Combination of (2.5)–(2.7) leads to the inequality:

$$\partial_t\psi \leq -\eta\,\partial_t(\mu^{-1}) + \mu^{-1}\bar{\boldsymbol{h}} \cdot \nabla\mu - \pi\,\partial_t\rho + \boldsymbol{\xi} \cdot \nabla(\partial_t\rho), \tag{2.8}$$

which replaces (2.3) as a filter for thermodynamically incompatible constitutive choices. We assume that, in addition to the independent variables ρ, $\nabla\rho$ and $\partial_t\rho$, the mappings delivering π, ξ, η, and $\bar{\boldsymbol{h}}$ depend also on μ; moreover, we choose:

$$\psi = \widehat{\psi}(\rho, \nabla\rho, \mu) = -\mu\,\rho + f(\rho) + \frac{1}{2}|\nabla\rho|^2. \tag{2.9}$$

We remark that it makes sense to impose the C-N compatibility of these constitutive assumptions with (2.8), because,

- given that we have two independent controls γ and $\bar{\sigma}$ at our disposal, we are in a position to guarantee the free linear continuation in time of any given process $t \mapsto (\rho, \mu)(t)$ at any fixed space point.

We find out that:

$$\widehat{\pi}(\rho, \nabla\rho, \partial_t\rho, \mu) = \mu - f'(\rho) - \widehat{\kappa}(\rho, \nabla\rho, \partial_t\rho)\partial_t\rho, \quad \widehat{\boldsymbol{\xi}}(\rho, \nabla\rho, \partial_t\rho, \mu) = \nabla\rho,$$
$$\widehat{\eta}(\rho, \nabla\rho, \partial_t\rho, \mu) = -\mu^2\rho, \quad \widehat{\bar{\boldsymbol{h}}}(\rho, \nabla\rho, \partial_t\rho, \mu) \equiv \mathbf{0}. \tag{2.10}$$

The last of these findings implies a crucial mathematical simplification: the microenergy balance – generally, a PDE – becomes an ODE. Under the additional assumptions that the mobility is a positive constant and the external distance microforce is null, the microforce balance (2.2) becomes:

$$\kappa\, \partial_t\rho - \Delta\rho + f'(\rho) = \mu, \tag{2.11}$$

while microenergy balance reads:

$$\partial_t(-\mu^2\rho) = \mu \left(\kappa\, (\partial_t\rho)^2 + \bar{\sigma}\right), \tag{2.12}$$

where $\bar{\sigma} = \bar{\sigma}(x, t)$ is a given source term.

In [3], we consider the nonlinear evolution system consisting of the parabolic PDE (2.11) and the first-order-in time ODE (2.12), supplemented by the homogeneous Neumann boundary condition:

$$\partial_n\rho = 0 \quad \text{on the body's boundary} \tag{2.13}$$

(here ∂_n denotes the outward normal derivative) and by the initial conditions:

$$\rho|_{t=0} = \rho_0 \quad \text{bounded away from } 0\,, \quad \mu|_{t=0} = \mu_0 \geq 0\,. \tag{2.14}$$

This initial/boundary-value problem is to be solved for the order-parameter field ρ and for the chemical potential field μ.

Note that the microentropy field $\eta = -\mu^2\rho$ cannot exceed the level 0 from below; thus, the prescribed initial field:

$$\eta|_{t=0} = \eta_0\,, \ \text{ with } \eta_0 = -\mu_0^2\rho_0, \tag{2.15}$$

is nonpositive-valued. Note also that taking $\mu \equiv 0$ in (2.11) yields the standard Allen-Cahn equation.

