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Global existence of a solution to a phase field model for supercooling

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Abstract

In this work, we will derive a macroscopic model of phase field type for supercooling. The phase transition process is described by the evolution of the temperature and the volume fraction of the liquid phase. This phase field model can also be interpreted as the approximation of some generalized Stefan problem.

We will prove the existence of solutions to an initial–boundary value problem for the resulting system by using a time discrete scheme.

1 Introduction and derivation of the model

When pure water is cooled down carefully, it often does not freeze at the freezing temperature but stays liquid at some temperatures below the melting point. This supercooled water freezes if ice seeds are included in the water or if some movement of the water initiates the freezing process.

We are now going to derive a macroscopic model of phase field type for supercooling, which can also be interpreted as the approximation of some generalized Stefan problem. The corresponding system of partial differential equations will be subsequently discussed from the point of view of existence of solutions.

1.1 Thermomechanical derivation

We consider the solidification of supercooled water in a smooth bounded domain $\Omega \subset \mathbb{R}^3$ with boundary Γ. We assume that there are no macroscopic movements and that the macroscopic density ρ_0 is constant. Moreover, we assume that there are no exterior forces. Hence, our state quantities are the volume fraction of the liquid phase β and the absolute temperature θ.

Although the macroscopic movements are supposed to be zero, there are microscopic movements. We want to take into account the power of the microscopic movements during the phase transition without using a new state quantity. Hence, $\partial_t \beta$ is the only quantity which is connected to the microscopic movements. Let p_i be the volume density of the power of the interior forces corresponding to these movements. Following [BFL, FGS98], we introduce two fields B and $\vec{H}$ such that

$$p_i = -B\partial_t\beta - \vec{H} \bullet \nabla\partial_t\beta, \tag{1.1}$$

with the scalar B and the vector $\vec{H}$ representing new interior forces. Hence, the overall power $\mathcal{P}_i$ of the interior forces is

$$\mathcal{P}_i(\partial_t\beta) = \int_\Omega p_i \, \mathrm{d}x = -\int_\Omega \left(B\partial_t\beta + \vec{H} \bullet \nabla\partial_t\beta\right) \mathrm{d}x \,. \tag{1.2}$$

We assume that there is no macroscopic power of the microscopic accelerations and that no work is provided to the system by microscopic actions (as electrical, chemical or radiative external actions). Using the principle of virtual power, provided $\vec{H}$ is sufficiently smooth we get

$$\begin{aligned} \forall\, \phi: \quad 0 = \mathcal{P}_i(\phi) &= -\int_\Omega \left(B\phi + \vec{H} \bullet \nabla\phi\right) \mathrm{d}x \\ &= -\int_\Omega \left(B - \operatorname{div}\vec{H}\right)\phi \, \mathrm{d}x - \int_\Gamma \vec{H} \bullet \vec{n}\phi \, \mathrm{d}\sigma \,, \end{aligned} \tag{1.3}$$

where $\vec{n}$ denotes the outward normal vector to Γ. This leads to the new equations of motion

$$\operatorname{div}\vec{H} - B = 0, \text{ in } \Omega, \quad \text{and} \quad \vec{H} \bullet \vec{n} = 0, \text{ on } \Gamma. \tag{1.4}$$

Let us emphasize that the boundary condition has a physical meaning, since $\vec{H} \bullet \vec{n}$ is the amount of the work provided to the system by local actions (and with our assumptions such amount is zero). The vector $\vec{H}$ is a work flux vector. The energy balance is

$$\frac{\partial U}{\partial t} + \operatorname{div}\vec{q} = f - p_i, \tag{1.5}$$

where U is the density of the internal energy, $\vec{q}$ is the heat flux, and f accounts for heat sources and sinks. To formulate the constitutive laws, a density $\Psi = \Psi(\beta, \nabla\beta, \theta)$ of the free energy and a pseudo–potential of dissipation $\Phi = \Phi(\partial_t\beta, \nabla\beta, \theta)$ will be introduced. Let us recall that $\Phi(\partial_t\beta, \nabla\beta, \theta)$ is a pseudo–potential of dissipation whenever it is a non–negative function, convex with respect to $\partial_t\beta$, with value 0 for $\partial_t\beta = 0$, i.e., $\Phi(0, \nabla\beta, \theta) = 0$. Now, we specify the constitutive laws

$$B = \frac{\partial\Psi}{\partial\beta} + \frac{\partial\Phi}{\partial(\partial_t\beta)}, \quad \vec{H} = \frac{\partial\Psi}{\partial(\nabla\beta)}, \quad \vec{q} = -\kappa\nabla\theta, \tag{1.6}$$

where $\kappa > 0$ is the specific heat conductivity. Moreover, if S denotes the density of the entropy, we have the classical state equations

$$S = -\frac{\partial\Psi}{\partial\theta}, \quad U = \Psi + \theta S = \Psi - \theta\frac{\partial\Psi}{\partial\theta}. \tag{1.7}$$

Therefore, thanks to the constitutive laws in (1.6), it is easy to see that

$$\frac{\partial U}{\partial t} = \theta\frac{\partial S}{\partial t} + \left(B - \frac{\partial\Phi}{\partial(\partial_t\beta)}\right)\partial_t\beta + \vec{H} \bullet \partial_t\nabla\beta, \quad \vec{q} \bullet \nabla\theta \le 0. \tag{1.8}$$

It results that the energy balance (1.5), the equality (1.1), and the conditions on Φ yield that

$$\frac{\partial S}{\partial t} + \operatorname{div}\left(\frac{\vec{q}}{\theta}\right) - \frac{f}{\theta} = \frac{1}{\theta}\left(-\vec{q}\bullet\nabla\theta + \frac{\partial\Phi}{\partial(\partial_t\beta)}\partial_t\beta\right) \geq 0, \tag{1.9}$$

which proves that the second law of thermodynamics is satisfied. We choose

$$\Psi(\beta,\nabla\beta,\theta) = -\frac{L}{\theta_C}(\theta-\theta_C)\beta + \frac{\mu}{2}(\nabla\beta)^2 + I_{[0,1]}(\beta) - c_0\theta\ln(\theta), \tag{1.10}$$

where L is the latent heat of the phase transition, $\theta_C > 0$ is the melting temperature, $c_0 > 0$ is the specific heat, $\mu > 0$ is the interfacial energy coefficient, and $I_{[0,1]}$ is the indicator function of the interval $[0,1]$. As pseudo–potential of dissipation, we take

$$\Phi(\partial_t\beta,\nabla\beta,\theta) = \frac{1}{2}\eta(\theta,\nabla\beta)(\partial_t\beta)^2, \tag{1.11}$$

where $\eta : \mathbb{R}\times\mathbb{R}^3 \to [0,\infty)$ is some given non negative relaxation parameter function, so that the conditions for a pseudo–potential of dissipation are satisfied. Combining the constitutive laws (1.6) and the equations of motion (1.4), we get

$$0 \ni \eta(\theta,\nabla\beta)\partial_t\beta - \mu\,\Delta\beta + \partial I_{[0,1]}(\beta) - \frac{L}{\theta_C}(\theta-\theta_C), \text{ in } \Omega, \tag{1.12}$$

$$\frac{\partial\beta}{\partial n} = 0, \text{ on } \Gamma. \tag{1.13}$$

The energy balance (1.5), the equality (1.1), the constitutive laws (1.6), and the state relations (1.7) give

$$c_0\partial_t\theta + L\frac{\theta}{\theta_C}\partial_t\beta - \kappa\,\Delta\theta = f + \eta(\theta,\nabla\beta)\left(\partial_t\beta\right)^2, \text{ in } \Omega. \tag{1.14}$$

Within the small perturbation assumption

$$\frac{\theta}{\theta_C} \approx 1, \quad \eta(\theta,\nabla\beta)\left(\partial_t\beta\right)^2 \approx 0, \tag{1.15}$$

we get the final equation

$$c_0\partial_t\theta + L\partial_t\beta - \kappa\,\Delta\theta = f, \text{ in } \Omega. \tag{1.16}$$

Remark 1.1. This classical small perturbation assumption has been widely used, for instance, to replace the material derivatives $\frac{\mathrm{de}}{\mathrm{d}t}$ by the partial derivatives $\partial_t\beta$.

