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A SEMIDISCRETIZATION SCHEME FOR A PHASE-FIELD TYPE MODEL FOR SOLIDIFICATION

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Abstract: A mathematical analysis of a time discretization scheme for an initial-boundary value problem for a phase-field type model for phase transitions is presented. Convergence of the solutions of the proposed discretized scheme is proved and existence and regularity results for the original problem are derived. The long time behavior of the constructed solutions is also considered.

1 – Introduction

Phase transitions are important phenomena occurring in many physical situations, and, for this, they have been extensively studied along decades by many researchers. Although there are many complex possibilities for phase change, in this work, we restrict ourselves to the analysis of a problem involving only solidification and melting, that is, solid-liquid phase changes.

We start by observing that there are basically three methodological approaches for modelling such phase transitions, namely, the Stefan's, the enthalpy and the phase-field methodologies.

In a simplified and very brief way, we can say that the main point in the derivation of the model equations using the Stefan's approach is the assumption that each solid-liquid interface is a sharp smooth surface (see for instance Alexiades [1].)

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Then, based on conservation principles, the governing equations for thermodynamic variables are independently formulated in each phase. Next, conservation laws are imposed of the interface, and by a limit process the so-called Stefan's conditions are obtained, which supply additional equations governing the evolution of the interfaces. The result is a highly non-linear free-boundary problem since the location of each interface is not *a priori* known.

In this approach, the inclusion of several important effects, like surface tension, must be done directly on the Stefan's conditions for the interfaces, leading to the so-called modified Stefan problems. Surface tension effects, for instance, can be incorporated by using a Gibbs–Thompson-type condition (see Colli [11] and Mullis [31]). However, other important effects may be harder to incorporate in a clear and satisfactory physical way to the Stefan's conditions. More detailed discussion of the Stefan-type problem may be found in Alexiades [1] and Rubinstein [35].

From a computational viewpoint, perhaps the most difficult aspect of the Stefan's approach is the fact that it requires that the interfaces be tracked numerically. And this is a very difficult task in realistic situations where the interfaces evolve in complex ways, forming for instance dendrities.

Another aspect is that the real physical situation may be more complex than indicated by the classical Stefan's approach. The very concept of a sharp interface separating the different phases may be physically unrealistic. In fact, there are many situations where such interfaces are transitions layers with nonzero thickness and even internal structure; there are situations where mushy zones are formed, and so on.

A possibility to avoid the last appointed difficulties is to resort to the concept of enthalpy. In this approach, the phases are determined by the values of the enthalpy alone, with no explicit mentioning of the interface locations. The idea is that the transition layers are determined by certain level sets of the enthalpy. This allows the possibility of complex geometry and the existence of both thin layers and extended mushy zones. From the computational point of view, this formulation does not require that the interfaces be tracked numerically, which in practical situations brings advantages to the enthalpy method, as compared to the Stefan formulation (see Alexiades [1], p. 257.) However, the enthalpy method has certain physical limitations, excluding for instance problems with special interface conditions, such as supercooling problems (see Wheeler *et al* [39]).

Another formulation extends this last idea by using more general order parameters than the enthalpy to specify the phases in terms of level sets. These order parameters are called phase-fields and not necessarily have direct physical meanings. The roots of this approach are originally in statistical physics, since its involved the construction of the Landau–Ginzburg free energy functional (see Landau [24]). This approach has the same advantages than the enthalpy approach as compared to the one by Stefan, including the computational advantages, and has much more flexibility than the enthalpy method, permitting the modelling of more complex physical situations.

The phase-field methodology was firstly proposed for the study of solidification processes by Fix [14]; then Caginalp extensively studied several phase-field models for solidification ([5, 7, 8].) He employed a free energy functional in the derivation of the kinetic equation for the phase-field; the usual conservation laws were used for the derivation for the thermodynamic variables. An alternative derivation for the phase-field equation was proposed by Peronse and Fife [32, 33]; they constructed an entropy functional, and postulated kinetic equations for the phase-field and the temperature that ensure that the entropy increase monotonically in time. Peronse and Fife exhibit a specific choice of entropy density which essentially recovers the phase-field model employed by Caginalp [4]. Thus, phase-field models provides a simple and elegant description the phase transition processes, and physical aspects can be naturally incorporated in the derivation of model equations. An important example of the utility such models is the numerical studies of dentritic growth (see Caginalp [7] and Kobayshi [21]).

Several papers have been devoted to the mathematical analysis of phase-field models for solidification. Questions like existence, uniqueness, regularity, and large time behavior of their solutions have been examined by many authors (e.g. [4, 17, 27, 26, 30, 3].)

In this work, we are also interested in performing this kind of mathematical analysis, in a situation where the phase-field variable is related to the fraction of solidified material (see Beckermann [2]). In this case, the enthalpy, h, of the material is expressed by $h = e+(L/2)(1-f_s)$, where e is the internal energy, which depends on the temperature, L is the latent heat and f_s is the solid fraction (and thus, $(1-f_s)$ is the liquid fraction). Since this solid fraction may be functionally dependent on the phase-field variable and the temperature, the usual balance of energy arguments couple the temperature equation to the phase-field equation. In [3], this kind of situation was analyzed under the simplifying assumption that the solid fraction depended only on the phase-field variable. In that work, in a context that also included the possibility of convection of the melted material, a mathematical analysis of the resulting model was performed, and existence and regularity for its solutions were proved. However, the techniques employed in [3] were not enough to manage the case in which the solid fraction was function both of the phase-field and temperature, even in the situation without convection of the melted material.

The purpose of this paper is analyze a phase-field model for which the solid fraction is explicitly functionally dependent of both the phase-field variable and the temperature (without the possibility of convection of the melted material; the inclusion of this possibility will be addressed in a future work.) For this, we will employ a technique that constructs approximations by using semidiscretization in time, and then we will be able to prove existence and regularity of solutions of the original problem under rather natural physical conditions. We remark that this kind of technique was also employed in previous papers (e.g. [20, 19, 38]) addressing other types of phase-field problems.

The paper is organized as follows. The next section is dedicated to present the model equations, formulate our general assumptions and fix both the notations and the basic functional spaces to be used. In this section, we also define what we understand by a generalized solution of our problem, introduce the time-discretization scheme and state the main results of the paper. Section 3 has the proof of existence of the discrete solution, that is, the solution of the discretized scheme, as well as certain regularity results. Section 4 contains a collection of estimates, which are uniform with respect to the time-discretization step. These estimates will allow us to pass to the limit in Section 5 and obtain our main results. In Section 6, we comment on the long time behavior of the constructed solutions.

Finally, we remark that, as it is usual in this sort of work, during the computations of the estimates, we will often use a generic C to denote constants depending only on known quantities.

2 – Model equations, technical hypotheses and main results

Let us consider the following initial-boundary value problem:

$$\tag{2.1} \begin{aligned} \frac{\partial\varphi}{\partial t} - \alpha\,\Delta\varphi &= a(x)\varphi + b(x)\varphi^2 - \varphi^3 + \theta && \text{in } Q\,, \\ \frac{\partial\theta}{\partial t} - \kappa\,\Delta\theta &= \frac{\ell}{2}\,\frac{\partial}{\partial t} f_s(\theta,\varphi) && \text{in } Q\,, \end{aligned}$$

$$\tag{2.2} \begin{aligned} &\frac{\partial\varphi}{\partial\eta} = 0\,, \quad \theta = 0 && \text{on } S\,, \\ &\varphi(x,0) = \varphi_0(x)\,, \quad \theta(x,0) = \theta_0(x) && \text{in } \Omega\,. \end{aligned}$$

This system is a mathematical model for the evolution in time of a process of solidification/melting of a pure material. We assume that the process is occurring in a region $\Omega \subset \mathbb{R}^n$, and the time interval of interest is $[0, T]$, with $T > 0$. The variables φ and θ are respectively the phase-field and temperature. The *mass solid fraction* $f_s(\theta, \varphi)$ is supposed to be a known function of the temperature and phase-field. The initial data $\varphi_0(x), \theta_0(x)$ and $a(x), b(x)$ are also known functions. The parameters ℓ, and κ are positive constants corresponding respectively to the latent heat and thermal conductivity coefficients divided by the specific heat of the material. $\alpha > 0$ is a constant related to the thickness of the transition layers, and $\partial/\partial\eta$ denotes the outward normal derivative at $\partial\Omega$.

The first equation in (2.1) describes the evolution of the phase-field variable φ; it is exactly as in Hoffman and Jiang [17]. The function $g(x, s) = a(x)s + b(x)s^2 - s^3$ at the the right-hand side of this equation is classical and comes from the choice of a double-well potential as an interaction potential between the phases for the free-energy of the system. Other possibilities could be considered; see for instance [12]. For a detailed discussions of the phase-field transition system, we refer to [4] and [13]. The second equation in (2.1) results from energy conservation.

In the following, we will very briefly describe our notations and functional spaces to be used.

Let $\Omega \subset \mathbb{R}^n$ be an open and bounded domain with sufficiently smooth boundary $\partial\Omega$; (C^2-regularity will be enough for the purposes of this paper); let T be a finite positive number, and denote $Q = \Omega\times(0, T)$ the space-time cylinder with lateral surface $S = \partial\Omega\times(0, T)$.

For a nonnegative integer m and $1 \le q \le +\infty$, $W_q^m(\Omega)$ is the traditional Sobolev space consisting of the functions $u(x)$ having generalized derivatives up to order m in $L_q(\Omega)$. Such space is supplied with the usual norm. For $q = 2$ this space is denoted by $H^p(\Omega)$. $\overset{0}{W}{}_q^m(\Omega)$ is the closure in this norm of the set of all infinitely differentiable functions with compact support in Ω. For non integers m, similar spaces can be defined by interpolation, for instance.

$W_q^{2,1}(Q)$ is a Banach space consisting of functions $u(x, t)$ in $L_q(Q)$ whose generalized derivatives $D_x u, D_x^2 u, u_t$ are L_q-integrable ($q \ge 1$). The norm in $W_q^{2,1}(Q)$ is defined by

$$\|u\|_{q,Q}^{(2)} = \|u\|_{q,Q} + \|D_x u\|_{q,Q} + \|D_x^2 u\|_{q,Q} + \|u_t\|_{q,Q} \tag{2.3}$$

where D_x^s denotes any partial derivatives with respect to variables $x_1, x_2, ..., x_n$ of order $s = 1, 2$ and $\|\cdot\|_q$ the usual norm in the space $L_q(Q)$.

The space $W_2^{1,0}(Q)$ consist of the functions $u(x,t)$ in $L_2(Q)$ having generalized derivatives $D_x u$ in $L_2(Q)$. We denote by $\overset{0}{W}{}_2^{1,0}(Q)$ the subspace of $W_2^{1,0}(Q)$ whose functions vanish on S in the sense of traces.

The space $W_2^{1,1}(Q)$ consist of the functions $u(x,t)$ in $L_2(Q)$ having generalized derivatives $D_x u$ and u_t in $L_2(Q)$. We denote by $\overset{0}{W}{}_2^{1,1}(Q)$ the subspace of $W_2^{1,1}(Q)$ whose functions vanish on S in the sense of traces.

More details about the above spaces are given in [23]. Other classical functional spaces will also be used, with standard notations and definitions.

All along this work we will be using the following technical hypotheses:

(H_1) $\Omega \subset \mathbb{R}^n$, $n=2$ or 3, is an open and bounded domain with a C^2 boundary.

(H_2) $a(x)$, $b(x)$ are given functions in $L_\infty(\Omega)$; f_s is a known function in $C_b^{1,1}(\mathbb{R}^2)$ such that $0 \le f_s(y,z) \le 1$ $\forall\,(y,z) \in \mathbb{R}^2$ and such that for each $z \in \mathbb{R}$, $y \mapsto f_s(y,z)$ is non increasing.

(H_3) $\varphi_0 \in W_2^{(3/2)+\delta}(\Omega)$ for some $\delta \in (0,1)$; $\dfrac{\partial \varphi_0}{\partial \eta} = 0$ on $\partial\Omega$; $\theta_0 \in \overset{0}{W}{}_2^{1}(\Omega)$.