2.3 Accounting for thermal effects in the manner of [4]

As is well-known (see e.g. [10]), the classic heat equation can be arrived at by coupling the *energy balance*

$$\partial_t\varepsilon = -\operatorname{div} \bar{\boldsymbol{h}} \tag{2.16}$$

and the *entropy imbalance*

$$\partial_t\eta \geq -\operatorname{div} \boldsymbol{h}, \quad \boldsymbol{h} = \vartheta^{-1}\bar{\boldsymbol{h}}, \tag{2.17}$$

with the following *constitutive prescriptions*:

$$\psi = \varepsilon - \vartheta\eta, \quad \psi = \bar{\psi}(\vartheta) = -c_v\vartheta(\ln\vartheta - 1), \tag{2.18}$$

where the absolute temperature field ϑ is positive-valued and the specific heat c_v is a positive constant. To account for

- thermal effects on the phenomenology of phase segregation by atomic rearrangement,

we compare the formats (2.16)–(2.18) and (2.5)–(2.9). A way to match them, *in the light of the relationships of temperature and chemical potential to entropy provided by statistical mechanics*, is to assume that:

(i) the microenergy balance keeps the form (2.5);

(ii) the energy and entropy influxes and the free energy have the mutually consistent forms:

$$\boldsymbol{h} = (\vartheta^{-1}\mu)\bar{\boldsymbol{h}}, \quad \boxed{\psi = \varepsilon - (\vartheta\mu^{-1})\eta,} \quad \psi = \widehat{\psi}(\rho, \nabla\rho, \mu, \vartheta). \tag{2.19}$$

The second assumption is the main element of novelty. With that measure, the dissipation inequality replacing for (2.8) is:

$$\partial_t\psi \leq -\eta\,\partial_t(\vartheta\mu^{-1}) + (\vartheta\mu^{-1})\bar{\boldsymbol{h}}\cdot\nabla(\vartheta^{-1}\mu) - \pi\,\partial_t\rho + \boldsymbol{\xi}\cdot\nabla(\partial_t\rho), \tag{2.20}$$

where, in addition to $(2.19)_3$ for the free energy,

- the distance force, the microscopic stress, the entropy, and the microenergy influx, are assumed to depend on the list of variables $\{\rho, \nabla\rho, \mu, \vartheta; \partial_t\rho, \nabla\vartheta\}$.

We point out that the last two variables in the list give way to incorporate in the model the dissipation mechanisms relative to, respectively, atom-rearrangement without diffusion and heat conduction. Indeed, it is clear that postulating (2.19) covers both special cases when either temperature or chemical potential are space-time constants.

When C-N compatibility of the current constitutive prescriptions with (2.20) is sought, a delicate modeling issue emerges, because

- this time, we cannot count on as many controls as needed to guarantee the free local continuation in time of any given process $t \mapsto (\rho, \mu, \vartheta)(t)$ at any fixed point in space.

We do get the counterparts of the first, second, and fourth of (2.10), namely,

$$\widehat{\pi} = -\partial_\rho\psi - \kappa\partial_t\rho, \quad \widehat{\boldsymbol{\xi}} = \partial_{\nabla\rho}\psi = \nabla\rho, \quad \widehat{\bar{\boldsymbol{h}}} \equiv \boldsymbol{0}; \tag{2.21}$$

moreover, we are left with the following residual inequality:

$$(\partial_\mu\psi - \vartheta\mu^{-2}\eta)\partial_t\mu + (\partial_\vartheta\psi + \mu^{-1}\eta)\partial_t\vartheta \leq 0. \tag{2.22}$$

Now, were it possible to choose both $\partial_t \mu$ and $\partial_t \vartheta$ arbitrarily, (2.22) would yield the double equality:

$$\eta = \vartheta^{-1}\mu^2 \partial_\mu \psi = -\mu\, \partial_\vartheta \psi. \tag{2.23}$$

This observation motivates our decision to complement the balances of microforce and energy with another field equation, namely,

- the *thermodynamic consistency condition*

$$\boxed{\mu\, \partial_\mu \psi + \vartheta\, \partial_\vartheta \psi = 0.} \tag{2.24}$$