Remark 1.2. For a constant η, the system (1.12), (1.16) is a special version of the *standard phase field system*, which has been investigated in a number of papers, see [BE93, BE94, Cag86, Cag89, CL87, EG94] to name only a few.

Systems like (1.12), (1.16) and similar systems with η depending on the direction of $\nabla\beta$ have been investigated, for example in [EG96, WMS93], to simulate the dendritic solidification of liquids when one takes into account the latent heat of solidification.

If the temperature θ is supposed to be a known function, one needs only to consider the equation (1.12). If one adds the term $-\frac{1}{\mu}\beta$ on the left–hand side of (1.12), one gets a double–obstacle Allen–Cahn equation. This equation with η depending on the direction of $\nabla\beta$ is considered in [EGK96, EPS96, ES97].

1.2 Derivation as approximation of a generalized Stefan problem

The above system can also be interpreted as the approximation of a generalized Stefan problem. In the context of a Stefan problem, we assume that at every time t there are open disjoint smooth subsets $\Omega_{liq}(t)$, $\Omega_{ice}(t)$ of Ω, such that $\overline{\Omega_{liq}(t) \cup \Omega_{ice}(t)} = \overline{\Omega}$, $\Omega_{liq}(t)$ is filled with liquid, and $\Omega_{ice}(t)$ is filled with ice. Hence, we see that ice and water are separated by a freezing surface $\Gamma(t) = \partial\Omega_l(t) \cap \partial\Omega_i(t)$.

As in [Fré95], we assume that the normal velocity of the thin interface is temperature–dependent and consider the following model for the solidification of an supercooled liquid. Let

$$c_0 \partial_t \theta - \kappa\, \Delta\theta = f \quad \text{in the water and in the ice,} \tag{1.17}$$

$$\kappa \left.\frac{\partial\theta}{\partial n}\right|_{water} - \kappa \left.\frac{\partial\theta}{\partial n}\right|_{ice} = -L W_N \quad \text{on} \quad \Gamma(t), \tag{1.18}$$

$$c(\theta) W_N = \frac{L(\theta_C - \theta)}{\theta_C} \quad \text{on} \quad \Gamma(t), \tag{1.19}$$

where W_N is the normal velocity of the phase interface with respect to the normal vector pointing into the liquid phase and $c : \mathbb{R} \to [0, \infty)$ is a given function, supposed to describe the temperature dependence of the normal velocity of the freezing line. In the case $c \equiv 0$, the above problem corresponds to the classical Stefan problem.

Defining $\beta = 0$ in ice and $\beta = 1$ in water, we have

$$(\partial_t\beta, \phi)_{\mathcal{D}'(\Omega_T)\times\mathcal{D}(\Omega_T)} = -\int_0^T \int_{\Gamma(t)} W_N \phi \,\mathrm{d}\Gamma(t)\,\mathrm{d}t, \tag{1.20}$$

for all $\phi \in \mathcal{D}(\Omega_T) = C_0^\infty(\Omega_T)$, where $\Omega_T := \Omega \times (0,T)$ and $T > 0$ denotes the final time. Hence, we can rewrite (1.17) and (1.18) as

$$c_0 \partial_t\theta + L\partial_t\beta - \kappa\,\Delta\theta = f \quad \text{in} \quad \mathcal{D}'(\Omega_T), \tag{1.21}$$

and (1.19) leads to

$$(\partial_t\beta, \phi)_{\mathcal{D}'(\Omega_T)\times\mathcal{D}(\Omega_T)} = \int_0^T \int_{\Gamma(t)} \frac{L}{\theta_C}\frac{\theta - \theta_C}{c(\theta)} \phi \,\mathrm{d}\Gamma(t)\,\mathrm{d}t, \quad \forall\, \phi \in \mathcal{D}(\Omega_T). \tag{1.22}$$

Since β jumps from 0 to 1 on the freezing line $\Gamma(t)$, in a formal way we have

$$(|\nabla\beta(\cdot,t)|_2\,, \phi)_{\mathcal{D}'(\Omega)\times\mathcal{D}(\Omega)} = \int_{\Gamma(t)} \phi \,\mathrm{d}\Gamma(t), \quad \forall\, \phi \in \mathcal{D}(\Omega), \tag{1.23}$$

where $|\cdot|_2$ denotes the Euclidean norm in $\mathbb{R}^3$. Combining (1.22) and (1.23), by a naive computation we should get

$$\partial_t\beta - \frac{L}{\theta_C}\frac{\theta - \theta_C}{c(\theta)}\,|\nabla\beta| = 0 \quad \text{in } \mathcal{D}'(\Omega_T). \tag{1.24}$$

A rigorous derivation of (1.24) from (1.18) and (1.19) can be found in [FGS98]. This equation leads to

$$\frac{c(\theta)}{|\nabla\beta|_2}\partial_t\beta = \frac{L(\theta-\theta_C)}{\theta_C} \quad \text{in } \mathcal{D}'(\Omega_T). \tag{1.25}$$

In order to impose the constraint $0 \le \beta \le 1$, equation (1.25) will be approximated by adding $\partial I_{[0,1]}(\beta)$ on the left–hand side, where $I_{[0,1]}$ is the indicator function of $[0,1]$. Moreover, the equation is mollified by including the term $-\mu\,\Delta\beta$ on the left–hand side, and replacing $\frac{c(\theta)}{|\nabla\beta|_2}$ by some continuous approximation $\eta(\theta,\nabla\beta)$, e.g.

$$\eta(\theta,\nabla\beta) = \frac{c(\theta)}{|\nabla\beta|_2+\delta} \quad \text{or} \quad \eta(\theta,\nabla\beta) = \frac{c(\theta)}{\sqrt{|\nabla\beta|_2^2+\delta}}, \tag{1.26}$$

where $\delta > 0$ is some small parameter. Thus, we obtain

$$\eta(\theta,\nabla\beta)\partial_t\beta - \mu\,\Delta\beta + \partial I_{[0,1]}(\beta) \ni \frac{L}{\theta_C}(\theta-\theta_C), \quad \text{a.e. in} \quad \Omega_T, \tag{1.27}$$

which coincides with (1.12). Hence, it is clear that (1.16) and (1.12) can be considered as approximation of the generalized Stefan problem in (1.17)–(1.19), but until now no convergence result to the Stefan problem could be derived.

Remark 1.3. In [FGS98], one deals with the energy balance (1.16) combined with a modified version of (1.27), in which $\eta \equiv 1$ and the right–hand side is replaced by $W(\theta)\,|\nabla\beta|_2$ for some continuous function $W : \mathbb{R} \to \mathbb{R}$ having compact support.