Remark. The monotony condition on $f_s(\,.\,z)$ required in (H_2) is natural since for most materials the solid fraction is not expected to increase with an increase of temperature. □

In the following we will explain in what sense we will understand a solution of (2.1)–(2.2) (see [23], p. 26).

Definition 2.1. By a **generalized solution** of problem (2.1)–(2.2), we mean a pair of functions $(\varphi,\theta) \in W_2^{1,1}(Q) \times \overset{0}{W}{}_2^{1,1}(Q)$ satisfying (2.1)–(2.2) in the following sense

$$
\begin{aligned}
-\int_Q \varphi\,\beta_t\;dxdt + \alpha\int_Q \nabla\varphi\,\nabla\beta\;dxdt &= \\
= \int_Q \Big(a(x)\varphi + b(x)\varphi^2 - \varphi^3\Big)\beta\;dxdt &+ \int_Q \theta\beta\;dxdt + \int_\Omega \varphi_0(x)\,\beta(x,0)\,dx\;,
\end{aligned}
$$

$$
\begin{aligned}
-\int_Q \theta\,\xi_t\;dxdt + \kappa\int_Q \nabla\theta\,\nabla\xi\;dxdt &= \\
= \frac{\ell}{2}\int_Q \Big(\frac{\partial f_s}{\partial t}(\theta,\varphi)\Big)\xi\;dxdt &+ \int_\Omega \theta_0(x)\,\xi(x,0)\,dx\;,
\end{aligned}
$$

for all β in $W_2^{1,1}(Q)$ such that $\beta(x,T) = 0$ and for all ξ in $\overset{0}{W}{}_2^{1,1}(Q)$ such that $\xi(x,T) = 0$. □

Note that due to our technical hypotheses and choice of functional spaces, all of the integrals in Definition 2.1 are well defined.

In the sequel, we introduce a time-discretization scheme (see [23], p. 241) for the phase-field type model (2.1)–(2.2).

Let N be an integer and $\mathcal{P}$ be a partition of the time interval [0,T] such that $\mathcal{P} = \{t_0, t_1, ..., t_N\}$ with $0 = t_0 < t_1 < ... < t_m < ... < t_N = T$ where $t_m = m\tau$, $0 \le m \le N$ and $\tau = T/N$ is the time-step.

For $m = 1, 2, ..., N$, we consider the differential-difference equations

$$\delta_t\varphi^m - \alpha\,\Delta\varphi^m \;=\; a(x)\varphi^m + b(x)(\varphi^m)^2 - (\varphi^m)^3 + \theta^m \qquad \text{a.e. in } \Omega\,, \tag{2.4}$$

$$\delta_t\theta^m - \kappa\,\Delta\theta^m \;=\; \frac{\ell}{2}\left(\frac{f_s(\theta^m,\varphi^m) - f_s(\theta^{m-1},\varphi^{m-1})}{\tau}\right) \qquad \text{a.e. in } \Omega\,, \tag{2.5}$$

$$\frac{\partial\varphi^m}{\partial n} \;=\; 0\,, \qquad \theta^m = 0 \qquad \text{a.e. in } \partial\Omega\,, \tag{2.6}$$

assuming

$$\varphi^0 = \varphi_0\,, \qquad \theta^0 = \theta_0\,. \tag{2.7}$$

Here, we used the notation

$$\delta_t\varphi^m \;=\; \frac{1}{\tau}\left(\varphi^m - \varphi^{m-1}\right) \tag{2.8}$$

$$\delta_t\theta^m \;=\; \frac{1}{\tau}\left(\theta^m - \theta^{m-1}\right), \tag{2.9}$$

and φ^m and θ^m, $m = 1, ..., N$, are expected to be approximations of $\varphi(x, t_m)$ and $\theta(x, t_m)$, respectively.

Definition 2.2. (φ^m, θ^m), $m = 1, 2, ..., N$, is said to be solution to the scheme (2.4)–(2.7) if $\varphi^m \in W_2^1(\Omega)$, $\theta^m \in \overset{0}{W}{}_2^1(\Omega)$ for every $m = 1, 2, ..., N$, (2.7) is true, and relations (2.4)–(2.6) are satisfied in the following sense

$$\int_\Omega \delta_t\varphi^m\,\widehat{\beta}(x)\,dx \,+\, \alpha\int_\Omega \nabla\varphi^m\,\nabla\widehat{\beta}\;dx \;=\; \\ = \int_\Omega \Big(a\varphi^m + b(\varphi^m)^2 - (\varphi^m)^3\Big)\widehat{\beta}(x)\;dx \,+\, \int_\Omega \theta^m\widehat{\beta}(x)\;dx\,,$$

$$\int_\Omega \delta_t\theta^m\widehat{\xi}(x)\,dx \,+\, \kappa\int_\Omega \nabla\theta^m\,\nabla\widehat{\xi}\;dx \;=\; \frac{\ell}{2}\int_\Omega \frac{f_s(\theta^m,\varphi^m) - f_s(\theta^{m-1},\varphi^{m-1})}{\tau}\,\widehat{\xi}(x)\;dx$$

for all $\widehat{\xi} \in \overset{0}{W}{}_2^1(\Omega)$ and $\widehat{\beta} \in W_2^1(\Omega)$. □

The following existence result for the discrete scheme given by (2.4)–(2.7) will be proved in the next section.

Theorem 2.1. *Assume that* (H_1), (H_2) *and* (H_3) *hold. Then, there is a generalized solution of the discrete scheme* (2.4)–(2.6) *in sense of Definition* 2.2. *Moreover, this solution is unique when the time-step* τ *is small enough.*

Using this result, we may introduce the corresponding piecewise constant interpolating functions φ_τ, θ_τ and also the corresponding linear interpolate functions $\widetilde{\varphi}_\tau$, $\widetilde{\theta}_\tau$:

Definition 2.3. Consider a partition $\mathcal{P} = \{t_0, t_1, ..., t_{N-1}, t_N\}$ such that $t_m = m\tau$ for $1 \leq m \leq N$ and $\tau = T/N$. Then, given $\{\gamma^m\}_{m=0}^N \in L_2(\Omega)$, we define the interpolations functions $\gamma_\tau\,, \widetilde{\gamma}_\tau\colon\ [0,T] \to L_2(\Omega)$ as follows: for a.e. $x \in \Omega$ and for $t \in [(m-1)\tau, m\tau]$, we set

$$\begin{aligned} \gamma_\tau(x,t) \;&=\; \gamma^m\;, \\ \widetilde{\gamma}_\tau(x,t) \;&=\; \gamma^m + \left(\frac{t-t_m}{\tau}\right)\left(\gamma^m - \gamma^{m-1}\right). \;\square \end{aligned}$$

In Section 5, we will prove the following result

Theorem 2.2. *Assume that* (H_1), (H_2) *and* (H_3) *holds. Let* φ_τ, $\widetilde{\varphi}_\tau$, θ_τ, $\widetilde{\theta}_\tau$ *be functions as in Definition* 2.3 *and corresponding to the solution of the discrete scheme* (2.4)–(2.6) *that was obtained in Theorem* 2.1. *Then, as* $\tau \to 0$, *we have the following convergences:*

$$\begin{aligned} &\theta_\tau \rightharpoonup \theta, \quad \varphi_\tau \rightharpoonup \varphi \qquad \text{in} \quad L^2\big(0,T,W_2^2(\Omega)\big)\;, \\ &\theta_\tau \overset{*}{\rightharpoonup} \theta, \quad \varphi_\tau \overset{*}{\rightharpoonup} \varphi \qquad \text{in} \quad L^\infty\big(0,T,W_2^1(\Omega)\big)\;, \\ &\widetilde{\theta}_\tau \rightharpoonup \theta, \quad \widetilde{\varphi}_\tau \rightharpoonup \varphi \qquad \text{in} \quad L^2\big(0,T,W_2^1(\Omega)\big)\;, \\ &\theta_\tau \to \theta, \quad \varphi_\tau \to \varphi \qquad \text{in} \quad L_2(Q)\;. \end{aligned} \tag{2.10}$$

and the pair (φ,θ) *is a generalized solution of the problem* (2.1)–(2.2) *in the sense of the Definition* 2.1.

Moreover, when $\varphi_0 \in W_q^{2-2/q}(\Omega) \cap W_2^{3/2+\delta}(\Omega)$ *for some* $\delta \in (0,1)$ *and* $3 \leq q \leq 9$, *then such solution satisfies* $\varphi \in W_q^{2,1}(Q) \cap L_\infty(Q)$ *and* $\theta \in W_2^{2,1}(Q) \cap L_9(Q)$.

Finally, we mention that in Theorem 6.1 we will state a result concerning the long time behavior of the solutions given in Theorem 2.1.

3 – Discrete solutions

Our aim in this section is to prove the existence of the solution φ^m, θ^m of the system (2.4)–(2.6), for a fixed m and assuming that φ^{m-1} and θ^{m-1} are already known. For this, consider the following non-linear system:

$$\left\{\begin{aligned} -\tau\alpha\,\Delta\varphi+\varphi \;&=\; \tau\Big(a(x)\varphi+b(x)\varphi^2-\varphi^3+\theta\Big)+g(x)\;,\\ -\tau\kappa\,\Delta\theta+\theta \;&=\; \frac{\ell}{2}\,f_s(\theta,\varphi)+h(x)\,, \qquad \text{in}\;\;\Omega\;, \end{aligned}\right. \tag{3.1}$$

subject to the boundary conditions:

$$\frac{\partial\varphi}{\partial n}=0\,,\quad \theta=0 \qquad \text{on}\;\;\partial\Omega\;, \tag{3.2}$$

where $(\varphi,\theta)=(\varphi^m,\theta^m)$, $g(x)=\varphi^{m-1}$, and $h(x)=\big(\theta^{m-1}+f_s(\theta^{m-1},\varphi^{m-1})\big)$.

We will apply the Leray–Schauder degree theory (see [12]) to prove the existence of solutions of problem (3.1), (3.2). For this, we reformulate the problem as $T(1,\varphi,\theta)=(\varphi,\theta)$, where $T(\lambda,.)$ is a compact homotopy depending on a parameter $\lambda\in[0,1]$ defined as follows.

Consider the non-linear operator

$$T\colon\;\; [0,1]\times W^1_2(\Omega)\times \overset{0}{W}{}^1_2(\Omega) \to W^1_2(\Omega)\times \overset{0}{W}{}^1_2(\Omega)$$

defined as

$$T(\lambda,\phi,\omega)=(\varphi,\theta)\;, \tag{3.3}$$

where (φ,θ) is the unique solution of the following problem:

$$\left\{\begin{aligned} -\tau\alpha\,\Delta\varphi+\varphi \;&=\; \lambda\tau\Big(a(x)\phi+b(x)\phi^2-\phi^3+\omega\Big)+\lambda g(x)\;,\\ -\tau\kappa\,\Delta\theta+\theta \;&=\; \lambda\Big(\frac{\ell}{2}\,f_s(\omega,\phi)+h(x)\Big) \qquad \text{in}\;\;\Omega\;, \end{aligned}\right. \tag{3.4}$$

subject to the following boundary conditions

$$\frac{\partial\varphi}{\partial n}=0\,,\quad \theta=0 \qquad \text{on}\;\;\partial\Omega\;. \tag{3.5}$$

To verify that $T(\lambda,\cdot)$ is well defined, we observe that $a\phi+b\phi^2-\phi^3+\omega+g\in L_2(\Omega)$; thus, by the L_p-regularity theory for elliptic linear equations (see [22], Chapter 3), we conclude that the first equation of problem (3.4), (3.5) has a unique solution $\varphi\in W_2^2(\Omega)\cap(L_2(\Omega)/\mathbb{R})$. In addition, $f_s\in C_b^{1,1}(\mathbb{R}^2)$ and $h\in L_6(\Omega)$ imply again by the L_p-regularity theory for elliptic linear equation that there is a unique solution $\theta\in W_2^2(\Omega)$ of the second equation of (3.4)–(3.5).