With this, (2.22) can be written as

$$\vartheta(\partial_\mu \psi - \vartheta \mu^{-2}\eta)\partial_t(\vartheta^{-1}\mu) \leq 0, \tag{2.25}$$

and (2.23) follows, provided the time rate of $(\vartheta^{-1}\mu)$ can be chosen arbitrarily. Finally, we specify the free energy density $(2.19)_3$ as follows (cf. (2.9)):

$$\psi = \widehat{\psi}(\rho, \nabla\rho, \mu, \vartheta) = -\mu\, \rho + \varphi(\rho, \vartheta) + \frac{1}{2}|\nabla\rho|^2, \tag{2.26}$$

with

$$\varphi(\rho, \vartheta) = f(\rho) - c_v \vartheta(\ln \vartheta - 1) - c_0\, \rho(\vartheta - \vartheta_c) \quad \text{and} \quad c_0 > 0, \tag{2.27}$$

where the double-well potential and the purely caloric free energy are supplemented by a coupling term that is effective when and where the temperature differs from the characteristic temperature ϑ_c.

With the constitutive choice (2.27), the consistency condition (2.24) reduces to:

$$\mu\rho + c_0 \vartheta \rho + c_v \vartheta \ln \vartheta = 0\,; \tag{2.28}$$

moreover, the balance of microforces (2.2) becomes:

$$\kappa\, \partial_t \rho - \Delta\rho + f'(\rho) - c_0 \vartheta = \mu \tag{2.29}$$

where, with slight abuse of notation, we have written $f'(\rho)$ for $(f'(\rho) + c_0 \vartheta_c)$. As to the microenergy balance (2.5), we find:

$$\partial_t(-\vartheta^{-1}\mu^2 \rho) = \vartheta^{-1}\mu(\bar{\sigma} + \kappa(\partial_t \rho)^2), \tag{2.30}$$

an equation to be compared with (2.12). These field equations are complemented by the same boundary and the initial conditions as in, respectively, (2.13) and (2.14), with ϑ_0 recovered from (2.28) in terms of convenient assignments of μ_0 and ρ_0.

In conclusion, the mathematical model assembled in [4] regards

- processes of phase segregation by atomic re-arrangement in the presence of thermal effects as solutions of the system of equations (2.28), (2.29) and (2.30).

Needless to say, the relative initial-boundary value problem is more difficult to deal with than its isothermal version successfully tackled in [3], let alone the standard A-C equation (2.1).

3 Processes of A-C type, isothermal or not

In this section, we collect the well-posedness results we proved for the models proposed in [3] and [4] in the order, insisting on key ideas and flow of proofs, rather than on technicalities.

3.1 How to tackle the isothermal problem

3.1.1 Flow chart

For the mathematical investigation of *well-posedness of system* (2.11)–(2.14), the strategy exploited in [3] is

- to discuss the ODE first, then to solve the PDE.

In order to carry out this program, a change of variable is introduced that permits to give (2.12) plus (2.15) the form of a parametric initial-value problem. One sets:

$$\xi := -\eta, \quad \xi_0 := -\eta_0, \tag{3.1}$$

whence $\mu = \sqrt{\xi/\rho}$ and ξ should satisfy

$$\partial_t \xi + \frac{\kappa\,(\partial_t \rho)^2 + \bar{\sigma}}{\sqrt{\rho}}\sqrt{\xi} = 0, \quad \xi|_{t=0} = \xi_0, \tag{3.2}$$

that is, a Cauchy problem parameterized on the space variable x and on the field $\rho(x, \cdot)$. The general form of equation (3.2) entails the Peano phenomenon and allows the existence of infinitely many solutions; among them, a suitably defined *maximal solution* ξ is picked, having the desirable property of staying positive as long as is possible. It turns out that

- the maximal solution to (3.2) is uniquely determined and depends continuously on the coefficients of the ODE, in particular, on ρ and $\partial_t \rho$.

Next, (2.11) is transformed into

$$\kappa\,\partial_t \rho - \Delta\rho + f'(\rho) - \sqrt{\xi}\frac{1}{\sqrt{\rho}} = 0, \tag{3.3}$$

an Allen-Cahn equation for ρ with the additional term $-\sqrt{\xi/\rho}$. Note that the factor $\sqrt{\xi}$ is implicitly defined in terms of ρ as the maximal solution to (3.2), so that

- (3.3) may be viewed as an *integrodifferential equation.*

Existence, regularity and uniqueness of the solution to (3.3) subject to the boundary condition (2.13) and the initial condition $(2.14)_1$ are proved by using a fixed-point argument, which takes advantage of the iterated Contraction Mapping Principle. It is important to be able to count on the a priori uniform boundedness of $\partial_t \rho$ in the space-time domain; this fact is ascertained by applying standard regularity arguments for parabolic equations.

