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STABILITY AND CONVERGENCE OF TWO DISCRETE SCHEMES FOR A DEGENERATE SOLUTAL NON-ISOTHERMAL PHASE-FIELD MODEL *

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Abstract. We analyze two numerical schemes of Euler type in time and C^0 finite-element type with $\mathbb{P}_1$-approximation in space for solving a phase-field model of a binary alloy with thermal properties. This model is written as a highly non-linear parabolic system with three unknowns: phase-field, solute concentration and temperature, where the diffusion for the temperature and solute concentration may degenerate. The first scheme is nonlinear, unconditionally stable and convergent. The other scheme is linear but conditionally stable and convergent. A maximum principle is avoided in both schemes, using a truncation operator on the L^2 projection onto the $\mathbb{P}_0$ finite element for the discrete concentration. In addition, for the model when the heat conductivity and solute diffusion coefficients are constants, optimal error estimates for both schemes are shown based on stability estimates.

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1. Introduction

1.1. The model

The phase-field method provides a mathematical description for free-boundary problems associated to physical processes with phase transitions. It postulates the existence of a function, called the phase-field, whose value identifies the phase at a particular point in space and time. The method is particularly suitable for cases with complex growth structures occurring during phase transitions. The mathematical model studied in this work describes the solidification process occurring in a binary alloy with temperature-dependent properties. It is based on a highly non-linear parabolic system of partial differential equations with three dependent variables: phase-field, solute concentration and temperature. Moreover, the temperature and concentration equation have nonlinear degenerate diffusivity.

Keywords and phrases. Phase-field models, diffuse interface model, solidification process, degenerate parabolic systems, backward Euler schemes, finite elements, stability, convergence, error estimates.

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Let $\Omega \subseteq \mathbb{R}^d$ ($d = 2$ or 3) be a bounded domain with boundary Γ. Denote by $[0, T]$ the time interval ($T > 0$). We use the notation $Q = \Omega \times (0, T)$, $\Sigma = \Gamma \times (0, T)$ and $\boldsymbol{n}(\boldsymbol{x})$ is the outwards unit normal vector to Ω at the point $\boldsymbol{x} \in \Gamma$.

After some physical simplifications [5], we consider the following differential problem, related to a phase-field model of a binary alloy with thermal properties [1]:

$$\left\{\begin{array}{rcll} \alpha\varepsilon^2\phi_t - \varepsilon^2\Delta\phi & = & \dfrac{1}{2}(\phi - \phi^3) + \beta(\theta - \theta_A c - \theta_B(1-c)) & \text{in } Q, \\ C_V\theta_t + \dfrac{l}{2}\phi_t & = & \nabla\cdot[K_1(\phi)\nabla\theta] & \text{in } Q, \\ c_t & = & \nabla\cdot[K_2(\phi)(\nabla c + Mc(1-c)\nabla\phi)] & \text{in } Q. \end{array}\right. \tag{1.1}$$

This model is completed with the Neumann boundary conditions

$$\frac{\partial\phi}{\partial\boldsymbol{n}}\Big|_\Sigma = 0, \quad (K_1(\phi)\nabla\theta)\cdot\boldsymbol{n}\Big|_\Sigma = 0, \quad (K_2(\phi)\nabla c)\cdot\boldsymbol{n}\Big|_\Sigma = 0 \tag{1.2}$$

and the initial conditions

$$\phi(\boldsymbol{x}, 0) = \phi_0(\boldsymbol{x}), \qquad \theta(\boldsymbol{x}, 0) = \theta_0(\boldsymbol{x}), \qquad c(\boldsymbol{x}, 0) = c_0(\boldsymbol{x}) \quad \boldsymbol{x} \in \Omega. \tag{1.3}$$

The unknowns for this problem are: $\phi : Q \to \mathbb{R}$ (phase-field) is the state variable characterizing the different phases so that $\phi = 1$ represents the liquid phase and $\phi = -1$ represents the solid phase, $\theta : Q \to \mathbb{R}$ is the temperature of the material, $c : Q \to [0, 1]$ (concentration) represents the fraction of one of the two materials in the mixture. The parameter $\alpha > 0$ is the relaxation scaling; the parameter β is given by $\beta = \varepsilon[s]/3\sigma$, where $\varepsilon > 0$ is the measure of the interface width, σ the surface tension and $[s]$ the entropy density difference between phases; θ_A, θ_B are the melting temperatures of each of the two materials in the alloy; $C_V > 0$ is the specific heat; $l > 0$ the latent heat; $K_1 \geq 0$ the thermal conductivity; $K_2 \geq 0$ the solute diffusivity; $M \in \mathbb{R}$ is a constant related to the slopes of solid and liquid lines.