To check the continuity of $T(\lambda,\cdot)$, let $\lambda_n\to\lambda$ in [0,1] and $(\phi_n,\omega_n)\to(\phi,\omega)$ in $W_2^1(\Omega)\times\overset{0}{W}{}_2^1(\Omega)$. Denote $T(\lambda_n,\phi_n,\omega_n)=(\varphi_n^{\lambda_n},\theta_n^{\lambda_n})$, $T(\lambda,\phi_n,\omega_n)=(\varphi_n^{\lambda},\theta_n^{\lambda})$ and $T(\lambda,\phi,\omega)=(\varphi^{\lambda},\theta^{\lambda})$. From (3.3) and (3.4)–(3.5), we obtain

$$
\begin{cases}
-\tau\alpha\,\Delta(\varphi_n^{\lambda_n}-\varphi_n^{\lambda})+(\varphi_n^{\lambda_n}-\varphi_n^{\lambda}) \;=\; (\lambda_n-\lambda)\,\tau(a\phi_n+b\phi_n^2-\phi_n^3+\omega_n) \\
\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad +(\lambda_n-\lambda)g\,, \\
-\tau\kappa\,\Delta(\theta_n^{\lambda_n}-\theta_n^{\lambda})+(\theta_n^{\lambda_n}-\theta_n^{\lambda}) \;=\; (\lambda_n-\lambda)\left(\dfrac{\ell}{2}\,f_s(\omega_n,\phi_n)+h\right),
\end{cases}
\tag{3.6}
$$

subject to boundary conditions

$$
\frac{\partial}{\partial\eta}\big(\varphi_n^{\lambda_n}-\varphi_n^{\lambda}\big)=0\,,\quad \big(\theta_n^{\lambda_n}-\theta_n^{\lambda}\big)=0\qquad\text{on }\ \partial\Omega\,.
\tag{3.7}
$$

Applying the L_p-regularity theory for elliptic linear equations to the equations of problem (3.6)–(3.7), observing that $\phi\in W_2^1(\Omega)\subset L_6(\Omega)$ and using the fact that $f_s\in C_b^{1,1}(\mathbb{R}^2)$, we obtain the following estimates

$$
\begin{aligned}
\|\varphi_n^{\lambda_n}-\varphi_n^{\lambda}\|_{W_2^1(\Omega)} &\le C\,|\lambda_n-\lambda|\Big(\|\phi_n\|_{2,\Omega}+\|\phi_n\|_{2,\Omega}^3+\|\omega_n\|_{2,\Omega}+\|g\|_{2,\Omega}\Big)\,,\\
\|\theta_n^{\lambda_n}-\theta_n^{\lambda}\|_{W_2^1(\Omega)} &\le C\,|\lambda_n-\lambda|\Big(1+\|h\|_{2,\Omega}\Big)\,,
\end{aligned}
\tag{3.8}
$$

where C depends on Ω, α, κ, ℓ, τ, $\|a\|_\infty$, $\|b\|_\infty$ and $\|f_s\|_\infty$.

Since the sequences $\{\phi_n\}$ and $\{\omega_n\}$ are bounded in $W_2^1(\Omega)\times\overset{0}{W}{}_2^1(\Omega)$, we conclude that $\|\varphi_n^{\lambda_n}-\varphi_n^{\lambda}\|_{W_2^1(\Omega)}\longrightarrow 0$ and $\|\theta_n^{\lambda_n}-\theta_n^{\lambda}\|_{W_2^1(\Omega)}\longrightarrow 0$ as $n\to\infty$.

Again from (3.3) and (3.4)–(3.5), we obtain

$$
\begin{cases}
-\tau\alpha\,\Delta(\varphi_n^{\lambda}-\varphi^{\lambda})+(\varphi_n^{\lambda}-\varphi^{\lambda}) \;=\; \tau\lambda\Big(d_n(\phi_n-\phi)+\omega_n-\omega\Big)\,,\\
-\tau\kappa\,\Delta(\theta_n^{\lambda}-\theta^{\lambda})+(\theta_n^{\lambda}-\theta^{\lambda}) \;=\; \lambda\,\dfrac{\ell}{2}\Big(f_s(\omega_n,\phi_n)-f_s(\omega,\phi)\Big)\,,
\end{cases}
\tag{3.9}
$$

subject to boundary conditions

$$
\frac{\partial}{\partial\eta}\big(\varphi_n^{\lambda}-\varphi^{\lambda}\big)=0\,,\quad \big(\theta_n^{\lambda}-\theta^{\lambda}\big)=0\qquad\text{on }\ \partial\Omega\,,
\tag{3.10}
$$

where $d_n = a(x) + b(x)(\phi_n + \phi) - (\phi_n^2 + \phi_n\phi + \phi^2) \in L^3(\Omega)$.

As before, the L_p-regularity theory for elliptic linear equations implies the following estimates

$$\|\varphi_n^\lambda - \varphi^\lambda\|_{W_2^1(\Omega)} \le C\Big(\|d_n(\phi_n - \phi)\|_{2,\Omega} + \|\omega_n - \omega\|_{2,\Omega}\Big) ,$$
$$\|\theta_n^\lambda - \theta^\lambda\|_{W_2^1(\Omega)} \le C\Big(\|f_s(\omega_n, \phi_n) - f_s(\omega, \phi)\|_{2,\Omega}\Big) .$$

Since $f_s(y, z)$ is a Lipschitz function, we get

$$\begin{aligned} \|\varphi_n^\lambda - \varphi^\lambda\|_{W_2^1(\Omega)} &\le C\Big(\|d_n\|_{3,\Omega}\|\phi_n - \phi\|_{6,\Omega} + \|\omega_n - \omega\|_{2,\Omega}\Big) , \\ \|\theta_n^\lambda - \theta^\lambda\|_{W_2^1(\Omega)} &\le C\Big(\|\phi_n - \phi\|_{W_2^1(\Omega)} + \|\omega_n - \omega\|_{2,\Omega}\Big) . \end{aligned} \tag{3.11}$$

Thus, $\|\varphi_n^\lambda - \varphi^\lambda\|_{W_2^1(\Omega)} \longrightarrow 0$ and $\|\theta_n^\lambda - \theta^\lambda\|_{W_2^1(\Omega)} \longrightarrow 0$ as $n \to \infty$, and we obtain the continuity of $T(\lambda, \cdot)$.

The mapping $T(\lambda, \cdot)$ given by (3.3) is also compact. In fact, if $\{(\lambda_n, \phi_n, \omega_n)\}$ is any bounded sequence in $[0,1] \times W_2^1(\Omega) \times \overset{0}{W}{}_2^1(\Omega)$, the previous arguments can be applied to obtain exactly the same sort of estimates for $T(\lambda_n, \phi_n, \omega_n) = (\varphi_n, \theta_n)$. These estimates supply $\|\varphi_n\|_{W_2^1(\Omega)} \le C$ and $\|\theta_n\|_{W_2^1(\Omega)} \le C$.

By using this and applying again the L_p-regularity theory for elliptic equations, we obtain that for all n

$$\|\varphi_n\|_{W_2^2(\Omega)} \le C \quad \text{and} \quad \|\theta_n\|_{W_2^2(\Omega)} \le C , \tag{3.12}$$

where C depends only on Ω, α, κ, ℓ, τ, $\|a\|_\infty$ and $\|b\|_\infty$.

Estimates (3.12) show that the norms of the elements of the sequence $\{T(\lambda_n, \phi_n, \omega_n)\} = \{(\varphi_n, \theta_n)\}$ are uniformly bounded with respect to n in the functional space $W_2^2(\Omega) \times W_2^2(\Omega)$. Since the embedding of $W_2^2(\Omega) \times (W_2^2(\Omega) \cap \overset{0}{W}{}_2^1(\Omega))$ into $W_2^1(\Omega) \times \overset{0}{W}{}_2^1(\Omega)$ is compact, there exists a subsequence of $T(\lambda_n, \phi_n, \omega_n)$ converging in $W_2^1(\Omega) \times \overset{0}{W}{}_2^1(\Omega)$ and, the compactness of $T(\lambda, \cdot)$ is proved.

In the following, we will show that any possible fixed point of $T(\lambda, \cdot)$ can be estimated independently of $\lambda \in [0,1]$; that is, we will show that if $(\varphi, \theta) \in W_2^1(\Omega) \times \overset{0}{W}{}_2^1(\Omega)$ is such that $T(\lambda, \varphi, \theta) = (\varphi, \theta)$, for some $\lambda \in [0,1]$, then there exists a constant $\beta > 0$ such that

$$\|(\varphi, \theta)\|_{W_2^1(\Omega) \times W_2^1(\Omega)} < \beta . \tag{3.13}$$

For this, we recall that such fixed point $(\varphi,\theta) \in W_2^1(\Omega)\times \overset{0}{W}{}_2^1(\Omega)$ solves the problem

$$\left\{\begin{aligned} -\tau\alpha\,\Delta\varphi+\varphi \;&=\; \tau\lambda\big(a\varphi+b\varphi^2-\varphi^3+\theta\big)+\lambda g\;,\\ -\tau\kappa\,\Delta\theta+\theta \;&=\; \lambda\bigg(\frac{\ell}{2}f_s(\theta,\varphi)+h\bigg) \qquad \text{in}\quad \Omega\;, \end{aligned}\right. \tag{3.14}$$

subject to the following boundary conditions

$$\frac{\partial\varphi}{\partial n}=0\,,\quad \theta=0 \qquad \text{on}\;\;\partial\Omega\;. \tag{3.15}$$

By multiplying the first equation in (3.14) by φ, integrating over Ω, using Green's formula and Young's inequality, we obtain

$$\tau\alpha\int_\Omega|\nabla\varphi|^2\,dx\;+\;\frac{1}{4}\int_\Omega|\varphi|^2\,dx\;\leq\;C\tau+\frac{\tau^2}{2}\|\theta\|^2_{2,\Omega}+\frac{1}{2}\|g\|^2_{2,\Omega}\;. \tag{3.16}$$

Here we also used that $\max\limits_{s\in\mathbb{R},\;x\in\Omega}\big(a(x)s^2+b(x)s^3-s^4\big)$ is finite.

By multiplying the second equation in (3.14) by θ, integrating over Ω, using Green's formula and Young's inequality, we get

$$\tau\kappa\int_\Omega|\nabla\theta|^2\,dx\;+\int_\Omega|\theta|^2\,dx\;\leq\;C\big(\|f_s(\theta,\varphi)\|^2_{2,\Omega}+\|h\|^2_{2,\Omega}\big)\;. \tag{3.17}$$

By using the fact that $f_s\in C_b^{1,1}(\mathbb{R}^2)$, we conclude that

$$\|\theta\|_{W_2^1(\Omega)}\;\leq\;C\big(1+\|h\|_{2,\Omega}\big)\,. \tag{3.18}$$

Now, by combining (3.16) and (3.18), we obtain

$$\|\varphi\|_{W_2^1(\Omega)}\;\leq\;C\big(1+\|g\|_{2,\Omega}+\|h\|_{2,\Omega}\big) \tag{3.19}$$

with C depending only on Ω, α, κ, ℓ, τ, $\|a\|_\infty$, $\|b\|_\infty$ and $\|f_s\|_\infty$.