As to the *long-time behavior of solutions*, it is verified in [3] that

- $\sqrt{\xi}$ uniquely converges to some function φ_∞, while any element ρ_∞ of the $\omega-$limit set solves the stationary problem

$$-\Delta\rho_\infty + f'(\rho_\infty) - \varphi_\infty \frac{1}{\sqrt{\rho_\infty}} = 0, \tag{3.4}$$

supplemented by a homogeneous Neumann boundary condition.

3.1.2 Main results

The system under study consists of equations (3.2) and (3.3), to be satisfied over space-time domains $Q_t := \Omega \times [0, t)$, $t \in (0, +\infty)$, for Ω a smooth bounded domain of $\mathbb{R}^N (N \geq 1)$ with boundary Γ. Recall that the mobility κ is a given positive constant. As to the initial data ρ_0, ξ_0 and the energy source $\bar{\sigma}$, it is assumed that

$$\rho_0, \xi_0 \in L^\infty(\Omega), \quad 0 < \rho_0 < 1 \quad \text{and} \quad \xi_0 \geq 0 \quad \text{a.e. in } \Omega,$$
$$\bar{\sigma} \in L^2(Q_T) \quad \text{for all } \; T > 0.$$

The *coarse-grain free energy* f is split as follows:

$$0 \leq f = f_1 + f_2, \quad \text{where} \quad f_1, f_2 : (0,1) \to \mathbb{R} \quad \text{are } C^2\text{-functions},$$
$$f_1 \text{ is convex}, \quad f_2' \text{ is bounded}, \quad \lim_{r \searrow 0} f'(r) = -\infty, \quad \text{and} \quad \lim_{r \nearrow 1} f'(r) = +\infty.$$

A simple and significant example for f_1 is:

$$f_1(r) = r \ln r + (1 - r) \ln(1 - r) \quad \text{for } r \in (0, 1)\,,$$

while f_2 stands for a smooth perturbation of this principal convex part.

In the first place, it is to be observed that, in the forward Cauchy problem (3.2), the unknown ξ must be nonnegative. Moreover, (i) if one looks for a strictly positive ξ (for given $\rho > 0$ and $\xi_0 > 0$), then that problem admits a unique local solution; (ii) uniqueness is no longer guaranteed if ξ is only required to be nonnegative; and, (iii) every nonnegative local solution can be extended to a global solution. All this considered, a (global) solution to problem (3.2) is selected according to the following *maximality criterion*:

$$\sqrt{\xi(x,t)} = \sup\left\{w(x,t) : \; w \in \mathcal{S}^*(\bar{\sigma}, \xi_0, \rho)\right\} \quad \text{for } (x,t) \in Q_T, \tag{3.5}$$

where

$$\mathcal{S}^*(\bar{\sigma}, \xi_0, \rho) := \Big\{ w \in W^{1,1}(0, T; L^1(\Omega)) : \; w(0) = \sqrt{\xi_0}, \quad w \geq 0 \quad \text{a.e. in } Q_T,$$
$$\partial_t w = -\big(\kappa\,(\partial_t \rho)^2 + \bar{\sigma}\big)/(2\rho^{1/2}) \quad \text{a.e. where } w > 0 \Big\}.$$

Thus, the maximal ξ satisfies:

$$\sqrt{\xi(x,t)} = \sqrt{\xi_0(x)} - \int_0^t a^*(x,s)\, ds\,,$$

with $a^*(x,s)$ specified by

$$a^*(x,s) := \begin{cases} \dfrac{\kappa\,|\partial_t\rho(x,s)|^2 + \bar\sigma(x,s)}{2\sqrt{\rho(x,s)}} & \text{if } \ \xi(x,s) > 0, \\ 0 & \text{otherwise.} \end{cases}$$