2 Main results

This section is concerned with the system of PDE's which has been discussed above. Now, we add boundary and initial conditions for both variables, give a precise formulation of the problem, and state our main existence theorems. Then, we deal with the system **(P)**:

$$c_0\partial_t\theta + L\partial_t\beta - \kappa\,\Delta\theta = f, \quad \text{a.e. in} \quad \Omega_T, \tag{2.1a}$$

$$\eta(\theta,\nabla\beta)\partial_t\beta - \mu\,\Delta\beta + \chi = \frac{L}{\theta_C}(\theta-\theta_C), \quad \text{a.e. in} \quad \Omega_T, \tag{2.1b}$$

$$\beta \in [0,1], \quad \chi \in \partial I_{[0,1]}(\beta), \quad \text{a.e. in} \quad \Omega_T, \tag{2.1c}$$

$$-\kappa\frac{\partial\theta}{\partial n} = \alpha(\theta-\theta_{\text{ext}}), \quad \frac{\partial\beta}{\partial n} = 0, \quad \text{a.e. in} \quad \Gamma\times(0,T), \tag{2.1d}$$

$$\theta(\cdot,0) = \theta^0, \quad \beta(\cdot,0) = \beta^0, \quad \text{a.e. in} \quad \Omega. \tag{2.1e}$$

Here $\alpha > 0$ is a constant, $\theta_{\text{ext}} : \Gamma\times(0,T) \to \mathbb{R}$ is the external temperature, and β^0, θ^0 are initial values.

The following assumptions will be used.

(A1): There exists a positive constant C_η such that

$$\eta : \mathbb{R} \times \mathbb{R}^3 \to (0, C_\eta] \quad \text{is continuous},$$
$$\beta^0 \in H^1(\Omega), \quad 0 \le \beta^0 \le 1, \quad \text{a.e. in} \quad \Omega.$$

(A2): There exists a positive constant B_η such that

$$\eta(u, \vec{v}) \ge B_\eta, \quad \forall\, u \in \mathbb{R},\, \vec{v} \in \mathbb{R}^3,$$
$$\theta^0 \in H^1(\Omega), \quad \theta_{\text{ext}} \in L^2(0,T; H^{\frac{1}{2}}(\Gamma)) \cap H^1(0,T;L^2(\Omega)), \quad f \in L^2(0,T;L^2(\Omega)).$$

Under these assumptions, we can show the validity of the following existence result.

Theorem 1. *If assumptions (A1) and (A2) are satisfied, then there exists a strong solution* (θ, β, χ) *to the system **(P)** in the sense that*

$$\theta, \beta \in H^1(0,T;L^2(\Omega)) \cap C^0([0,T];H^1(\Omega)) \cap L^2(0,T;H^2(\Omega)), \tag{2.2a}$$
$$\chi \in L^\infty(0,T;L^2(\Omega)), \tag{2.2b}$$

and (2.1) *hold.*

Note that if $\eta(\theta, \nabla\beta)$ yields some approximation of $\frac{c(\theta)}{|\nabla\beta|_2}$ as in (1.26), then **(A2)** is not fulfilled. Hence, we consider also the alternative assumption below and introduce there the functional F, which is used in the generalized weak formulation (2.5a) of the energy balance. Actually, this formulation coincides with the normal weak formulation of (2.1a), if F is defined by

$$(F(t), v)_{H^1(\Omega)^* \times H^1(\Omega)} = \int_\Omega f(t,x) v \,\mathrm{d}x + \alpha \int_\Gamma \theta_{ext}(t,\sigma) v \,\mathrm{d}\sigma\,, \qquad \forall\, v \in H^1(\Omega), \text{ for a.e. } t \in (0,T), \tag{2.3}$$

with $f \in L^2(0,T;L^2(\Omega))$ and $\theta_{ext} \in L^2(0,T;L^2(\Gamma))$.

(A3): There is a positive constant B^*_η such that

$$\eta(u, \vec{v})\,(|\vec{v}|_2 + 1) \ge B^*_\eta, \quad \forall\, u \in \mathbb{R},\, \vec{v} \in \mathbb{R}^3,$$
$$\theta_0 \in L^2(\Omega), \quad F \in L^2(0,T;H^1(\Omega)^*).$$

In the case when **(A3)** substitutes **(A2)**, we can only prove the existence of a weak solution to **(P)**.

Theorem 2. *If assumptions (A1) and (A3) are satisfied, then there exists a solution* (θ, β, χ) *to the generalized weak formulation of problem **(P)**, i.e., we have*

$$\theta \in H^1(0,T;H^1(\Omega)^*) \cap C^0([0,T];L^2(\Omega)) \cap L^2(0,T;H^1(\Omega)), \tag{2.4a}$$
$$\beta \in H^1(0,T;L^{\frac{4}{3}}(\Omega)) \cap L^\infty(0,T;H^1(\Omega)) \cap L^2(0,T;H^2(\Omega)), \tag{2.4b}$$

$$\sqrt{\eta(\theta,\nabla\beta)}\beta_t \in L^2(0,T;L^2(\Omega)), \tag{2.4c}$$
$$\chi \in L^\infty(0,T;L^2(\Omega)), \tag{2.4d}$$

and the equations and conditions

$$c_0\left(\partial_t\theta, v\right)_{H^1(\Omega)^*\times H^1(\Omega)} + \int_\Omega L\left(\partial_t\beta\right) v\,\mathrm{d}x + \int_\Omega \kappa\nabla\theta \bullet \nabla v\,\mathrm{d}x + \int_\Gamma \alpha\theta v\,\mathrm{d}\sigma$$
$$= \left(F, v\right)_{H^1(\Omega)^*\times H^1(\Omega)}, \quad \forall\, v \in H^1(\Omega), \quad a.e.\ in \quad (0,T), \tag{2.5a}$$
$$\frac{\partial\beta}{\partial n} = 0, \quad a.e.\ in \quad \Gamma\times(0,T), \tag{2.5b}$$

(2.1b)*,* (2.1c)*, and* (2.1e) *hold.*

Remark 2.1. If we replace in **(A1)** the assumption that there is a uniform upper bound for η, by the weaker assumption that there is a positive constant C^*_η with

$$\eta(u,\vec{v}) \leq C^*_\eta(u + |\vec{v}|_2 + 1), \quad \forall\, u \in \mathbb{R}, \vec{v} \in \mathbb{R}^3, \tag{2.6}$$

we can still show existence by considering first the problem with η modified by some cut–off function, then deriving uniform a priori estimates, and afterwards carring out some limit procedure. Since we can still obtain (2.4a), (2.4c), (2.4d) as well as $\beta \in L^\infty(0,T;H^1(\Omega))$, then by comparison we just get $\Delta\beta \in L^2(0,T;L^{\frac{4}{3}}(\Omega))$, whence $\beta \in L^2(0,T;W^{2,\frac{4}{3}}(\Omega))$, while it is no longer clear whether the last inclusion in (2.4b) holds.

Remark 2.2. Until now, we do not know of any uniqueness result for the system **(P)** .

Remark 2.3. The asymptotic behaviour of our solution to **(P)** as $\mu \to 0$ or as $\eta(\theta,\nabla\beta)$ converges in some sense (cf. (1.26)) to $\frac{c(\theta)}{|\nabla\beta|_2}$ remains an open question. The authors wonder whether if would be possible to show that the limit of such sequences is a viscosity solution of some problem.