Thus, it is enough to take β as any constant satisfying

$$\beta\;>\;\max\Big\{C\big(1+\|h\|_{2,\Omega}\big),\,C\big(1+\|g\|_{2,\Omega}+\|h\|_{2,\Omega}\big)\Big\}$$

to obtain the stated result. By denoting

$$B_\beta\;=\;\Big\{(\varphi,\theta)\in W_2^1(\Omega)\times\overset{0}{W}{}_2^1(\Omega)\;;\;\;\|(\varphi,\theta)\|_{W_2^1(\Omega)\times W_2^1(\Omega)}<\beta\Big\}\;,$$

(3.13) ensures in particular that

$$T(\lambda,\varphi,\theta) \neq (\varphi,\theta) \qquad \forall\,(\varphi,\theta)\in\partial B_\beta, \quad \forall\,\lambda\in[0,1]\;. \tag{3.20}$$

According to property (3.20) and the compactness of $T(\lambda,\cdot)$, we may consider the Leray–Schauder degree $D(Id-T(\lambda,\cdot),B_\beta,0)$, $\forall\,\lambda\in[0,1]$ (see Deimling [12]). The homotopy invariance of the degree implies

$$D\big(Id-T(0,\cdot),B_\beta,0\big) \;=\; D\big(Id-T(1,\cdot),B_\beta,0\big)\;. \tag{3.21}$$

Now, by choosing $\beta>0$ large enough so that the ball B_β contains the unique solution of the linear equation $T(0,\varphi,\theta)=(\varphi,\theta)$ given by

$$\begin{cases} -\tau\alpha\,\Delta\varphi+\varphi \;=\; 0 \\ -\tau\kappa\,\Delta\theta+\theta \;=\; 0 \end{cases} \quad \text{in } \;\Omega\;,$$

subject to the following boundary conditions

$$\frac{\partial\varphi}{\partial n}=0\,, \quad \theta=0 \qquad \text{on } \;\partial\Omega\;.$$

Therefore $D(Id-T(0,\cdot),B_\beta,0)=1$, and, from (3.21), we conclude that problem (3.1), (3.2) has a solution $(\varphi,\theta)\in W_2^1(\Omega)\times \overset{0}{W}{}_2^1(\Omega)$.

By the L_p-regularity theory for elliptic linear equations and the fact that $f_s\in C_b^{1,1}(\mathbb{R}^2)$, it is easy to conclude that $\theta\in W_2^2(\Omega)\cap C^{1,\sigma}(\overline{\Omega})$ for $\sigma=1-n/4$. Also, $a\varphi+b\varphi^2-\varphi^3+\theta+g\in L_2(\Omega)$ and by applying again the L_p-regularity theory, we obtain that $\varphi\in W_2^2(\Omega)\cap C^{1,\sigma}(\overline{\Omega})$, with $\sigma=1-n/4$.

To prove the uniqueness of such solutions, let φ_i and θ_i with $i=1$ or 2 be to two solutions of the problem (3.1)–(3.2). By writing the corresponding problems for both (φ_1,θ_1) , (φ_2,θ_2); denoting $\hat\varphi=\varphi_1-\varphi_2$, $\hat\theta=\theta_1-\theta_2$, and adding the two resulting equations, we infer that

$$\begin{cases} -\tau\alpha\,\Delta\hat\varphi+\hat\varphi \;=\; \tau\Big(a+b(\varphi_1{+}\varphi_2)-(\varphi_1^2+\varphi_1\varphi_2+\varphi_2^2)\Big)\hat\varphi+\tau\hat\theta\;, \\ -\tau\kappa\,\Delta\hat\theta+\hat\theta \;=\; \dfrac{\ell}{2}\Big(f_s(\theta_1,\varphi_1)-f_s(\theta_2,\varphi_2)\Big) \qquad \text{in } \;\Omega\;, \end{cases} \tag{3.22}$$

subject to the boundary conditions

$$\frac{\partial\varphi}{\partial n}=0\,, \quad \theta=0 \qquad \text{on } \;\partial\Omega\;. \tag{3.23}$$

By multiplying the first equation in (3.22)–(3.23) by $\hat{\varphi}$, integrating over Ω, using Green's formula, that $a(.), b(.), \varphi_1, \varphi_2 \in L_\infty(\Omega)$, Holder's inequality and Young's inequality, we obtain

$$\tau\alpha \int_\Omega |\nabla\hat{\varphi}|^2\,dx + \frac{1}{2}\int_\Omega |\hat{\varphi}|^2\,dx \le C_1\,\tau\|\hat{\varphi}\|^2_{2,\Omega} + \frac{\tau^2}{2}\|\hat{\theta}\|^2_{2,\Omega}\,. \tag{3.24}$$

By choosing τ small enough such that $\tau \le 1/(4C_1)$, we obtain

$$\tau\alpha \int_\Omega |\nabla\hat{\varphi}|^2\,dx + \frac{1}{4}\int_\Omega |\varphi|^2\,dx \le \frac{\tau^2}{2}\|\hat{\theta}\|^2_{2,\Omega}\,. \tag{3.25}$$

Next,we multiply the second equation in (3.22)–(3.23) by $\hat{\theta} = \theta_1 - \theta_2$, and proceed as usual to obtain

$$\tau\kappa \int_\Omega |\nabla\hat{\theta}|^2\,dx + \int_\Omega |\hat{\theta}|^2\,dx = \frac{\ell}{2}\int_\Omega \big(f_s(\theta_1,\varphi_1) - f_s(\theta_2,\varphi_2)\big)\,(\theta_1-\theta_2)\,dx\,. \tag{3.26}$$

Now, we observe that the integral at the right-hand side of (3.26) can be rewritten as

$$\int_\Omega \big(f_s(\theta_1,\varphi_1) - f_s(\theta_2,\varphi_2)\big)\,(\theta_1-\theta_2)\,dx =$$

$$= \int_\Omega \big(f_s(\theta_1,\varphi_1) - f_s(\theta_2,\varphi_1)\big)\,(\theta_1-\theta_2)\,dx + \int_\Omega \big(f_s(\theta_2,\varphi_1) - f_s(\theta_2,\varphi_2)\big)\,(\theta_1-\theta_2)\,dx\,.$$

By recalling that for each $z \in \mathbb{R}$ the function $y \mapsto f_s(y,z)$ is non-increasing, and using that f_s is a Lipschitz function together with Young's inequality, we can conclude that

$$\frac{\ell}{2}\int_\Omega \big(f_s(\theta_2,\varphi_1) - f_s(\theta_2,\varphi_2)\big)\,(\theta_1-\theta_2)\,dx \le C_2\,\|\hat{\varphi}\|^2_{2,\Omega} + \frac{1}{2}\,\|\hat{\theta}\|^2_{2,\Omega}\,.$$

By combining this result with estimate (3.26), we obtain

$$\tau\kappa \int_\Omega |\nabla\hat{\theta}|^2\,dx + \frac{1}{2}\int_\Omega |\hat{\theta}|^2\,dx \le C_2\,\|\hat{\varphi}\|^2_{2,\Omega}\,.$$

Now, we add this last result to (3.25) multiplied by $5C_2$ to obtain

$$\tau\alpha\,\|\nabla\hat{\varphi}\|^2_{2,\Omega} + \tau\kappa\,\|\nabla\hat{\theta}\|^2_{2,\Omega} + \frac{1}{4}C_2\,\|\hat{\varphi}\|^2_{2,\Omega} + \|\hat{\theta}\|^2_{2,\Omega} \le \frac{5}{2}C_2\tau^2\,\|\hat{\theta}\|^2_{2,\Omega}\,. \tag{3.27}$$

Thus, by taking $\tau \le \min\big\{1/(4C_1), 1/\sqrt{5C_2}\big\}$, we conclude that

$$\tau\alpha\,\|\nabla\hat{\varphi}\|^2_{2,\Omega} + \tau\kappa\,\|\nabla\hat{\theta}\|^2_{2,\Omega} + \frac{1}{4}C\ell\,\|\hat{\varphi}\|^2_{2,\Omega} + \frac{1}{2}\,\|\hat{\theta}\|^2_{2,\Omega} \le 0\,,$$

which implies that $\hat{\varphi} = 0$, $\hat{\theta} = 0$ and thus the uniqueness of solution.

This completes the proof the Theorem 2.1. ∎

Remark. We observe that the fact that the solid fraction function f_s is non-increasing with respect to the temperature was not used in the part of the proof that shows the existence of discrete solutions; it is only used to obtain the uniqueness of such solutions. However, this monotony hypothesis will play an important role in what follows, namely in the proof of certain estimates that will be necessary to obtain the existence of the solutions of the original continuous model. □

4 – *A priori* estimates

In this section we will be interested in obtaining *a priori* estimates, which are uniform with respect to τ.

We start by multiplying equation (2.5) by $\delta_t\theta^m$ (see (2.9)). After integration over Ω and the usual integration by parts, we obtain

$$\int_\Omega (\delta_t\theta^m)^2\,dx + \frac{\kappa}{\tau}\int_\Omega \nabla\theta^m(\nabla\theta^m - \nabla\theta^{m-1})\,dx = \\ = \frac{\ell}{2}\int_\Omega \left(\frac{f_s(\theta^m,\varphi^m) - f_s(\theta^{m-1},\varphi^{m-1})}{\tau}\right)\delta_t\theta^m\;dx\;.$$

By using the relation

$$2\int_\Omega \chi(\chi-\psi)\,dx = \int_\Omega |\chi|^2\,dx - \int_\Omega |\psi|^2\,dx + \int_\Omega |\chi-\psi|^2\,dx\;, \tag{4.1}$$

we get

$$\|\delta_t\theta^m\|^2_{2,\Omega} + \frac{\kappa}{2\tau}\Big(\|\nabla\theta^m\|^2_{2,\Omega} - \|\nabla\theta^{m-1}\|^2_{2,\Omega} + \|\nabla\theta^m - \nabla\theta^{m-1}\|^2_{2,\Omega}\Big) = \\ = \frac{\ell}{2}\int_\Omega \left(\frac{f_s(\theta^m,\varphi^m) - f_s(\theta^{m-1},\varphi^{m-1})}{\tau}\right)\delta_t\theta^m\;dx\;. \tag{4.2}$$

Now, the integral of the right-hand side of this expression can be written as

$$\int_\Omega \left(\frac{f_s(\theta^m,\varphi^m) - f_s(\theta^{m-1},\varphi^{m-1})}{\tau}\right)\delta_t\theta^m\;dx = \\ = \int_\Omega \left(\frac{f_s(\theta^m,\varphi^m) - f_s(\theta^{m-1},\varphi^{m})}{\tau}\right)\delta_t\theta^m\;dx \\ + \int_\Omega \left(\frac{f_s(\theta^{m-1},\varphi^m) - f_s(\theta^{m-1},\varphi^{m-1})}{\tau}\right)\delta_t\theta^m\;dx\;. \tag{4.3}$$

Working as before, that is, by using the fact that for each fixed $z \in \mathbb{R}$ the function $y \mapsto f_s(y,z)$ is non increasing Lipschitz function, and Young's inequality, we conclude that

$$\frac{\ell}{2}\int_\Omega \left(\frac{f_s(\theta^m,\varphi^m)-f_s(\theta^{m-1},\varphi^{m-1})}{\tau}\right)\delta_t\theta^m\,dx \;\le\; C\,\|\delta_t\varphi^m\|^2_{2,\Omega}+\frac{1}{2}\,\|\delta_t\theta^m\|^2_{2,\Omega}\;.$$

Combining this result with estimates (4.2), we obtain

$$\tau\,\|\delta_t\theta^m\|^2_{2,\Omega}+\Big(\|\nabla\theta^m\|^2_{2,\Omega}-\|\nabla\theta^{m-1}\|^2_{2,\Omega}+\|\nabla\theta^m-\nabla\theta^{m-1}\|^2_{2,\Omega}\Big)\;\le\; C\tau\,\|\delta_t\varphi^m\|^2_{2,\Omega}\;.$$

By adding these relations for $m=1,2,...,r$, for $1\le r\le N$, we obtain

$$\begin{aligned}\tau\sum_{m=1}^{r}\|\delta_t\theta^m\|^2_{2,\Omega}+\|\nabla\theta^r\|^2_{2,\Omega}+\sum_{m=1}^{r}\|\nabla\theta^m-\nabla\theta^{m-1}\|^2_{2,\Omega}\;\le&\\ \le C\left(\|\nabla\theta_0\|^2_{2,\Omega}+\tau\sum_{m=1}^{r}\|\delta_t\varphi^m\|^2_{2,\Omega}\right)&\;.\end{aligned}\tag{4.4}$$

where C depends only on Ω, ℓ and κ.