Next, on replacing μ by $\sqrt{\xi/\rho}$ in (2.11), (3.3) is arrived at. When this equation is supplemented with the boundary and initial conditions for ρ given by, respectively, (2.13) and the first of (2.14), an initial/boundary-value problem is obtained, whose variational formulation in the framework of the spaces $V := H^1(\Omega)$ and $H := L^2(\Omega)$ is: find

$$\rho \in H^1(0,T;H) \cap C^0([0,T];V) \tag{3.6}$$

satisfying

$$\rho(0) = \rho_0, \quad 0 < \rho < 1 \quad \text{a.e. in } Q_T, \quad \frac{1}{\rho} + \frac{1}{1-\rho} \in L^\infty(Q_T)\,; \tag{3.7}$$

and solving the equation

$$\kappa \int_\Omega \partial_t\rho(t)\,z + \int_\Omega \nabla\rho(t)\cdot\nabla z + \int_\Omega f'(\rho(t))\,z - \int_\Omega \big(\xi(t)/\rho(t)\big)^{1/2} z = 0$$
$$\text{for a.a. } t \in (0,T), \text{ for every } z \in V, \text{ and for } \xi \text{ given by (3.5).} \tag{3.8}$$

Problem (3.6)–(3.8) can be regarded as

- an essentially integrodifferential Allen-Cahn equation in the sole unknown ρ.

Note, in particular, that (3.8) has a well-defined meaning, because $\xi^{1/2}$ is in $L^2(Q_T)$ and $\rho^{-1/2}$ belongs to $L^\infty(Q_T)$ (at least) whenever ρ satisfies (3.6) and $\bar\sigma \in L^2(Q_T)$.

The first result proved in [3] concerns existence and uniqueness of the solution.

Theorem 3.1 *In addition to the already specified assumptions on the data f, $\bar\sigma$, ρ_0, ξ_0, assume that*

$$\bar\sigma \in L^\infty(Q_\infty) \quad \textit{and} \quad \bar\sigma^- \in L^1(0,\infty;L^\infty(\Omega)); \quad \frac{1}{\rho_0} + \frac{1}{1-\rho_0} \in L^\infty(\Omega),$$
$$\rho_0 \in H^2(\Omega), \quad \partial_n\rho_0 = 0 \quad \textit{on } \Gamma, \quad \textit{and} \quad \Delta\rho_0 \in L^\infty(\Omega).$$

Then, for every $T \in (0,+\infty)$, problem (3.6)–(3.8) has a unique solution. Furthermore,

$$\rho \in L^p(0,T;W^{2,p}(\Omega)) \quad \textit{for every } p < +\infty,$$
$$\partial_t\rho \in L^\infty(Q_T), \quad \textit{and} \quad \xi \in L^\infty(Q_T). \tag{3.9}$$

Finally, there exist constants $\rho_*, \rho^* \in (0,1)$ and $\xi^* \geq 0$, independent of T, such that

$$\rho_* \leq \rho \leq \rho^*, \quad \xi \leq \xi^* \quad \textit{a.e. in } Q_T. \tag{3.10}$$

The second result proved in [3] has to do with the long-time behavior of the solution ρ to problem (3.6)–(3.8): the elements of the ω-limit of every trajectory turn out to be steady-state solutions to the system under study.

Let $\varphi_\infty : \Omega \to [0, +\infty)$ be defined by

$$\varphi_\infty(x) := \lim_{t\to+\infty} \sqrt{\xi(x,t)} \quad \text{for a.a. } x \in \Omega, \quad \text{where } \sqrt{\xi} \text{ is given by (3.5).}$$

The stationary problem associated to (3.6)–(3.8)reads: find

$$\rho_\infty \in V \;\; \text{such that} \;\; \rho_* \le \rho_\infty \le \rho^* \quad \text{a.e. in } \Omega \tag{3.11}$$

and

$$\int_\Omega \nabla\rho_\infty \cdot \nabla z + \int_\Omega f'(\rho_\infty)\, z - \int_\Omega \frac{\varphi_\infty}{\sqrt{\rho_\infty}}\, z = 0 \quad \text{for every } z \in V. \tag{3.12}$$