3 Proof of Theorem 2

3.1 A time discrete scheme

In this section, we assume that **(A1)** and **(A3)** hold, and we deal with $K \in \mathbb{N}$ sufficiently large, in order that

$$h := \frac{T}{K} < \frac{c_0^2\theta_C^2}{4L^4}. \tag{3.1}$$

We consider the scheme $(\mathbf{D_K})$:

For $1 \le m \le K$, find $\theta_m \in H^1(\Omega)$, $\beta_m \in H^2(\Omega)$, $\chi_m \in L^2(\Omega)$ such that

$$\int_\Omega \left(c_0 \frac{\theta_m - \theta_{m-1}}{h} + L \frac{\beta_m - \beta_{m-1}}{h} \right) v \,\mathrm{d}x + \kappa \int_\Omega \nabla\theta_m \bullet \nabla v \,\mathrm{d}x + \alpha \int_\Gamma \theta_m v \,\mathrm{d}\sigma \tag{3.2a}$$
$$= (F_m, v)_{H^1(\Omega)^* \times H^1(\Omega)} \quad \forall\, v \in H^1(\Omega),$$

$$\left(\eta_m + \sqrt{h}\right) \frac{\beta_m - \beta_{m-1}}{h} - \mu\,\Delta\beta_m + \chi_m = \frac{L}{\theta_C}(\theta_{m-1} - \theta_C), \quad \text{a.e. in} \quad \Omega, \tag{3.2b}$$

$$\beta_m \in [0,1], \quad \chi_m \in \partial I_{[0,1]}(\beta_m), \quad \text{a.e. in} \quad \Omega, \tag{3.2c}$$

$$\frac{\partial \beta_m}{\partial n} = 0, \quad \text{a.e. on } \Gamma, \tag{3.2d}$$

$$\beta_0 := \beta^0, \quad \theta_0 := \theta^0, \quad \text{a.e. in} \quad \Omega, \tag{3.2e}$$

where, for $1 \le m \le K$, $F_m \in H^1(\Omega)^*$ and $\eta_m \in L^\infty(\Omega)$ are defined by

$$F_m := \frac{1}{h} \int_{(m-1)h}^{mh} F(t)\,\mathrm{d}t\,, \tag{3.3}$$

$$\eta_m(x) := \eta\left(\theta_{m-1}(x), \nabla\beta_{m-1}(x)\right) > 0 \quad \text{for a.e. } x \in \Omega. \tag{3.4}$$

Let us point out that the explicit treatment of the right–hand side of (3.2b) is similar to those considered for the approximation of the standard phase field model in [EG96]. Instead, we remark that in the approximation of the Penrose–Fife system (see [Hor93, Kle]), one has to deal with an implicit coupling term to get a priori estimates.

For the scheme (3.2), we can prove the following statement.

Lemma 3.1. *The scheme* $(\boldsymbol{D}_{\mathbf{K}})$ *has a unique solution.*

Proof. By **(A1)** and **(A3)**, we see that (3.2e) defines $\theta_0 \in L^2(\Omega)$ and $\beta_0 \in H^1(\Omega)$ uniquely.

To prove the existence of a unique solution to the scheme by induction, let $\theta_{m-1} \in L^2(\Omega)$, $\beta_{m-1} \in H^1(\Omega)$ be given for some $m \in \{1, \dots K\}$.

We can rewrite the discrete order parameter equation (3.2b), (3.2c), the boundary condition for β_m in (3.2d), and the regularity conditions for β_m and χ_m as

$$\frac{1}{\sqrt{h}}\beta_m + \frac{\eta_m}{h}\beta_m + A\beta_m \ni \frac{L}{\theta_C}(\theta_{m-1} - \theta_C) + \frac{\eta_m + \sqrt{h}}{h}\beta_{m-1}, \tag{3.5}$$

$$\chi_m = \frac{L}{\theta_C}(\theta_{m-1} - \theta_C) - \left(\eta_m + \sqrt{h}\right)\frac{\beta_m - \beta_{m-1}}{h} + \mu\,\Delta\beta_m, \quad \text{a.e. in} \quad \Omega, \tag{3.6}$$

where $A : D(A) \subset L^2(\Omega) \to 2^{L^2(\Omega)}$ is the nonlinear operator defined by

$$Au = -\mu\,\Delta u + \left\{ v \in L^2(\Omega) : v \in \partial I_{[0,1]}(u) \quad \text{a.e. in} \quad \Omega \right\}, \tag{3.7}$$

$$D(A) = \left\{ u \in H^2(\Omega) : 0 \le u \le 1 \quad \text{a.e. in} \quad \Omega, \quad \frac{\partial u}{\partial n} = 0 \quad \text{a.e. on } \Gamma \right\}. \tag{3.8}$$

Applying [Bré71, Cor. 13], we see that this operator is maximal monotone. In the light of (3.4), as $\eta_m \in L^\infty(\Omega)$, we see that $L^2(\Omega) \ni \beta \mapsto \eta_m \beta$ is a continuous monotone operator from $L^2(\Omega)$ to $L^2(\Omega)$. Thanks to a theorem on the sum of monotone operators (see, e.g., [Bar76, Chap. II, Cor. 1.3]), we deduce that $D(A) \ni \beta \mapsto \frac{1}{h}\eta_m \beta + A\beta$ is a maximal monotone operator as well. Owing to maximality, we see that (3.5) has a unique solution $\beta_m \in H^2(\Omega)$. Subsequently, $\chi_m \in L^2(\Omega)$ is uniquely determined by (3.6).

Next, thanks to the Lax–Milgram lemma, we conclude that the discrete energy balance (3.2a) has a unique solution θ_m.

Therefore, the lemma is completely proved. □

3.2 Uniform estimates

Now, we are going to derive some uniform a priori estimates for the solution to the scheme.

In the sequel, C_i, for $i \in \mathbb{N}$, will always denote generic positive constants, independent of K. We will use $\|\cdot\|_2$ for the $L^2(\Omega)$–norm and $\|\cdot\|_{2,3}$ for the the $\left(L^2(\Omega)\right)^3$–norm.

The following norm equivalence is well known: there exists two positive constants C_1, C_2 such that

$$C_1 \|v\|^2_{H^1(\Omega)} \le \kappa \|\nabla v\|^2_{2,3} + \frac{\alpha}{2} \|v\|^2_{L^2(\Gamma)} \le C_2 \|v\|^2_{H^1(\Omega)}, \quad \forall\, v \in H^1(\Omega). \tag{3.9}$$

Lemma 3.2. *There is a positive constant C_3 such that*

$$\begin{aligned}
&\max_{0\le m\le K} \left(\|\theta_m\|_2^2 + \|\beta_m\|^2_{H^1(\Omega)}\right) + \sum_{m=1}^K h \|\theta_m\|^2_{H^1(\Omega)} + \sum_{m=1}^K h \left\| \sqrt{\eta_m}\, \frac{\beta_m - \beta_{m-1}}{h}\right\|_2^2 \\
&+ \sqrt{h} \sum_{m=1}^K h \left\| \frac{\beta_m - \beta_{m-1}}{h}\right\|_2^2 + \sum_{m=1}^K \|\theta_m - \theta_{m-1}\|_2^2 + \sum_{m=1}^K \|\beta_m - \beta_{m-1}\|^2_{H^1(\Omega)} \le C_3.
\end{aligned} \tag{3.10}$$

Proof. We consider (3.2a) with $v = h\theta_m$, test (3.2b) by $\theta_C\left(\beta_m - \beta_{m-1}\right)$, and add the two equations. Afterwards, we apply (AP.6) (see the Appendix), (3.2d), (3.4), (3.2c), $0 \in \partial I_{[0,1]}(\beta_{m-1})$, and Young's inequality to obtain

$$\begin{aligned}
&\frac{c_0}{2}\left(\|\theta_m\|_2^2 - \|\theta_{m-1}\|_2^2 + \|\theta_m - \theta_{m-1}\|_2^2\right) + \kappa h \|\nabla\theta_m\|^2_{2,3} + \alpha h \|\theta_m\|^2_{L^2(\Gamma)} \\
&+ \theta_C h \left\| \sqrt{\eta_m}\, \frac{\beta_m - \beta_{m-1}}{h}\right\|_2^2 + \sqrt{h}\theta_C h \left\| \frac{\beta_m - \beta_{m-1}}{h}\right\|_2^2 \\
&+ \frac{\mu}{2}\theta_C \left(\|\nabla\beta_m\|^2_{2,3} - \|\nabla\beta_{m-1}\|^2_{2,3} + \|\nabla\left(\beta_m - \beta_{m-1}\right)\|^2_{2,3}\right) + \theta_C \|\chi_m\left(\beta_m - \beta_{m-1}\right)\|_{L^1(\Omega)} \\
= {}& h\left(F_m, \theta_m\right)_{H^1(\Omega)^*\times H^1(\Omega)} + L \int_\Omega \left(\theta_{m-1} - \theta_C - \theta_m\right)\left(\beta_m - \beta_{m-1}\right) \mathrm{d}x
\end{aligned}$$

$$\leq h\frac{1}{2C_1}\|F_m\|^2_{H^1(\Omega)^*}+h\frac{C_1}{2}\|\theta_m\|^2_{H^1(\Omega)}$$
$$-L\int_\Omega\theta_C\left(\beta_m-\beta_{m-1}\right)\,\mathrm{d}x\,+\frac{c_0}{4}\|\theta_m-\theta_{m-1}\|_2^2+\frac{1}{c_0}L^2\|\beta_m-\beta_{m-1}\|_2^2\,.$$