Now, by multiplying equation (2.5) by θ^m, integrating over Ω and using Green's formula, we obtain

$$\begin{aligned}\frac{1}{\tau}\int_\Omega\theta^m(\theta^m-\theta^{m-1})\,dx+\kappa\int_\Omega|\nabla\theta^m|^2\,dx\;=&\\ =\;\frac{\ell}{2}\int_\Omega\left(\frac{f_s(\theta^m,\varphi^m)-f_s(\theta^{m-1},\varphi^{m-1})}{\tau}\right)\theta^m\,dx&\;,\end{aligned}$$

which as before implies that

$$\begin{aligned}\frac{1}{2\tau}\Big(\|\theta^m\|^2_{2,\Omega}-\|\theta^{m-1}\|^2_{2,\Omega}+\|\theta^m-\theta^{m-1}\|^2_{2,\Omega}\Big)+\kappa\,\|\nabla\theta^m\|^2_{2,\Omega}\;\le&\\ \le\;\frac{\ell}{2}\int_\Omega\left(\frac{f_s(\theta^m,\varphi^m)-f_s(\theta^{m-1},\varphi^{m-1})}{\tau}\right)\theta^m\,dx&\;.\end{aligned}$$

We can treat the last term in this expression as we did before, by using the fact that f_s is a Lipschitz function, that $f_s(z,\cdot)$ is non-increasing and Young's inequality, to obtain

$$\begin{aligned}\frac{1}{2}\Big(\|\theta^m\|^2_{2,\Omega}-\|\theta^{m-1}\|^2_{2,\Omega}+\|\theta^m-\theta^{m-1}\|^2_{2,\Omega}\Big)+\tau\kappa\,\|\nabla\theta^m\|^2_{2,\Omega}\;\le&\\ \le\;C_1\tau\,\|\delta_t\varphi^m\|^2_{2,\Omega}+C\tau\,\|\theta^m\|^2_{2,\Omega}&\;.\end{aligned}\tag{4.5}$$

Now, we multiply the equation (2.4) by $\delta_t\varphi^m$, integrate over Ω and use Green's formula together with the convexity of $h(s)=s^4$, which implies $(\varphi^m)^4-(\varphi^{m-1})^4\le 4(\varphi^m)^3(\varphi^m-\varphi^{m-1})$, to obtain

$$\begin{aligned}\int_\Omega (\delta_t\varphi^m)^2\,dx \;+\; \frac{\alpha}{\tau}\int_\Omega \nabla\varphi^m(\nabla\varphi^m-\nabla\varphi^{m-1})\,dx\\ +\;\frac{1}{\tau}\int_\Omega (\varphi^m)^4\,dx \;-\;\frac{1}{\tau}\int_\Omega(\varphi^{m-1})^4\,dx \;=\\ =\int_\Omega a(x)\varphi^m\,\delta_t\varphi^m\,dx \;+\int_\Omega b(x)(\varphi^m)^2\delta_t\varphi^m\,dx\;+\int_\Omega \theta^m\,\delta_t\varphi^m\,dx\;.\end{aligned}$$

In this last expression, now we use Hölder's and Young's inequality and apply the relation (4.1) to find

$$\begin{aligned}\tau\,\|\delta_t\varphi^m\|^2_{2,\Omega}\;+\;\alpha\Big(\|\nabla\varphi^m\|^2_{2,\Omega}-\|\nabla\varphi^{m-1}\|^2_{2,\Omega}+\|\nabla\varphi^m-\nabla\varphi^{m-1}\|^2_{2,\Omega}\Big)\\ +\;\frac{1}{4}\Big(\|\varphi^m\|^4_{4,\Omega}-\|\varphi^{m-1}\|^4_{4,\Omega}\Big)\;\le\\ \le\; C_2\tau\,\|\varphi^m\|^4_{4,\Omega}+C\tau\Big(\|\varphi^m\|^2_{2,\Omega}+\|\theta^m\|^2_{2,\Omega}\Big)\,.\end{aligned}$$

By multiplying this expression by $2\,C_1$ and adding the result to estimate (4.5), we obtain

$$\begin{aligned}\alpha\Big(\|\nabla\varphi^m\|^2_{2,\Omega}-\|\nabla\varphi^{m-1}\|^2_{2,\Omega}+\|\nabla\varphi^m-\nabla\varphi^{m-1}\|^2_{2,\Omega}\Big)\\ +\;\|\theta^m\|^2_{2,\Omega}-\|\theta^{m-1}\|^2_{2,\Omega}+\|\theta^m-\theta^{m-1}\|^2_{2,\Omega}+\tau\kappa\,\|\nabla\theta^m\|^2_{2,\Omega}\\ +\;\tau\,\|\delta_t\varphi^m\|^2_{2,\Omega}+\frac{1}{4}\Big(\|\varphi^m\|^4_{4,\Omega}-\|\varphi^{m-1}\|^4_{4,\Omega}\Big)\;\le\\ \le\; C_2\tau\,\|\varphi^m\|^4_{4,\Omega}+C\tau\Big(\|\varphi^m\|^2_{2,\Omega}+\|\theta^m\|^2_{2,\Omega}\Big)\,.\end{aligned}\tag{4.6}$$

Now, we multiply equation (2.4) by φ^m, integrate over Ω, and use Green's formula to get

$$\begin{aligned}\frac{1}{\tau}\int_\Omega\big(\varphi^m-\varphi^{m-1}\big)\,\varphi^m\,dx\;+\;\alpha\int_\Omega|\nabla\varphi^m|^2\,dx\;+\;\frac{1}{2}\int_\Omega(\varphi^m)^4\,dx\;=\\ =\int_\Omega\Big(a(x)+b(x)\varphi^m-\frac{1}{2}(\varphi^m)^2\Big)(\varphi^m)^2\;dx\;+\int_\Omega\theta^m\varphi^m\,dx\;.\end{aligned}$$

By using relation (4.1) and that $\max\limits_{s\in\mathbb{R},\;x\in\Omega}\big(a(x)+b(x)s-\frac{1}{2}s^2\big)$ is finite, together with Young's inequality, we are left with

$$\begin{aligned}\|\varphi^m\|^2_{2,\Omega}-\|\varphi^{m-1}\|^2_{2,\Omega}+\|\varphi^m-\varphi^{m-1}\|^2_{2,\Omega}+\tau\alpha\|\nabla\varphi^m\|^2_{2,\Omega}+\tau\|\varphi^m\|^4_{4,\Omega}\;\le\\ \le\; C\tau\Big(\|\varphi^m\|^2_{2,\Omega}+\|\theta^m\|^2_{2,\Omega}\Big)\;.\end{aligned}$$

By multiplying this last expression by $2\,C_2$ and adding the result to estimate (4.6), we get

$$\begin{aligned}
\|\varphi^m\|^2_{2,\Omega} - \|\varphi^{m-1}\|^2_{2,\Omega} &+ \|\varphi^m - \varphi^{m-1}\|^2_{2,\Omega} \\
&+ \|\theta^m\|^2_{2,\Omega} - \|\theta^{m-1}\|^2_{2,\Omega} + \|\theta^m - \theta^{m-1}\|^2_{2,\Omega} \\
&+ \|\nabla\varphi^m\|^2_{2,\Omega} - \|\nabla\varphi^{m-1}\|^2_{2,\Omega} + \|\nabla\varphi^m - \nabla\varphi^{m-1}\|^2_{2,\Omega} \\
&+ \tau\,\|\nabla\varphi^m\|^2_{2,\Omega} + \tau\,\|\nabla\theta^m\|^2_{2,\Omega} + \tau\,\|\varphi^m\|^4_{4,\Omega} \\
&+ \|\delta_t\varphi^m\|^2_{2,\Omega} + \|\varphi^m\|^4_{4,\Omega} - \|\varphi^{m-1}\|^4_{4,\Omega} \;\le \\
&\qquad\le\; C\tau\Big(\|\varphi^m\|^2_{2,\Omega} + \|\theta^m\|^2_{2,\Omega}\Big)\;.
\end{aligned}$$

By adding these relations for $m = 1, 2, ..., r$, with $1 \le r \le N$, we finally get

$$\begin{aligned}
\|\varphi^r\|^2_{W^1_2(\Omega)} &+ \|\theta^r\|^2_{2,\Omega} + \|\varphi^r\|^4_{4,\Omega} \\
&+ \sum_{m=1}^{r}\Big(\|\varphi^m - \varphi^{m-1}\|^2_{W^1_2(\Omega)} + \|\theta^m - \theta^{m-1}\|^2_{2,\Omega}\Big) \\
&+ \;\tau\sum_{m=1}^{r}\Big(\|\nabla\varphi^m\|^2_{2,\Omega} + \|\nabla\theta^m\|^2_{2,\Omega}\Big) \\
&+ \;\tau\sum_{m=1}^{r}\|\varphi^m\|^4_{4,\Omega} \;+\; \tau\sum_{m=1}^{r}\|\delta_t\varphi^m\|^2_{2,\Omega} \;+\; \|\varphi^r\|^4_{4,\Omega} \;\le \\
\le\; C\Big(\|\varphi_0\|^2_{W^1_2(\Omega)} &+ \|\varphi_0\|^4_{4,\Omega} + \|\theta_0\|^2_{2,\Omega}\Big) + C\tau\sum_{m=1}^{r}\Big(\|\varphi^m\|^2_{2,\Omega} + \|\theta^m\|^2_{2,\Omega}\Big)\;.
\end{aligned} \tag{4.7}$$

where C depends only on Ω, α, κ, ℓ, $\|a\|_\infty$ and $\|b\|_\infty$.

Now, we apply Gronwall's lemma in a discrete form (see for instance [18, 34]) to conclude that

$$\|\varphi^r\|^2_{W^1_2(\Omega)} + \|\theta^r\|^2_{2,\Omega} \;\le\; C\Big(\|\varphi_0\|^2_{W^1_2(\Omega)} + \|\varphi_0\|^4_{4,\Omega} + \|\theta_0\|^2_{2,\Omega}\Big)\;, \tag{4.8}$$

for $r = 0, 1, ..., N$.

By going back to (4.7), we obtain the following estimates:

$$\tau\sum_{m=1}^{r}\Big(\|\nabla\varphi^m\|^2_{2,\Omega} + \|\nabla\theta^m\|^2_{2,\Omega}\Big) \;\le\; C\;, \tag{4.9}$$

$$\sum_{m=1}^{r}\Big(\|\varphi^m - \varphi^{m-1}\|^2_{W^1_2(\Omega)} + \|\theta^m - \theta^{m-1}\|^2_{2,\Omega}\Big) \;\le\; C\;, \tag{4.10}$$

$$\tau \sum_{m=1}^{r} \|\varphi^m\|_{4,\Omega}^4 \le C \,, \tag{4.11}$$

$$\tau \sum_{m=1}^{r} \|\delta_t \varphi^m\|_{2,\Omega}^2 \le C \,, \tag{4.12}$$

$$\max_{1\le r\le N} \|\varphi^r\|_{W_2^1(\Omega)} \le C \,. \tag{4.13}$$

$$\max_{1\le r\le N} \|\varphi^r\|_{4,\Omega} \le C \,. \tag{4.14}$$

Combining (4.4) with (4.12), we obtain

$$\tau \sum_{m=1}^{r} \|\delta_t \theta^m\|_{2,\Omega}^2 + \|\nabla \theta^r\|_{2,\Omega}^2 \le C \qquad \text{for} \;\; r = 1, ..., N \,. \tag{4.15}$$

Similarly, we obtain

$$\max_{1\le r\le N} \|\theta^r\|_{W_2^1(\Omega)} \le C \,. \tag{4.16}$$

Now, by multiplying equation (2.4) by $-\Delta\varphi^m$, integrating over Ω, using Green's formula, we get

$$\begin{aligned} \alpha \int_\Omega |\Delta\varphi^m| \, dx \,+\, 3 \int_\Omega |\nabla\varphi^m|^2 (\varphi^m)^2 \, dx \;\le \\ \le \int_\Omega |a| \, |\varphi^m| \, |\Delta\varphi^m| \, dx + \int_\Omega |b| \, |\varphi^m|^2 \, |\Delta\varphi^m| \, dx \\ + \int_\Omega |\theta^m| \, |\Delta\varphi^m| \, dx + \int_\Omega |\delta_t\varphi^m| \, |\Delta\varphi^m| \, dx \,. \end{aligned} \tag{4.17}$$