Theorem 3.2 *Under the same assumptions as in Theorem 3.1, let ρ denote the unique global solution to problem* (3.6)–(3.8)*. Then, the limit $\varphi_\infty(x)$ exists for a.a. $x \in \Omega$, and $\varphi_\infty \in L^\infty(\Omega)$. Moreover, the ω-limit, defined by*

$$\omega(\rho) := \{\rho^\infty \in H : \; \|\rho^\infty - \rho(t_n)\|_H \to 0 \;\; \text{for some} \;\; \{t_n\} \nearrow +\infty\}, \tag{3.13}$$

is non-empty, compact, and connected in the strong topology of H. Finally, every element $\rho^\infty \in \omega(\rho)$ is actually a solution ρ_∞ to problem (3.11)–(3.12)*.*

The reader is referred to [3] for detailed proofs of Theorems 3.1 and 3.2, as well as for an informal but more complete discussion of the employed techniques.

3.2 How to handle temperature changes

3.2.1 Flow chart

In [4], the strategy is to repeat, for as much as is possible, the procedure that proved successful in [3]: the ODE (2.30), together with the relative initial condition, is discussed first, then one passes to the system composed by the PDE and the transcendental equation, together with the proper boundary and initial conditions.

In order to carry out the first part of the program, a change of variable is adopted, to give (2.30) plus (2.15) the form of a parametric initial-value problem. For ϑ_0 the initial value of ϑ, one sets:

$$-\eta = \vartheta^{-1}\xi = \vartheta^{-1}\mu^2\rho, \quad \xi_0 = -\vartheta_0\eta_0, \quad \eta_0 = -\vartheta_0^{-1}\mu_0^2\rho_0.$$

Accordingly, for

$$\mu = \sqrt{\xi/\rho}, \tag{3.14}$$

the following Cauchy problem is arrived at:

$$\vartheta\partial_t(\vartheta^{-1}\xi) + \frac{\kappa\,(\partial_t\rho)^2 + \bar\sigma}{\sqrt{\rho}}\sqrt{\xi} = 0, \quad (\vartheta^{-1}\xi)|_{t=0} = -\eta_0. \tag{3.15}$$

Next,

- attention is restricted to the class of processes such that

$$\vartheta\partial_t(\vartheta^{-1}\xi) \simeq \partial_t\xi;$$

- problem (3.15) is replaced by the simpler problem (cf. (3.2)):

$$\partial_t\xi + \frac{\kappa\,(\partial_t\rho)^2 + \bar{\sigma}}{\sqrt{\rho}}\,\sqrt{\xi} = 0, \quad \xi|_{t=0} = \xi_0, \tag{3.16}$$

  parameterized on both the space variable x and the field $\rho(x,\cdot)$.

Although simpler, the Cauchy problem (3.16) is far from trivial, because it can exhibit the Peano phenomenon and have infinitely many solutions; just as before, a suitably defined *maximal solution* ξ (or $\sqrt{\xi}$) is singled out, having the important property to stay positive as long as is possible.

To complete the program, one observes that, with (3.14), (2.29) and (2.28) become, respectively,

$$\kappa\,\partial_t\rho - \Delta\rho + f'(\rho) - c_0\vartheta = \sqrt{\xi/\rho}\,, \tag{3.17}$$

and

$$\lambda(\rho,\vartheta) := c_0\rho\vartheta + c_v\vartheta\ln\vartheta = -\sqrt{\rho\xi}\,, \tag{3.18}$$

that is

- an *integro–differential system* for ρ and ϑ,

with $\sqrt{\xi}$ implicitly defined in terms of ρ as the maximal solution to (3.16). This system is to be supplemented with the boundary condition (2.13), the initial condition for ρ in (2.14), and a compatible initial condition for ϑ.