Summing this inequality from $m=1$ to $m=k$ and using (3.9), (3.3), (3.2e), **(A1)**, **(A3)**, and (3.2c) we get

$$\frac{c_0}{2}\|\theta_k\|_2^2+\frac{c_0}{4}\sum_{m=1}^k\|\theta_m-\theta_{m-1}\|_2^2+\frac{1}{2}C_1\sum_{m=1}^k h\|\theta_m\|^2_{H^1(\Omega)}+\sqrt{h}\theta_C\sum_{m=1}^k h\left\|\frac{\beta_m-\beta_{m-1}}{h}\right\|_2^2$$
$$+\theta_C\sum_{m=1}^k h\left\|\sqrt{\eta_m}\,\frac{\beta_m-\beta_{m-1}}{h}\right\|_2^2+\frac{\mu}{2}\theta_C\|\beta_k\|^2_{H^1(\Omega)}+\frac{\mu}{2}\theta_C\sum_{m=1}^k\|\nabla\left(\beta_m-\beta_{m-1}\right)\|_{2,3}^2$$
$$\leq C_4+\frac{\sqrt{h}L^2}{c_0\theta_C}\sqrt{h}\theta_C\sum_{m=1}^k h\left\|\frac{\beta_m-\beta_{m-1}}{h}\right\|_2^2.$$

Applying (3.1), (3.2e), **(A1)**, and **(A3)**, we conclude that (3.10) is satisfied. □

Lemma 3.3. *There is a positive constant C_5 such that*

$$\max_{1\leq m\leq K}\|\chi_m\|_2^2+\sum_{m=1}^K h\left\|\frac{\beta_m-\beta_{m-1}}{h}\right\|_{\frac{4}{3}}^2+\sum_{m=1}^K h\left\|\eta_m\frac{\beta_m-\beta_{m-1}}{h}\right\|_2^2\leq C_5. \tag{3.11}$$

Proof. Testing formally (3.2b) by χ_m and using (3.2d), (3.2c), (3.4), $0\in\partial I_{[0,1]}(\beta_{m-1})$, and Young's inequality, we deduce

$$\|\chi_m\|_2^2\leq\frac{L}{\theta_C}\int_\Omega\left(\theta_{m-1}-\theta_C\right)\chi_m\,\mathrm{d}x\,\leq\frac{1}{2}\|\chi_m\|_2^2+\frac{L^2}{2\theta_C^2}\|\theta_{m-1}-\theta_C\|_2^2\,. \tag{3.12}$$

For a rigorous derivation of this inequality, one has to replace in (3.2c) the maximal monotone graph $\partial I_{[0,1]}$ by its Yosida approximation (see, e.g., [Bré71, p. 104]), test the modified version of (3.2c) by the approximations of β_m and χ_m, consider the passage to the limit, and use [Bar76, Chap. II, Prob. 1.1(iv)] .

Using (3.4), **(A3)**, and Hölder's inequality, we get

$$\left\|\frac{\beta_m-\beta_{m-1}}{h}\right\|_{\frac{4}{3}}^{\frac{4}{3}}\leq\frac{1}{\left(B_\eta^*\right)^{\frac{2}{3}}}\left\|\sqrt{\eta_m}\,\frac{\beta_m-\beta_{m-1}}{h}\right\|_2^{\frac{4}{3}}\left(\int_\Omega\left(|\nabla\beta_{m-1}|_2+1\right)^2\,\mathrm{d}x\right)^{\frac{1}{3}}.$$

Combining this with (3.12), (3.10), and $\eta_m\leq C_\eta$, we see that (3.11) is proved. □

Lemma 3.4. *There is a positive constant C_6 such that*

$$\sum_{m=1}^K h\left\|\frac{\theta_m-\theta_{m-1}}{h}\right\|^2_{H^1(\Omega)^*}+\sum_{m=1}^K h\|\beta_m\|^2_{H^2(\Omega)}\leq C_6. \tag{3.13}$$

Proof. Considering the terms in (3.2a) and the terms in (3.2b) and using (3.10), (3.9), (3.3), **(A3)**, and Young's inequality, it is not difficult to verify that

$$\sum_{m=1}^{K} h \left\| c_0 \frac{\theta_m - \theta_{m-1}}{h} + L \frac{\beta_m - \beta_{m-1}}{h} \right\|^2_{H^1(\Omega)^*} \leq C_7, \tag{3.14}$$

$$\mu^2 \sum_{m=1}^{K} h \, \| \Delta \beta_m \|_2^2 \leq C_8 + 2 \sum_{m=1}^{K} h \, \| \chi_m \|_2^2 + 2 \sum_{m=1}^{K} h \left\| \eta_m \frac{\beta_m - \beta_{m-1}}{h} \right\|_2^2 . \tag{3.15}$$

Hence, combining (3.14), (3.11), (AP.2), (3.15), (3.2d), and (AP.4) leads to (3.13). □

3.3 Convergence of the time–discrete scheme

From the solution to $(\mathbf{D_K})$, we define $\widehat{\theta}^K$ and $\widehat{\beta}^K$ in $H^1(0,T;L^2(\Omega))$ as the piecewise linear–in–time interpolation on [0,T] of $\theta_0, \ldots, \theta_K$ and $\beta_0, \ldots, \beta_K$ respectively, i.e., functions linear in time on $[(m-1)h, mh]$ for $m = 1, \ldots, K$ such that $\widehat{\theta}^K(\cdot, mh) = \theta_m$ and $\widehat{\beta}^K(\cdot, mh) = \beta_m$ respectively for $m = 0, \ldots, K$.

Let $\overline{\chi}^K \in L^\infty(0,T;L^2(\Omega))$ be the piecewise constant–in–time interpolation of $\chi_1, \ldots, \chi_K$, i.e., we define $\overline{\chi}^K(\cdot, t) = \chi_m$ for all $t \in (t_{m-1}, t_m]$ and $m = 1, \ldots, K$. The functions $\overline{\theta}^K \in L^2(0,T;H^1(\Omega))$, $\overline{\beta}^K \in L^2(0,T;H^2(\Omega))$, and $\overline{F}^K \in L^2(0,T;H^1(\Omega)^*)$ are specified analogously. Also, let $\underline{\theta}^K$ and $\underline{\beta}^K$ in $L^\infty(0,T;L^2(\Omega))$ be the piecewise constant–in–time interpolation of $\theta_0, \ldots, \theta_{K-1}$ and $\beta_0, \ldots, \beta_{K-1}$ respectively, i.e., we have $\underline{\theta}^K(\cdot, t) = \theta_{m-1}$ and $\underline{\beta}^K(\cdot, t) = \beta_{m-1}$ for all $t \in (t_{m-1}, t_m]$ and $m = 1, \ldots, K$.