By using Poincarè inequality and Young's inequality, we estimate the right-hand side of this expression by

$$\int_\Omega |a| \, |\varphi^m| \, |\Delta\varphi^m| \, dx \le C \, \|\nabla\varphi^m\|_{2,\Omega}^2 + \frac{\alpha}{2} \, \|\Delta\varphi^m\|_{2,\Omega}^2 \,,$$

$$\int_\Omega |b| \, |\varphi^m|^2 \, |\Delta\varphi^m| \, dx \le C \, \|\varphi^m\|_{4,\Omega}^4 + \frac{\alpha}{4} \, \|\Delta\varphi^m\|_{2,\Omega}^2 \,,$$

$$\int_\Omega |\theta^m| \, |\Delta\varphi^m| \, dx \le C \, \|\nabla\theta^m\|_{2,\Omega}^2 + \frac{\alpha}{8} \, \|\Delta\varphi^m\|_{2,\Omega}^2 \,,$$

$$\int_\Omega |\delta_t\varphi^m| \, |\Delta\varphi^m| \, dx \le C \, \|\delta_t\varphi^m\|_{2,\Omega}^2 + \frac{\alpha}{16} \, \|\Delta\varphi^m\|_{2,\Omega}^2 \,.$$

Therefore, (4.17) implies that

$$\tau\|\Delta\varphi^m\|_{2,\Omega}^2 \le C\tau\Big(\|\nabla\varphi^m\|_{2,\Omega}^2 + \|\varphi^m\|_{4,\Omega}^4 + \|\nabla\theta^m\|_{2,\Omega}^2 + \|\delta_t\varphi^m\|_{2,\Omega}^2\Big) .$$

By adding these relations for $m = 1, 2, ..., r$, with $1 \le r \le N$, we get

$$\begin{aligned}\tau\sum_{m=1}^{r}\|\Delta\varphi^m\|_{2,\Omega}^2 \le C\Bigg(&\tau\sum_{m=1}^{r}\|\nabla\varphi^m\|_{2,\Omega}^2 + \tau\sum_{m=1}^{r}\|\varphi^m\|_{4,\Omega}^4 \\ &+ \tau\sum_{m=1}^{r}\|\nabla\theta^m\|_{2,\Omega}^2 + \tau\sum_{m=1}^{r}\|\delta_t\varphi^m\|_{2,\Omega}^2\Bigg) .\end{aligned} \tag{4.18}$$

Combining (4.9), (4.11), (4.12) with (4.18), we obtain

$$\tau\sum_{m=1}^{r}\|\Delta\varphi^m\|_{2,\Omega}^2 \le C \qquad \text{for } r = 0, 1, ..., N , \tag{4.19}$$

where C depends on Ω, α, κ, ℓ, $\|a\|_\infty$ and $\|b\|_\infty$.

By multiplying equation (2.5) by $-\Delta\theta^m$, integrating over Ω, we get

$$\begin{aligned}\kappa\int_\Omega|\Delta\theta^m|\,dx \le \frac{\ell}{2}\int_\Omega&\left|\frac{f_s(\theta^m,\varphi^m) - f_s(\theta^{m-1},\varphi^{m-1})}{\tau}\right||\Delta\theta^m|\,dx \\ &+\int_\Omega|\delta_t\theta^m|\,|\Delta\theta^m|\,dx .\end{aligned}$$

By using that f_s is Lipschitz function and Young's inequality in in this expression, we obtain

$$\tau\|\Delta\theta^m\|_{2,\Omega}^2 \le C\tau\Big(\|\delta_t\theta^m\|_{2,\Omega}^2 + \|\delta_t\varphi^m\|_{2,\Omega}^2\Big) ,$$

which, by addition for $m = 1, 2, ..., r$, with $1 \le r \le N$, and the use of estimates (4.12), (4.15), gives

$$\tau\sum_{m=1}^{r}\|\Delta\theta^m\|_{2,\Omega}^2 \le C \qquad \text{for } r = 0, 1, ..., N , \tag{4.20}$$

where C depends on Ω, α, κ, ℓ, $\|a\|_\infty$ and $\|b\|_\infty$.

Finally, multiply equation (2.5) by $(1/\tau)\big(f_s(\theta^m,\varphi^m) - f_s(\theta^{m-1},\varphi^{m-1})\big)$ and integrate over Ω to obtain

$$\begin{aligned}&\frac{\ell}{2}\int_\Omega\bigg(\frac{f_s(\theta^m,\varphi^m) - f_s(\theta^{m-1},\varphi^{m-1})}{\tau}\bigg)^2 dx \le \\ &\qquad\le \kappa\int_\Omega\left|\frac{f_s(\theta^m,\varphi^m) - f_s(\theta^{m-1},\varphi^{m-1})}{\tau}\right||\Delta\theta^m|\,dx \\ &\qquad\quad+\int_\Omega\left|b\frac{f_s(\theta^m,\varphi^m) - f_s(\theta^{m-1},\varphi^{m-1})}{\tau}\right||\delta_t\theta^m|\,dx .\end{aligned}$$

By using that f_s is Lipschitz function and Young's inequality in this expression, we obtain

$$\tau\left\|\frac{f_s(\theta^m,\varphi^m)-f_s(\theta^{m-1},\varphi^{m-1})}{\tau}\right\|_{2,\Omega}^2 \leq C\tau\Big(\|\Delta\theta^m\|_{2,\Omega}^2+\|\delta_t\theta^m\|_{2,\Omega}^2+\|\delta_t\varphi^m\|_{2,\Omega}^2\Big)\ .$$

By adding these relations for $m=1,2,...,N$, and using the estimates (4.12), (4.15), (4.20), we get

$$\tau\sum_{m=1}^{N}\left\|\frac{f_s(\theta^m,\varphi^m)-f_s(\theta^{m-1},\varphi^{m-1})}{\tau}\right\|_{2,\Omega}^2 \leq C\ , \tag{4.21}$$

where C depends on Ω, α, κ, ℓ, $\|a\|_\infty$ and $\|b\|_\infty$.

5 – Proof of Theorem 2.2

With the notations of Definition 2.3, we may rewrite the scheme (2.4)–(2.6) in terms of φ_τ, $\widetilde{\varphi}_\tau$, θ_τ, $\widetilde{\theta}_\tau$ as follows.

$$\begin{cases} \dfrac{\partial\widetilde{\varphi}_\tau}{\partial t}-\alpha\,\Delta\varphi_\tau \,=\, a(x)\varphi_\tau+b(x)\varphi_\tau^2-\varphi_\tau^3+\theta_\tau & \text{in } \ Q\ , \\[2mm] \dfrac{\partial\widetilde{\theta}_\tau}{\partial t}-\kappa\,\Delta\theta_\tau \,=\, \dfrac{\ell}{2}\,\dfrac{\partial\widetilde{f}_{s\tau}}{\partial t} & \text{in } \ Q\ , \end{cases} \tag{5.1}$$

$$\begin{cases} \dfrac{\partial\varphi_\tau}{\partial\eta}=0\,, \quad \theta_\tau=0 & \text{on } \ S\ , \\[2mm] \widetilde{\varphi}_\tau(x,0)=\varphi_0(x)\,, \quad \widetilde{\theta}_\tau(x,0)=\theta_0(x) & \text{in } \ \Omega\ . \end{cases} \tag{5.2}$$

Here, $\widetilde{f}_{s\tau}$ denotes the interpolation function as in Definition 2.3 and corresponding to $\{f_s(\theta^m,\varphi^m)\}_{m=0}^N$.

By rewriting the estimates obtained in the last section in terms of the interpolations functions φ_τ, $\widetilde{\varphi}_\tau$, θ_τ, $\widetilde{\varphi}_\tau$, $\widetilde{f}_{s\tau}$, we obtain

Lemma 5.1.

$$\begin{aligned} &\|\varphi_\tau\|_{L^\infty(0,T;W_2^1(\Omega))}+\|\widetilde{\varphi}_\tau\|_{L^\infty(0,T;W_2^1(\Omega))} \,\leq\, C\ , \\ &\|\varphi_\tau\|_{L^2(0,T;W_2^2(\Omega))}+\|\widetilde{\varphi}_\tau\|_{L^2(0,T;W_2^2(\Omega))} \,\leq\, C\ , \\ &\|\theta_\tau\|_{L^\infty(0,T;W_2^1(\Omega))}+\|\widetilde{\theta}_\tau\|_{L^\infty(0,T;W_2^1(\Omega))} \,\leq\, C\ , \\ &\|\theta_\tau\|_{L^2(0,T;W_2^2(\Omega))}+\|\widetilde{\theta}_\tau\|_{L^2(0,T;W_2^2(\Omega))} \,\leq\, C\ , \\ &\|\varphi_\tau\|_{4,Q} \,\leq\, C\ , \end{aligned} \tag{5.3}$$

$$
\begin{aligned}
&\left\| \frac{\partial \widetilde{\varphi}_\tau}{\partial t} \right\|_{2,Q} + \left\| \frac{\partial \widetilde{\theta}_\tau}{\partial t} \right\|_{2,Q} \le C \,, \\
&\left\| \frac{\partial \widetilde{f}_{s\tau}}{\partial t} \right\|_{2,Q} \le C \,.
\end{aligned} \tag{5.4}
$$

Proof: By using estimate (4.12), we obtain

$$
\left\| \frac{\partial \widetilde{\varphi}_\tau}{\partial t} \right\|^2_{2,Q} = \sum_{m=1}^{N} \int_{(m-1)\tau}^{m\tau} \|\varphi^m_t\|^2_{2,\Omega}\, dt \;\le\; \tau \sum_{m=1}^{N} \|\varphi^m_t\|^2_{2,\Omega} \;\le\; C \,.
$$

Similarly, from (4.15) we conclude that $\left\| \frac{\partial \widetilde{\theta}_\tau}{\partial t} \right\|_{2,Q} \le C$.

By using estimates (4.9), (4.13) and (4.19), we obtain

$$
\|\nabla\varphi_\tau\|^2_{2,Q} = \sum_{m=1}^{N} \int_{(m-1)\tau}^{m\tau} \|\nabla\varphi^m\|^2_{2,\Omega}\, dt \;\le\; \tau \sum_{m=1}^{N} \|\nabla\varphi^m\|^2_{2,\Omega} \;\le\; C \,,
$$

$$
\|\Delta\varphi_\tau\|^2_{2,Q} = \sum_{m=1}^{N} \int_{(m-1)\tau}^{m\tau} \|\Delta\varphi^m\|^2_{2,\Omega}\, dt \;\le\; \tau \sum_{m=1}^{N} \|\Delta\varphi^m\|^2_{2,\Omega} \;\le\; C \,,
$$

$$
\|\varphi_\tau\|_{L^\infty(0,T;W^1_2(\Omega))} = \max_{1\le r\le N} \|\varphi_\tau\|^2_{W^1_2(\Omega)} \le C \,.
$$

Applying estimate (4.21), we obtain

$$
\begin{aligned}
\left\| \frac{\partial \widetilde{f}_{s\tau}}{\partial t} \right\|^2_{2,Q} &= \sum_{m=1}^{N} \int_{(m-1)\tau}^{m\tau} \left\| \frac{f_s(\varphi^m,\theta^m) - f_s(\varphi^{m-1},\theta^{m-1})}{\tau} \right\|^2_{2,\Omega} dt \\
&\le \tau \sum_{m=1}^{N} \left\| \frac{f_s(\varphi^m,\theta^m) - f_s(\varphi^{m-1},\theta^{m-1})}{\tau} \right\|^2_{2,\Omega} \le C \,.
\end{aligned}
$$

By similar arguments, using estimates (4.9), (4.11), (4.16) and (4.20), we obtain the other estimates of the statement. ∎