3.2.2 Main results

In view of the above discussion, one looks for suitably smooth triplets of time-dependent fields (ρ,ξ,ϑ) over a regular region Ω with boundary Γ, such that:

$$0 < \rho < 1, \quad \xi \geq 0, \quad \text{and} \quad \vartheta > 0; \tag{3.19}$$

$$\partial_t\rho - \Delta\rho + f'(\rho) - c_0\vartheta = \sqrt{\xi/\rho}\,, \quad \text{with } \partial_n\rho = 0 \text{ on } \Gamma; \tag{3.20}$$

$$\partial_t\xi + \frac{|\partial_t\rho|^2 + \bar{\sigma}}{\sqrt{\rho}}\,\sqrt{\xi} = 0; \tag{3.21}$$

$$\lambda(\rho,\vartheta) = -\sqrt{\rho\,\xi}; \tag{3.22}$$

$$\rho(0) = \rho_0, \quad \xi(0) = \xi_0\,, \quad \text{and} \quad \vartheta(0) = \vartheta_0\,; \tag{3.23}$$

and that, moreover,

$$\xi \text{ is maximal among the } \xi\text{'s satisfying (3.21) and the second of (3.23).} \tag{3.24}$$

The problem's structure is the same as in Subsection 3.2, apart for the modifications due to the presence of the temperature variable ϑ.

Two items deserve a supplemental discussion. The first is that, just as in [3], we assume that

$$0 \le f = f_1 + f_2, \quad \text{where} \quad f_1, f_2 : (0,1) \to \mathbb{R} \quad \text{are } C^2\text{-functions}, \tag{3.25}$$
$$f_1 \text{ convex}, \quad f_2' \text{ bounded}, \quad \lim_{r\searrow 0} f'(r) = -\infty, \quad \lim_{r\nearrow 1} f'(r) = +\infty, \tag{3.26}$$

with the constant $c_0\vartheta_c$ thought of as incorporated in $f_2'(\rho)$. The second has to do with the admissible choices of initial data: not only they must agree with (3.19), and hence fulfill the conditions

$$0 < \rho_0 < 1, \quad \xi_0 \ge 0, \quad \vartheta_0 > 0, \tag{3.27}$$

but also they have to comply with (3.22), that is to say, they have to satisfy

$$\lambda(\rho_0, \vartheta_0) = -\sqrt{\rho_0\xi_0}\,. \tag{3.28}$$

To see what restrictions this last requirement implies on the choice of ϑ_0, it is convenient to study the function $\lambda_r : s \mapsto \lambda(r,s) = c_0 r s + c_v s \ln s$ on $(0,+\infty)$ for a given $r \in (0,1)$. Clearly,

(i) λ_r is strictly convex and tends to 0 as s tends to 0;

(ii) the equation $\lambda_r(s) = 0$ has in $(0,+\infty)$ a unique solution, denoted by $\bar{s}(r)$;

(iii) λ_r has a unique minimum point, denoted by $\underline{s}(r)$;

in summary, for each fixed $r \in (0,1)$,

$$0 < \underline{s}(r) < \bar{s}(r), \quad \lambda(r, \bar{s}(r)) = 0, \quad \text{and} \quad \frac{\partial\lambda}{\partial s}(r, \underline{s}(r)) = 0. \tag{3.29}$$

A simple computation shows that

$$\begin{aligned} &\underline{s}(r) = e^{-1-c_* r}, \quad \bar{s}(r) = e^{-c_* r}, \quad \text{and} \\ &\lambda(r, \underline{s}(r)) = -c_v e^{-1-c_* r}, \quad \text{where} \quad c_* := c_0/c_v\,. \end{aligned} \tag{3.30}$$

Therefore, a necessary condition for the compatibility of initial data is that

$$\sqrt{\rho_0\xi_0} \le c_v e^{-1-c_*\rho_0} \quad \text{a.e. in } \Omega, \tag{3.31}$$

i.e., that $\sup\zeta \le 0$, where $\zeta := \sqrt{\rho_0\xi_0} - c_v e^{-1-c_*\rho_0}$.