Hence, we can rewrite (3.2a)–(3.2e) as

$$\left(c_0 \partial_t \widehat{\theta}^K + L \partial_t \widehat{\beta}^K, v \right)_{H^1(\Omega)^* \times H^1(\Omega)} + \kappa \int_\Omega \nabla \overline{\theta}^K \bullet \nabla v \, \mathrm{d}x + \alpha \int_\Gamma \overline{\theta}^K v \, \mathrm{d}\sigma$$
$$= \left(\overline{F}^K, v \right)_{H^1(\Omega)^* \times H^1(\Omega)}, \quad \forall \, v \in H^1(\Omega), \quad \text{a.e. in} \quad (0,T), \tag{3.16a}$$

$$\left(\eta \left(\underline{\theta}^K, \nabla \underline{\beta}^K \right) + \sqrt{h} \right) \partial_t \widehat{\beta}^K - \mu \, \Delta \overline{\beta}^K + \overline{\chi}^K = \frac{L}{\theta_C} \left(\underline{\theta}^K - \theta_C \right), \quad \text{a.e. in} \quad \Omega_T, \tag{3.16b}$$

$$\overline{\beta}^K \in [0,1], \quad \overline{\chi}^K \in \partial I_{[0,1]} \left(\overline{\beta}^K \right), \quad \text{a.e. in} \quad \Omega_T, \tag{3.16c}$$

$$\frac{\partial \overline{\beta}^K}{\partial n} = 0, \quad \text{a.e. in} \quad \Gamma \times (0,T), \tag{3.16d}$$

$$\widehat{\theta}^K(\cdot, 0) = \theta^0, \quad \widehat{\beta}^K(\cdot, 0) = \beta^0, \quad \text{a.e. in} \quad \Omega. \tag{3.16e}$$

Thanks to **(A3)** and (3.3), as $K \to \infty$ we have the strong convergence

$$\overline{F}^K \longrightarrow F \quad \text{in } L^2(0,T;H^1(\Omega)^*), \tag{3.17}$$

which can be verified by a density argument, for instance. In the light of the last three terms in estimate (3.10), let us point out that

$$\left\|\sqrt{h}\widehat{\beta}^K\right\|^2_{H^1(0,T;L^2(\Omega))} \leq \frac{1}{\sqrt{K}} C_9, \tag{3.18}$$

$$\left\|\overline{\theta}^K - \widehat{\theta}^K\right\|^2_{L^2(0,T;L^2(\Omega))} + \left\|\overline{\beta}^K - \widehat{\beta}^K\right\|^2_{L^2(0,T;H^1(\Omega))} \leq \frac{1}{K} C_{10}. \tag{3.19}$$

Then, using (3.10), (3.11), and (3.13), standard compactness arguments (see, e.g., [Zei90, Prop. 23.7, 23.19, Prob. 23.12]) allow us to deduce the existence of three functions θ, β, χ in $L^2(0,T;L^2(\Omega))$ such that, as $K \to \infty$, at least for some subsequence,

$$\widehat{\theta}^K \longrightarrow \theta \quad \text{weakly–star in} \quad H^1(0,T;H^1(\Omega)^*) \cap L^\infty(0,T;L^2(\Omega)), \tag{3.20}$$

$$\overline{\theta}^K \longrightarrow \theta \quad \text{weakly–star in} \quad L^\infty(0,T;L^2(\Omega)) \cap L^2(0,T;H^1(\Omega)), \tag{3.21}$$

$$\widehat{\beta}^K \longrightarrow \beta \quad \text{weakly–star in} \quad H^1(0,T;L^{\frac{4}{3}}(\Omega)) \cap L^\infty(0,T;H^1(\Omega)), \tag{3.22}$$

$$\overline{\beta}^K \longrightarrow \beta \quad \text{weakly–star in} \quad L^\infty(0,T;H^1(\Omega)) \cap L^2(0,T;H^2(\Omega)), \tag{3.23}$$

$$\overline{\chi}^K \longrightarrow \chi \quad \text{weakly–star in} \quad L^\infty(0,T;L^2(\Omega)). \tag{3.24}$$

Now, we are going to show that the triplet (θ, β, χ) is a solution of the generalized weak formulation of **(P)** introduced in Theorem 2. In view of the above convergences, we see that the regularity conditions (2.4b), (2.4d), and

$$\theta \in H^1(0,T;H^1(\Omega)^*) \cap L^2(0,T;H^1(\Omega))$$

are proved. From the last inclusion, for instance by interpolation, (2.4a) follows. Owing to (3.17) and (3.20)–(3.22), the passage to limit in (3.16a) yields (2.5a). Combining (3.16d) and (3.23), we get (2.5b). Recalling (3.16e), the weak convergences in (3.20), (3.22), and the regularity condition (2.4a) lead to (2.1e).

For $K \in \mathbb{N}$, we consider $\tilde{\theta}^K \in H^1(0,T;H^1(\Omega))$ with

$$\tilde{\theta}^K(x,t') := \overline{\theta}^K(x,t'),\ \tilde{\theta}^K(x,t) := \widehat{\theta}^K(x,t), \quad \forall\, t' \in [0,h),\ t \in [h,T],\ \ x \in \Omega. \tag{3.25}$$

Using (3.10) and (3.13), it is straightforward to deduce that this sequence is uniformly bounded in $L^2(0,T;H^1(\Omega))$ and in $H^1(0,T;H^1(\Omega)^*)$. Moreover, in view of the last part of estimate (3.10), we conclude (similarly as in the derivation of (3.19)) that

$$\left\|\tilde{\theta}^K - \widehat{\theta}^K\right\|^2_{L^2(0,T;L^2(\Omega))} + \left\|\tilde{\theta}^K - \underline{\theta}^K\right\|^2_{L^2(0,T;L^2(\Omega))} \leq C_{11}\frac{1}{K}. \tag{3.26}$$

Using the Aubin Lemma (c.f., e.g., [Sim87, Cor. 4]), we see that $\{\tilde{\theta}^K\}_{K\in\mathbb{N}}$ is relatively compact in $L^2(0,T;L^2(\Omega))$. Combining this with (3.20) and (3.26), we obtain, at least for the selected subsequence, that, as $K \to \infty$,

$$\underline{\theta}^K \longrightarrow \theta \quad \text{strongly in} \quad L^2(0,T;L^2(\Omega)). \tag{3.27}$$

Defining $\tilde{\beta}^K \in H^1(0,T;H^2(\Omega))$ analogously to $\tilde{\theta}^K$ and using (3.10), (3.11), and (3.13), we see that this sequence is uniformly bounded in $H^1(0,T;L^{\frac{4}{3}}(\Omega)) \cap L^2(0,T;H^2(\Omega))$ and that

$$\left\|\tilde{\beta}^K - \overline{\beta}^K\right\|^2_{L^2(0,T;H^1(\Omega))} + \left\|\tilde{\beta}^K - \underline{\beta}^K\right\|^2_{L^2(0,T;H^1(\Omega))} \leq C_{12}\frac{1}{K}. \tag{3.28}$$

Applying again the Aubin Lemma, from (3.23) and (3.28) we get, at least for the selected subsequence,

$$\overline{\beta}^K \longrightarrow \beta, \quad \underline{\beta}^K \longrightarrow \beta \quad \text{strongly in} \quad L^2(0,T;H^1(\Omega)), \tag{3.29}$$

as $K \to \infty$. Thanks to (3.27) and (3.29), we can finally find a subsequence of the subsequence such that, as $K \to \infty$,

$$\underline{\theta}^K \longrightarrow \theta, \quad \nabla\underline{\beta}^K \longrightarrow \nabla\beta \quad \text{a.e. in} \quad \Omega_T. \tag{3.30}$$