Now, by using the estimates (5.3)–(5.4), there exist subsequences, which for simplicity we still denote φ_τ, θ_τ, $\widetilde{\varphi}_\tau$, $\widetilde{\theta}_\tau$, such that as $\tau \to 0$ they satisfy

$$
\theta_\tau \rightharpoonup \theta, \quad \varphi_\tau \rightharpoonup \varphi \quad \text{in } L^2\big(0,T,W^2_2(\Omega)\big) \,, \tag{5.5}
$$

$$
\theta_\tau \overset{*}{\rightharpoonup} \theta, \quad \varphi_\tau \overset{*}{\rightharpoonup} \varphi \quad \text{in } L^\infty\big(0,T,W^1_2(\Omega)\big) \,, \tag{5.6}
$$

$$
\widetilde{\theta}_\tau \rightharpoonup \widetilde{\theta}, \quad \widetilde{\varphi}_\tau \rightharpoonup \widetilde{\varphi} \quad \text{in } L^2\big(0,T,W^1_2(\Omega)\big) \,, \tag{5.7}
$$

$$
\varphi_\tau \rightharpoonup \varphi \quad \text{in } L_4(Q) \,, \tag{5.8}
$$

$$
\frac{\partial \widetilde{\theta}_\tau}{\partial t} \rightharpoonup \frac{\partial \theta}{\partial t}, \quad \frac{\partial \widetilde{\varphi}_\tau}{\partial t} \rightharpoonup \frac{\partial \varphi}{\partial t} \quad \text{in } L_2(Q) \,. \tag{5.9}
$$

We must control the differences $\widetilde{\varphi}_\tau - \varphi_\tau$ and $\widetilde{\theta}_\tau - \theta_\tau$ with respect to suitable norms. From their definitions,

$$
\begin{aligned}
\|\widetilde{\varphi}_\tau - \varphi_\tau\|^2_{2,Q} &= \sum_{m=1}^{N} \int_{(m-1)\tau}^{m\tau} (t-t_m)^2 \,\|\delta_t \varphi^m\|^2_{2,\Omega} \\
&= \frac{\tau^2}{3}\left(\tau \sum_{m=1}^{N} \|\delta_t\varphi^m\|^2_{2,\Omega}\right) = \frac{\tau^2}{3}\left\|\frac{\partial \widetilde{\varphi}_\tau}{\partial t}\right\|^2_{2,Q} .
\end{aligned}
\tag{5.10}
$$

Therefore, from (5.4), we conclude that $\|\widetilde{\varphi}_\tau - \varphi_\tau\|_{L_2(Q)} \le C\tau$. Similarly, from (5.4) we deduce that $\|\widetilde{\theta}_\tau - \theta_\tau\|_{L_2(Q)} \le C\tau$. Thus, from (5.5) and (5.7), we obtain $\varphi = \widetilde{\varphi}$, $\theta = \widetilde{\theta}$ a.e. in Q.

This, (5.5) and (5.7) in particular imply

$$
\widetilde{\varphi}_\tau \rightharpoonup \varphi \quad \text{and} \quad \widetilde{\theta}_\tau \rightharpoonup \theta \qquad \text{in} \;\; L^2\big(0,T;W^1_2(\Omega)\big) \; . \tag{5.11}
$$

Using (5.9) and the Aubin–Lions Compactness Lemma (see for instance [36]), we derive also that

$$
\varphi_\tau \to \varphi \quad \text{and} \quad \theta_\tau \to \theta \qquad \text{in} \;\; L_2(Q) \; . \tag{5.12}
$$

Now, from (5.4) there exists $\mu \in L_2(Q)$ such that

$$
\frac{\partial \widetilde{f}_{s\tau}}{\partial t} \rightharpoonup \mu \qquad \text{in} \;\; L_2(Q) \; . \tag{5.13}
$$

We now claim that μ is in fact the weak derivative of $f_s(\theta,\varphi)$ with respect to time. Indeed, for any $\psi \in C_0^\infty(Q)$ with $\psi(\cdot,0) = \psi(\cdot,T) = 0$, we obtain

$$
\int_Q \frac{\partial \widetilde{f}_{s\tau}}{\partial t}\,\psi(x,t_m)\,dx\,dt = \tau \sum_{m=1}^{N} \int_\Omega \left(\frac{f_s(\theta^m,\varphi^m) - f_s(\theta^{m-1},\varphi^{m-1})}{\tau}\right)\psi(x,t_m)\,dx \, . \tag{5.14}
$$

By using the identity

$$
\sum_{m=0}^{N-1} y_m (z_{m+1} - z_m) \;=\; -\sum_{m=1}^{N} \big(z_m(y_m + y_{m-1})\big) + (yz)_N - (yz)_0
$$

at the right-hand side of (5.14), we get

$$
\begin{aligned}
\int_Q \frac{\partial \widetilde{f}_{s\tau}}{\partial t}\,\psi(x,t_m)\,dx\,dt &= -\tau \sum_{m=1}^{N} \int_\Omega f_s(\theta^m,\varphi^m)\left(\frac{\psi(x,t_m) - \psi(x,t_{m-1})}{\tau}\right) dx \\
&= -\int_Q f_s(\theta_\tau,\varphi_\tau)\,\widetilde{\psi}_t \;dx\,dt \; .
\end{aligned}
\tag{5.15}
$$

Since $f_s(\cdot,\cdot)$ is continuous and (5.12) is valid, extracting subsequences if necessary, we conclude that $f_s(\theta_\tau,\varphi_\tau) \to f_s(\theta,\varphi)$ almost everywhere in Q. Moreover, $\widetilde{\psi}_t \to \psi_t$ and $\left|f_s(\theta_\tau,\varphi_\tau)\widetilde{\psi}_t\right| < C$ a.e. in $\Omega\times[(m-1)\tau, m\tau]$. Therefore, by Lebesgue dominated convergence theorem we obtain that

$$\int_Q f_s(\theta_\tau,\varphi_\tau)\,\widetilde{\psi}_t\;dx\,dt \;\;\to\;\; \int_Q f_s(\theta,\varphi)\,\psi_t\;dx\,dt\;. \tag{5.16}$$

Thus, by passing to the limit in (5.15) and using (5.13) and (5.16), we conclude

$$\int_Q \mu\,\psi\;dx\,dt \;=\; -\int_Q f_s(\theta,\varphi)\,\psi_t\;dx\,dt$$

and also that μ is the weak derivative of $f_s(\theta,\varphi)$ with respect to time.

Now we are ready to pass to the limit in scheme (5.1)–(5.2) and to verify that (φ,θ) is in fact a generalized solution of (2.1)–(2.2).

To obtain this result, we take ξ in $\overset{0}{W}{}_2^{1,1}(Q)$ such that $\xi(\cdot,T)=0$ and $\beta\in C^1(0,T;W_2^1(\Omega))$ such that $\beta(\cdot,T)=0$. We use these functions to multiply the suitable equations and integrate over Q. Due to the kind of convergences we already have, the arguments to justify the passage to the limit in several of the terms of the resulting equations are rather standard. So, we just briefly describe this process for the nonlinear terms.

The convergence

$$\int_Q \left(\frac{\partial \widetilde{f}_{s\tau}}{\partial t}\right)\xi\;dx\,dt \;\;\to\;\; \int_Q \left(\frac{\partial f_s}{\partial t}\right)\xi\;dx\,dt$$

turns out to be an immediate consequence of (5.13).

By (5.8) and (5.12), we obtain

$$\int_Q \Big(a(x)\varphi_\tau + b(x)\varphi_\tau^2 - \varphi_\tau^3\Big)\,\beta\;dx\,dt \;\;\to\;\; \int_Q \Big(a(x)\varphi + b(x)\varphi^2 - \varphi^3\Big)\beta\;dx\,dt\;.$$

Thus,

$$\begin{aligned} -\int_Q \varphi\,\beta_t\;dx\,dt + \int_Q \nabla\varphi\,\nabla\beta\;dx\,dt \;=\; \\ \int_Q \Big(a(x)\varphi + b(x)\varphi^2 - \varphi^3\Big)\beta\;dx\,dt + \int_Q \theta\,\beta\;dx\,dt + \int_\Omega \varphi_0(x)\,\beta(x,0)\;dx\;, \end{aligned}$$

$$-\int_Q \theta\,\xi_t\;dx\,dt + \int_Q \nabla\theta\,\nabla\xi\;dx\,dt \;=\; \frac{\ell}{2}\int_Q \left(\frac{\partial f_s}{\partial t}\right)\xi\;dx\,dt + \int_\Omega \theta_0(x)\,\xi(x,0)\;dx\;,$$

and we conclude that (φ,θ) is a weak solution of (2.1)–(2.2).

To examine the regularity of (φ, θ), we use the following bootstrapping argument. By using the L_p-theory of parabolic linear equations (see [23], p. 351) with $\left(\dfrac{\partial f_s}{\partial \varphi}\dfrac{\partial \varphi}{\partial t} + \dfrac{\partial f_s}{\partial \theta}\dfrac{\partial \theta}{\partial t}\right) \in L_2(Q)$, we conclude that $\theta \in W_2^{2,1}(Q) \cap L_9(Q)$. This implies that $a\varphi + b\varphi^2 - \varphi^3 + \theta \in L_3(Q)$, and, by applying the L_p-regularity theory for parabolic linear equations again with $\varphi_0 \in W_3^{4/3}(\Omega) \cap W_2^{3/2+\delta}(\Omega)$ for some $\delta \in (0,1)$, we obtain $\varphi \in W_3^{2,1}(Q) \cap L_\infty(Q)$. Moreover, by using a similar bootstrapping argument starting with $\theta \in L_9(Q)$ and the known regularity of the given initial datum φ_0, we conclude that $\varphi \in W_q^{2,1}(Q)$ with $3 \le q \le 9$.

This completes the proof of Theorem 2.2. ∎

6 – Long time behavior of the solutions

In this section we will be interested in the long time behavior of the solutions constructed in the previous sections. We will show that when heat diffusion dominates (as we will explain later on), the construct solutions approach the set of the corresponding stationary solution as time increases.

For this, we start by observing that the stationary solutions of Problem 2.1 are solutions of the following system:

$$\begin{cases} -\alpha\, \Delta\varphi = g(.,\varphi) - \theta & \text{in } \Omega\,, \\ -\kappa\, \Delta\theta = 0 & \text{in } \Omega\,, \\ \partial\varphi/\partial\eta = 0\,, \quad \theta = \theta_1 & \text{on } \partial\Omega\,, \end{cases} \tag{6.1}$$

where $g(x,s) = a(x)s + b(x)s^2 - s^3$.

As it can be seen, the existence of such stationary solutions is rather easy to prove. In fact, since the second of the above equations is a very simple linear decoupled equation, the existence of θ is immediate. Using this θ just obtained, the first equation then decouples, and we recognize it as a Chafee–Infante equation [9], with Neumann boundary conditions. Results on existence of its solutions, and some of their properties, can then be obtained for instance using the techniques of Henry [16]. See also Caginalp [4].

Here, we consider the long time behavior of transient solutions, and as before, for simplicity of exposition, we will take the case with homogeneous boundary condition for the temperature, that is,

$$\theta = \theta_1 = 0 \quad \text{on } \partial\Omega\,. \tag{6.2}$$

The general case can be obtained in a standard way.

The idea now is to construct a suitable Liapunov function for our system. For this, let (φ,θ) be any solutions of (2.1) constructed as in the previous sections, and we observe that if we multiply the first equation in (2.1) by φ_t, integrate over Ω and use Hölder and Poincaré inequality, after some computations we end up with:

$$\int_\Omega \varphi_t^2 + \alpha\,\frac{d}{dt}\int_\Omega |\nabla\varphi|^2 + \frac{d}{dt}\int_\Omega 2\,G(.,\varphi) \;\le\; C_p^2\int_\Omega |\nabla\theta|^2\;, \tag{6.3}$$

where C_p denotes the constant associated to the Poincaré inequality and G is defined as $G(x,y) = -\displaystyle\int_0^y g(x,s)\,ds$.