If such a condition is satisfied, and if we want to solve (a.e. in Ω) the equation $\lambda(\rho_0(x), s) = 0$ for s, then uniqueness holds if $\zeta(x) = 0$, and $\underline{s}(\rho_0(x))$ is the unique solution. Otherwise, if the strict inequality holds, then there are two solutions, the one in the interval $(0, \underline{s}(\rho_0(x)))$ the other in $(\underline{s}(\rho_0(x)), \bar{s}(\rho_0(x)))$. For the existence of a local-in-time solution (ρ, ξ, ϑ), a modest reinforcement of condition (3.31) and a proper choice of ϑ_0 suffice, namely,

$$\sup\left(\sqrt{\rho_0 \xi_0} - c_v e^{-1-c_* \rho_0}\right) < 0 \quad \text{and} \quad \vartheta_0 \geq \underline{s}(\rho_0) \quad \text{a.e. in } \Omega. \tag{3.32}$$

Under these assumptions, we can state the following result.

Theorem 3.3 *Let* (3.25)–(3.26) *and* (3.32) *hold. Moreover, assume that*

$$\begin{aligned}
&\bar{\sigma} \in L^\infty(\Omega \times (0, +\infty)), \quad (\bar{\sigma})^- \in L^\infty(0, \infty; L^1(\Omega));\\
&\rho_0, \xi_0, \vartheta_0 \in L^\infty(\Omega), \quad \inf \rho_0 > 0, \quad \sup \rho_0 < 1;\\
&\rho_0 \in H^3(\Omega), \quad \partial_n \rho_0|_\Gamma = 0, \quad \Delta \rho_0 \in L^\infty(\Omega);\\
&\xi_0 \geq 0, \quad \sqrt{\xi_0} \in H^1(\Omega), \quad \lambda(\vartheta_0, \rho_0) = -\sqrt{\rho_0 \xi_0}.
\end{aligned}$$

Then, there exist $T > 0$ and a triplet (ρ, ξ, ϑ) satisfying:

$$\rho \in H^1(0, T; L^2(\Omega)) \cap C^0([0, T]; H^1(\Omega)); \tag{3.33}$$

$$\rho \in L^p(0, T; W^{2,p}(\Omega)) \ \textit{for each } p < +\infty, \quad \partial_t \rho \in L^\infty(Q_T); \tag{3.34}$$

$$\xi \in L^\infty(Q_T) \cap W^{1,1}(0, T; L^1(\Omega)), \quad \vartheta\,,\, \partial_t \vartheta \in L^\infty(Q_T); \tag{3.35}$$

$$\inf \rho > 0, \quad \sup \rho < 1, \quad \inf \vartheta > 0, \tag{3.36}$$

and solving problem (3.20)–(3.24).

In [4] this existence result is proved by a fixed-point argument. The employed method relies on the application of the Tychonoff-Schauder theorem in a weak topology. By (3.32), one starts by choosing $\varepsilon_0 > 0$ such that

$$\sqrt{\rho_0 \xi_0} \leq c_v e^{-1-c_* \rho_0} - 2\varepsilon_0 \quad \text{a.e. in } \Omega, \tag{3.37}$$

and, as the result is local, by fixing a reference final time $T^* > 0$ (e.g., $T^* = 1$), taking $T \leq T^*$ in course of the proof. Next, by looking at (3.8)–(3.5) and (3.22) separately,

- two maps:
  $$\mathcal{F}_1 : \vartheta \mapsto (\rho, \xi) \quad \text{and} \quad \mathcal{F}_2 : (\rho, \xi) \mapsto \vartheta$$
  are constructed, with proper domains: the domain of $\mathcal{F}_1$ is a convex set $\mathcal{K}$ depending on T and on a further parameter M; the domain of $\mathcal{F}_2$ is the range $\mathcal{R}$ of $\mathcal{F}_1$.
- it is proved that a suitable choice of T and M ensures that the range of $\mathcal{F}_2$ is contained in $\mathcal{K}$.

With this, one is entitled to look for a fixed point of $\mathcal{F}_2 \circ \mathcal{F}_1$. To this aim, the Tychonoff-Schauder theorem is used and, accordingly, $\mathcal{K}$ is endowed with some weak topology. For details, the reader to Section 4 of [4].

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