Considering this subsequence, by **(A1)** and the Lebesgue dominated convergence theorem we obtain

$$\sqrt{\eta\left(\underline{\theta}^K, \nabla\underline{\beta}^K\right)} \longrightarrow \sqrt{\eta\left(\theta, \nabla\beta\right)}, \quad \eta\left(\underline{\theta}^K, \nabla\underline{\beta}^K\right) \longrightarrow \eta\left(\theta, \nabla\beta\right) \quad \text{strongly in} \quad L^p(\Omega_T)$$

as $K \to \infty$, for all $p \in [1,\infty)$. Now, for $0 < \varepsilon \leq \frac{1}{3}$ arbitrary, we recall (3.22) and (3.18) to show that, for this subsequence, as $K \to \infty$,

$$\sqrt{\eta\left(\underline{\theta}^K, \nabla\underline{\beta}^K\right)}\partial_t\widehat{\beta}^K \longrightarrow \sqrt{\eta\left(\theta, \nabla\beta\right)}\partial_t\beta \quad \text{weakly in} \quad L^{2-\varepsilon}(0,T;L^{\frac{4}{3}-\varepsilon}(\Omega)), \tag{3.31}$$

$$\left(\eta\left(\underline{\theta}^K, \nabla\underline{\beta}^K\right) + \sqrt{h}\right)\partial_t\widehat{\beta}^K \longrightarrow \eta\left(\theta, \nabla\beta\right)\partial_t\beta \quad \text{weakly in} \quad L^{2-\varepsilon}(0,T;L^{\frac{4}{3}-\varepsilon}(\Omega)). \tag{3.32}$$

We combine the last convergence with (3.16b), (3.23), (3.24), and (3.27) to show that (2.1b) is satisfied. Thanks to (3.16c), (3.24), (3.29), and [Bar76, Chap. II, Lemma 1.3], we deduce that (2.1c) holds. Since combining (3.31) and (3.10) yields by compactness that

$$\sqrt{\eta\left(\underline{\theta}^K, \nabla\underline{\beta}^K\right)}\partial_t\widehat{\beta}^K \longrightarrow \sqrt{\eta\left(\theta, \nabla\beta\right)}\partial_t\beta \quad \text{weakly in} \quad L^2(0,T;L^2(\Omega)), \tag{3.33}$$

we conclude that the remaining regularity condition (2.4c) is satisfied.

Therefore, Theorem 2 is proved. □

4 Proof of Theorem 1

In this section, we suppose that assumptions **(A1)** and **(A2)** are satisfied. Letting F be as in (2.3), we see that **(A3)** holds. Now, we consider $K \in \mathbb{N}$ sufficiently large, such that the inequality (3.1) is satisfied, and define, for $1 \le m \le K$, $f_m \in L^2(\Omega)$, $\theta_{\text{ext},m} \in H^{\frac{1}{2}}(\Gamma)$ by

$$f_m(x) := \frac{1}{h} \int_{(m-1)h}^{mh} f(x,t)\,\mathrm{d}t \quad \text{for a.e. } x \in \Omega, \tag{4.1}$$

$$\theta_{\text{ext},m}(\sigma) := \frac{1}{h} \int_{(m-1)h}^{mh} \theta_{\text{ext}}(\sigma,t)\,\mathrm{d}t \quad \text{for a.e. } \sigma \in \Gamma. \tag{4.2}$$

We see by (2.3), (3.3), (4.1), and (4.2) that

$$(F_m, v)_{H^1(\Omega)^* \times H^1(\Omega)} = \int_\Omega f_m v\,\mathrm{d}x + \alpha \int_\Gamma \theta_{\text{ext},m} v\,\mathrm{d}\sigma\,, \quad \forall\, v \in H^1(\Omega), \quad m = 1, \dots K. \tag{4.3}$$

The time–discrete scheme $(\mathbf{D_K})$ considered in the last section has a unique solution. For this solution there holds

Lemma 4.1. *For $m = 1, \dots, K$, we have $\theta_m \in H^2(\Omega)$,*

$$c_0 \frac{\theta_m - \theta_{m-1}}{h} + L \frac{\beta_m - \beta_{m-1}}{h} - \kappa\,\Delta\theta_m = f_m, \quad a.e.\ in \quad \Omega, \tag{4.4}$$

$$-\kappa \frac{\partial \theta_m}{\partial n} = \alpha(\theta_m - \theta_{ext,m}), \qquad a.e.\ on\ \Gamma. \tag{4.5}$$

Proof. Well–known results for elliptic equations (see, e.g., [Ama93, Theorem 9.2]) yield the existence of a unique function $\theta_m^* \in H^2(\Omega)$ such that (4.4) and (4.5), with θ_m replaced by θ_m^*, are satisfied. Now, testing (4.4) with $v \in H^1(\Omega)$ and using (4.5) and (4.3), we verify that θ_m^* is also a solution of (3.2a), which has a unique solution by the Lax–Milgram lemma. Hence, we have $\theta_m^* = \theta_m$ and the Lemma is proved. □

Lemma 4.2. *There are two positive constant C_{13}, C_{14} such that*

$$\sum_{m=1}^{K} h \left\| \frac{\beta_m - \beta_{m-1}}{h} \right\|_2^2 \le C_{13}, \tag{4.6}$$

$$\max_{0 \le m \le K} \|\theta_m\|_{H^1(\Omega)}^2 + \sum_{m=1}^{K} h \left\| \frac{\theta_m - \theta_{m-1}}{h} \right\|_2^2 + \sum_{m=1}^{K} \|\theta_m - \theta_{m-1}\|_{H^1(\Omega)}^2 \le C_{14}. \tag{4.7}$$

Proof. We see that (4.6) holds because of (3.10) and $\eta_m \ge B_\eta > 0$. Considering (3.2a) with $v = \theta_m - \theta_{m-1}$ (this is possible because of $\theta_0 \in H^1(\Omega)$), summing up the resulting equation from $m = 1$ to $m = k$, and using (4.3), (AP.6), (AP.5), (3.2e), and Young's inequality, we end up with

$$c_0 \sum_{m=1}^{k} h \left\| \frac{\theta_m - \theta_{m-1}}{h} \right\|_2^2 + \frac{\kappa}{2} \|\nabla \theta_k\|_{2,3}^2 + \frac{\alpha}{2} \|\theta_k\|_{L^2(\Gamma)}^2$$
$$+ \frac{\kappa}{2} \sum_{m=1}^{k} \|\nabla(\theta_m - \theta_{m-1})\|_{2,3}^2 + \frac{\alpha}{2} \sum_{m=1}^{k} \|\theta_m - \theta_{m-1}\|_{L^2(\Gamma)}^2$$