Now, if we multiply the second equation in (2.1) by θ_t and proceed as before, we obtain:

$$\int_\Omega \theta_t^2 + \kappa\,\frac{d}{dt}\int_\Omega |\nabla\theta|^2 - \int_\Omega \frac{\ell}{2}\,f_{s,\theta}\,\theta_t^2 \;\le\; \frac{\ell^2 M_2^2}{4}\int_\Omega \varphi_t^2\;, \tag{6.4}$$

where $M_2 = \sup\bigl\{|f_{s,\varphi}(z_1,z_2)|:\ z_1,z_2\in\mathbb{R}\bigr\}$. We also remark that due to hypothesis (H_2),

$$-\int_\Omega \frac{\ell}{2}\,f_{s,\theta}\,\theta_t^2 \;\ge\; 0\;. \tag{6.5}$$

If we multiply the second equation in (2.1) by θ, working as before, we obtain:

$$\frac{d}{dt}\int_\Omega \theta^2 + \kappa\int_\Omega |\nabla\theta|^2 \;\le\; \frac{\ell^2 M_1^2 C_p^2}{2\,\kappa}\int_\Omega \theta_t^2 + \frac{\ell^2 M_2^2 C_p^2}{2\,\kappa}\int_\Omega \varphi_t^2\;, \tag{6.6}$$

where $M_1 = \sup\bigl\{|f_{s,\theta}(z_1,z_2)|:\ z_1,z_2\in\mathbb{R}\bigr\}$.

By taking in consideration (6.5), if we multiply (6.4) by $(\ell^2 M_1^2 C_p^2)(\kappa)^{-1}$ and add the result to (6.6), we obtain

$$\frac{d}{dt}\int_\Omega \theta^2 + \kappa\int_\Omega |\nabla\theta|^2 + \frac{\ell^2 M_1^2 C_p^2}{2\kappa}\int_\Omega \theta_t^2 + \ell^2 M_1^2 C_p^2\,\frac{d}{dt}\int_\Omega |\nabla\theta|^2 \;\le\; D\int_\Omega \varphi_t^2\;,$$

where

$$D = \frac{\ell^2 M_2^2 C_p^2}{2\kappa}\left(\frac{\ell^2 M_1}{2} + 1\right).$$

By adding this last result to (6.3) multiplied by $2D$, we finally obtain:

$$\begin{aligned}\frac{d}{dt}\int_\Omega &\Bigl(2\,\alpha D|\nabla\varphi|^2 + 4\,DG(\cdot,\varphi) + \ell^2 M_1^2 C_p^2|\nabla\theta|^2 + \theta^2\Bigr)\\ &+ D\int_\Omega \varphi_t^2 + \frac{\ell^2 M_1^2 C_p^2}{2\,\kappa}\int_\Omega \theta_t^2 + \kappa\int_\Omega |\nabla\theta|^2 \;\le\; 2\,C_p^2 D\int_\Omega |\nabla\theta|^2\;.\end{aligned}$$

Now we impose the condition that $\kappa \geq 2C_p^2 D$, which requires

$$\kappa \;\geq\; \ell\, M_2 C_p^2 \left(\ell^2 M_1^2/2 + 1\right)^{1/2} \,, \tag{6.7}$$

and define the functional

$$J(\zeta,\psi) \;=\; \int_\Omega \Big(2\,\alpha D|\nabla\psi|^2 + 4\,DG(\cdot,\psi) + \ell^2 M_1^2 C_p^2 |\nabla\zeta|^2 + \zeta^2\Big)\,. \tag{6.8}$$

Under the condition (6.7), inequality (6) implies that

$$\frac{d}{dt}\,J\big(\theta(t),\phi(t)\big) \;\leq\; -E\int_\Omega |\phi_t|^2 + |\theta_t|^2\,dx \;=\; -E\,\Big(\|\phi_t\|^2_{L_2(\Omega)} + \|\theta_t\|^2_{L_2(\Omega)}\Big)\,,$$

where $E = \min\big\{D, (\ell^2 M_1^2 C_p^2)/(2\kappa)\big\} > 0$.

This in particular implies that $J(\theta(t),\varphi(t))$ is a decreasing function of time, and thus J is a Liapunov function for (2.1).

Moreover, due to the expression of $G(\cdot,\cdot)$, there are finite positive constants C_1 and C_2 such that for any $\psi \in H^1(\Omega)$ and $\zeta \in H^1(\Omega)$ there holds

$$-C_1 \;\leq\; J(\psi,\eta)\,,$$

$$\|\nabla\psi\|^2_{L_2(\Omega)} + \|\psi\|^4_{L_4(\Omega)} + \|\nabla\zeta\|^2 \;\leq\; C_2\Big\{J(\psi,\zeta)+1\Big\}\,. \tag{6.9}$$

From the first inequality and the fact that $J(\theta(t),\phi(t))$ is decreasing, we conclude that there is $\bar J \in \mathbb{R}$ such that

$$\lim_{t\to+\infty} J\big(\theta(t),\phi(t)\big) = \bar J\,, \tag{6.10}$$

and also

$$\lim_{t\to+\infty}\frac{d}{dt}\,J\big(\theta(t),\phi(t)\big) \;=\; \lim_{t\to+\infty} -\Big(\|\phi_t(t)\|^2_{L_2(\Omega)} + \|\theta_t(t)\|^2_{L_2(\Omega)}\Big) \;=\; 0\,. \tag{6.11}$$

On the other hand, due again to the regularity of the solutions obtained in the previous sections, by a modification in a set of zero measure if necessary, for all $t > 0$ there hold:

$$\begin{aligned}
&\varphi_t(t) - \Delta\varphi(t) \;=\; g\big(\cdot,\varphi(t)\big) + \theta(t) \qquad \text{in } \Omega\,,\\
&\theta_t(t) - \kappa\,\Delta\theta(t) = \frac{\ell}{2}\,f_{s,\theta}\big(\theta(t),\varphi(t)\big)\,\theta_t(t) + \frac{\ell}{2}\,f_{s,\varphi}\big(\theta(t),\varphi(t)\big)\,\varphi_t(t) \qquad \text{in } \Omega\,,\\
&\frac{\partial\varphi}{\partial n}(t) = 0\,,\quad \theta(t) = 0 \qquad \text{on } \partial\Omega\,.
\end{aligned} \tag{6.12}$$

Now consider a sequence $\{t_n\}_n$ of positive numbers such that $t_n \to +\infty$ as $n \to +\infty$. From (6.10), (6.9), (6.11) and usual compactness arguments, there is a subsequence, which for simplicity we still denote $\{t_n\}$, and functions $\bar\varphi$ and $\bar\theta$ such that:

$$\begin{aligned} \nabla\varphi(t_n) &\to \nabla\bar\varphi\,, && \text{weakly in } \big(H^1(\Omega)\big)^n\,, \\ \nabla\theta(t_n) &\to \nabla\bar\theta\,, && \text{weakly in } \big(H^1(\Omega)\big)^n\,, \end{aligned}$$

$$\begin{aligned} \varphi(t_n) &\to \bar\varphi\,, && \text{strongly in } L_p(\Omega)\,, \\ \theta(t_n) &\to \bar\theta\,, && \text{strongly in } L_p(\Omega)\,, \end{aligned} \tag{6.13}$$

any $1 \le p < 6$ for $n \le 3$ (obviously better results hold for $n = 1$ or 2),

$$\begin{aligned} \varphi(t_n) &\to \bar\varphi\,, && \text{a.e.}\,, \\ \theta(t_n) &\to \bar\theta\,, && \text{a.e.}\,, \end{aligned}$$

$$\begin{aligned} \varphi_t(t_n) &\to 0, && \text{strongly in } L_2(\Omega)\,, \\ \theta_t(t_n) &\to 0, && \text{strongly in } L_2(\Omega)\,. \end{aligned}$$

Now, by taking $t = t_n$ in (6.12) and taking to the limit as $n \to +\infty$, with the help of the previous convergence, we obtain that $(\bar\varphi, \bar\theta)$ satisfy the first two equations of (6.1). Moreover, since

$$\begin{aligned} \Delta\varphi(t_n) &= -g\big(\cdot, \varphi(t_n)\big) - \theta(t_n) + \varphi_t(t_n)\,, \\ \kappa\,\Delta\theta(t_n) &= -(\ell/2)\, f_{s,\theta}\big(\theta(t_n), \varphi(t)\big)\,\theta_t(t_n) \\ &\quad -(\ell/2)\, f_{s,\varphi}\big(\theta(t_n), \varphi(t_n)\big)\,\varphi_t(t_n) + \theta_t(t_n)\,, \end{aligned}$$

the previous convergences imply that $\Delta\varphi(t_n)$ and $\Delta\theta(t_n)$ converge in $L_2(\Omega)$. These results and (6.13) imply that

$$\begin{aligned} \varphi(t_n) &\to \bar\varphi && \text{in } H^2(\Omega)\,, \\ \theta(t_n) &\to \bar\theta && \text{in } H^2(\Omega)\,, \end{aligned}$$

which imply that the boundary conditions are also satisfied and that $(\bar\varphi, \bar\theta)$ is a stationary solution.

We conclude that the w-limit set associated to any of the constructed transient solution is contained in the set of the stationary solutions, and thus, under the condition (6.7) we can state the following:

Theorem 6.1. *Let* $\kappa \geq 2\,\ell M_2(\ell^2 M_1^2/2+1)^{1/2}$, *where* $M_1 = \sup\big\{|\partial_\theta f_s(z_1,z_2)|: z_1,z_2\in\mathbb{R}\big\}$ *and* $M_2 = \sup\big\{\,|\partial_\varphi f_s(z_1,z_2)|: z_1,z_2\in\mathbb{R}\big\}$.

Then, any of the solutions $\big(\varphi(\cdot,t),\theta(\cdot,t)\big)$ *given in Theorem* 2.2 *is attracted to set of stationary solutions in the space* $H^1(\Omega)\times H^1(\Omega)$. *In particular, under the previous condition, when each stationary solution is isolated, any transient solution converges to a unique stationary solution.*

Remark. The question concerning the structure of the set of the stationary solutions, including the question whether they are isolated, is easy to answer in general terms. However, when the temperature at the boundary is a constant θ_1, the stationary problem reduces to the isothermal case ($\theta\equiv\theta_1$). If in addition the functions $a(\cdot)$ and $b(\cdot)$ appearing in $g(\cdot)$ are constants, then the first equation in (6.1) becomes an autonomous scalar equation. If we are also in the one-dimensional case, for which phase-plane analysis is available, then better results are known. For instance, in [37] it is proved that under these conditions, the first equation in (6.1) can have at most one non constant solution (for the homogeneous Neumann boundary conditions for φ, as in our case.). Thus, our stationary problem can have at most four stationary solutions (corresponding to three constants and at most a non constant φ.) *A fortiori*, the associated stationary solutions are isolated, and the second statement in the last theorem can be applied in this particular case. □

Remark. Observe that the steady state solutions for the discretized scheme (2.4)–(2.7), which corresponds to the case when $(\theta^m,\varphi^m) = (\theta^{m-1},\varphi^{m-1})$, for all $m\geq 1$, are the same as the steady state solutions of the original problem, that is, of (6.1). Now, recall that for simplicity we are considering the case when the boundary datum for the temperature is $\theta|_{\partial\Omega}=\theta_1=0$; and, therefore, such steady states solutions are such that the temperature is $\theta\equiv 0$, and the phase field φ satisfies $-\alpha\,\Delta\varphi = g(.,\varphi)$. On the other hand, the the critical points of the Liapunov functional (6.8) satisfy the conditions $\ell^2 M_1^2 C_p^2\Delta\zeta+\zeta=0$, with $\zeta|_{\partial\Omega}=0$ and $\alpha\,\Delta\psi - g(\cdot,\psi)=0$, with $(\partial/\partial n)\,\psi|_{\partial\Omega}=0$. Since these also imply that $\zeta\equiv 0$, we see that, as should be, the critical points of the proposed Liapunov functional are exactly the steady state solutions of both the original problem and the discretized scheme. Thus, it is expected that, under suitable conditions, (6.8) be also a Liapunov functional for the given discretized scheme. However, we were not able to prove that, and it would be very interesting to know whether this is indeed true. □

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