$$
\begin{aligned}
=&\frac{\kappa}{2}\left\|\nabla\theta_0\right\|_{2,3}^2+\frac{\alpha}{2}\left\|\theta_0\right\|_{L^2(\Gamma)}^2-L\sum_{m=1}^{k}h\int\limits_{\Omega}\frac{\beta_m-\beta_{m-1}}{h}\frac{\theta_m-\theta_{m-1}}{h}\,\mathrm{d}x\\
&+\sum_{m=1}^{k}h\int\limits_{\Omega}f_m\frac{\theta_m-\theta_{m-1}}{h}\,\mathrm{d}x+\alpha\int\limits_{\Gamma}\theta_{\mathrm{ext},k}\theta_k\,\mathrm{d}\sigma-\alpha\int\limits_{\Gamma}\theta_{\mathrm{ext},1}\theta_0\,\mathrm{d}\sigma\\
&-\alpha\sum_{m=1}^{k-1}h\int\limits_{\Gamma}\frac{\theta_{\mathrm{ext},m+1}-\theta_{\mathrm{ext},m}}{h}\theta_m\,\mathrm{d}\sigma\\
\le&\frac{\kappa}{2}\left\|\nabla\theta^0\right\|_{2,3}^2+\frac{\alpha}{2}\left\|\theta^0\right\|_{L^2(\Gamma)}^2+\frac{L^2}{c_0}\sum_{m=1}^{k}h\left\|\frac{\beta_m-\beta_{m-1}}{h}\right\|_2^2+\frac{1}{c_0}\sum_{m=1}^{k}h\left\|f_m\right\|_2^2\\
&+\frac{c_0}{2}\sum_{m=1}^{k}h\left\|\frac{\theta_m-\theta_{m-1}}{h}\right\|_2^2+\alpha\left\|\theta_{\mathrm{ext},k}\right\|_{L^2(\Gamma)}^2+\frac{\alpha}{4}\left\|\theta_k\right\|_{L^2(\Gamma)}^2+\alpha\left\|\theta_{\mathrm{ext},1}\right\|_{L^2(\Gamma)}\left\|\theta^0\right\|_{L^2(\Gamma)}\\
&+\frac{\alpha}{2}\sum_{m=1}^{k-1}h\left\|\frac{\theta_{\mathrm{ext},m+1}-\theta_{\mathrm{ext},m}}{h}\right\|_{L^2(\Gamma)}^2+\frac{\alpha}{2}\sum_{m=1}^{k-1}h\left\|\theta_m\right\|_{L^2(\Gamma)}^2.
\end{aligned}
$$

Hence, applying (3.9), **(A2)**, (4.6), (4.1), (4.2), and (3.10), we conclude that (4.7) holds. □

Lemma 4.3. *There is a positive constant C_{15} such that*

$$
\sum_{m=1}^{K}h\left\|\theta_m\right\|_{H^2(\Omega)}^2\le C_{15}. \tag{4.8}
$$

Proof. Comparing the terms in (4.4) and using (4.7), (4.6), (4.1), and **(A2)**, we see that

$$
\sum_{m=1}^{K}h\left\|\Delta\theta_m\right\|_2^2\le C_{16}.
$$

Therefore, with the help of (AP.3), (4.5), (4.2), **(A2)**, and (3.10), we deduce that (4.8) holds. □

Defining the functions $\overline{f}^K\in L^2(0,T;L^2(\Omega))$, and $\overline{\theta}_{\mathrm{ext}}^K\in L^2(0,T;L^2(\Gamma))$ analogously to $\overline{F}^K\in L^2(0,T;L^2(\Omega))$, we see by (4.4) and (4.5) that

$$
c_0\partial_t\widehat{\theta}^K+L\partial_t\widehat{\beta}^K-\kappa\,\Delta\overline{\theta}^K=\overline{f}^K,\quad\text{a.e. in}\quad\Omega_T, \tag{4.9}
$$

$$
-\kappa\frac{\partial\overline{\theta}^K}{\partial n}=\alpha\left(\overline{\theta}^K-\overline{\theta}_{\mathrm{ext}}^K\right),\qquad\text{a.e. on }\Gamma\times(0,T). \tag{4.10}
$$

Thanks to **(A2)**, (4.1), and (4.2), we can use a density argument to show the strong convergences

$$
\overline{f}^K\longrightarrow f\quad\text{in }L^2(0,T;L^2(\Omega)),\quad\overline{\theta}_{\mathrm{ext}}^K\longrightarrow\theta_{ext}\quad\text{in }L^2(0,T;H^{\frac{1}{2}}(\Gamma)), \tag{4.11}
$$

as $K \to \infty$. Coming back now to the passage to the limit of the last section, here from (4.6)–(4.8), (3.20)–(3.22), and compactness it follows that

$$\widehat{\beta}^K \longrightarrow \beta \quad \text{weakly in} \quad H^1(0,T;L^2(\Omega)), \tag{4.12}$$

$$\widehat{\theta}^K \longrightarrow \theta \quad \text{weakly–star in} \quad H^1(0,T;L^2(\Omega)) \cap L^\infty(0,T;H^1(\Omega)), \tag{4.13}$$

$$\overline{\theta}^K \longrightarrow \theta \quad \text{weakly–star in} \quad L^\infty(0,T;H^1(\Omega)) \cap L^2(0,T;H^2(\Omega)), \tag{4.14}$$

for the selected subsequence, as $K \to \infty$. Owing to these convergences, (2.4b), (2.4d), and the embedding of $H^1(0,T;L^2(\Omega)) \cap L^2(0,T;H^2(\Omega))$ in $C^0([0,T];H^1(\Omega))$, we infer that the regularity condition (2.2) is satisfied. Moreover, thanks to (4.11)–(4.14), we see that (4.9), (4.10), and (2.5b) imply that (2.1a) and (2.1d) are fulfilled. Since (2.1b), (2.1c), and (2.1e) have already been shown, Theorem 1 is proved. □

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Appendix

For convenience, we list some inequalities and equalities used throughout the paper.

Lemma AP.1 (Young's inequality). *For $a \geq 0$, $b \geq 0$, $p > 1$, $q := \frac{p}{p-1}$, and $\sigma > 0$, there holds*

$$ab \leq \frac{1}{p}a^p + \frac{1}{q}b^q, \quad ab \leq \frac{1}{p}\sigma^{-(p-1)}a^p + \frac{1}{q}\sigma b^q.$$

Thanks to Sobolev's embedding theorem, we have

Lemma AP.2. *For a bounded domain $\Omega \subset \mathbb{R}^3$ with Lipschitz boundary, there is a positive constant C such that*

$$\|v\|_{L^6(\Omega)} \leq C\,\|v\|_{H^1(\Omega)}\,, \quad \forall\, v \in H^1(\Omega). \tag{AP.1}$$

Moreover, we have

$$L^p(\Omega) \subset H^1(\Omega)^*, \quad \forall\, p \geq \frac{6}{5}. \tag{AP.2}$$

The following classical elliptic estimate can be found in [Ama93, Remark 9.3 d].

Lemma AP.3. *For a smooth bounded domain $\Omega \subset \mathbb{R}^N$ with $N \in \mathbb{N}$ and boundary Γ, there is a positive constant C such that*

$$\|v\|^2_{H^2(\Omega)} \leq C\left(\|\Delta v\|^2_{L^2(\Omega)} + \left\|\frac{\partial v}{\partial n}\right\|^2_{H^{\frac{1}{2}}(\Gamma)} + \|v\|^2_{L^2(\Omega)}\right), \quad \forall\, v \in H^2(\Omega). \tag{AP.3}$$

In particular, for all $v \in H^2(\Omega)$ with $\frac{\partial v}{\partial n} = 0$ a.e. on Γ,

$$\|v\|^2_{H^2(\Omega)} \leq C\left(\|\Delta v\|^2_{L^2(\Omega)} + \|v\|^2_{L^2(\Omega)}\right). \tag{AP.4}$$

Elementary calculations lead to

Lemma AP.4. *For $n \in \mathbb{N}$, $a_0, a_1, \ldots, a_n$, $b_0, b_1, \ldots, b_n \in \mathbb{R}$, we have that*

$$\sum_{m=1}^{n} a_m(b_m - b_{m-1}) = a_n b_n - a_1 b_0 - \sum_{m=1}^{n-1}(a_{m+1} - a_m)\, b_m. \tag{AP.5}$$

Lemma AP.5. *Let H be a Hilbert space with scalar-product $\langle\cdot,\cdot\rangle_H$ and norm $\|\cdot\|_H$. Then we have*

$$\langle a, a-b\rangle_H = \frac{1}{2}\|a\|^2_H - \frac{1}{2}\|b\|^2_H + \frac{1}{2}\|a-b\|^2_H\,, \quad \forall\, a, b \in H. \tag{AP.6}$$