We will assume that $K_1 = K_1(\phi)$ and $K_2 = K_2(\phi)$ are two globally Lipschitz continuous functions satisfying

$$0 \leq K_1(r) \leq b_1, \quad 0 \leq K_2(r) \leq b_2 \quad \forall\, r \in \mathbb{R},$$

with $b_1, b_2 > 0$. In this sense, the problem is singular with respect to the temperature and concentration when $K_1(\phi) = 0$ or $K_2(\phi) = 0$, respectively. As physically the diffusion of material in the solid phase can be considered close to zero [5]; this leads to a degenerate solute diffusion. Such a phenomenon is included in this model, assuming that $K_2(\phi) = 0$ if $\phi = -1$. On the other hand, although the heat conductivity is nonzero in both solid and liquid phases, we also consider a degenerate diffusion for the temperature with the aim of considering a more general model. Moreover, this may help the development of numerical methods for systems with similar characteristics.

The phase-field model for solidification (1.1) is used to treat phenomena such as crystal growth and the fusion of materials.

Now we introduce the definition of weak solutions similar to that given in [1,12] which take into account the heat and solute degenerate diffusivity, respectively. Moreover, the maximum principle for the concentration equation says us that $0 \leq c \leq 1$ in Q if $0 \leq c_0 \leq 1$ in Ω.

Definition 1.1. A triplet (ϕ, θ, c) is called a weak solution of (1.1)–(1.3) in $(0, T)$ if:

(1) $\phi \in L^2(0, T; H^2(\Omega)) \cap L^\infty(0, T, H^1(\Omega))$, $\phi_t \in L^2(Q), \phi(0) = \phi_0$, $\dfrac{\partial\phi}{\partial\boldsymbol{n}} = 0$ *a.e.* on Σ,
(2) $\theta \in L^\infty(0, T; L^2(\Omega))$, $\theta_t \in L^2(0, T, H^1(\Omega)')$, $\theta(0) = \theta_0$,
(3) $c \in L^\infty(0, T; L^2(\Omega))$, $c_t \in L^2(0, T; H^1(\Omega)')$, $c(0) = c_0$, $0 \leq c \leq 1$ *a.e.* in Q,
(4) $J_1 := \nabla(K_1(\phi)\theta) - \theta\nabla K_1(\phi) \in L^2(Q)$,
(5) $J_2 := \nabla(K_2(\phi)c) - c\nabla K_2(\phi) \in L^2(Q)$,

verifying

$$\alpha\varepsilon^2\phi_t - \varepsilon^2\Delta\phi = \frac{1}{2}(\phi - \phi^3) + \beta(\theta - \theta_A c - \theta_B(1-c)) \quad a.e. \text{ in } Q,$$

$$C_V \int_0^T \langle \theta_t, \eta\rangle \,\mathrm{d}t + \frac{l}{2}\int_0^T \Big(\phi_t, \eta\Big)\,\mathrm{d}t + \int_0^T \Big(J_1, \nabla\eta\Big) = 0,$$

$$\int_0^T \langle c_t, \eta\rangle \,\mathrm{d}t + \int_0^T \Big(J_2, \nabla\eta\Big)\,\mathrm{d}t + M\int_0^T \Big(K_2(\phi)c(1-c)\nabla\phi, \nabla\eta\Big) = 0,$$

for each $\eta \in L^2(0,T;H^1(\Omega))$. If, in addition, $K_1, K_2 \geq b_0 > 0$, then $\theta, c \in L^2(0,T;H^1(\Omega))$ and $J_1 = K_1(\phi)\nabla\theta$, $J_2 = K_1(\phi)\nabla c$.

Here and in what follows, $\Big(\cdot,\cdot\Big)$ denotes the inner product in $L^2(\Omega)$ and $\langle\cdot,\cdot\rangle$ denotes the duality between $H^1(\Omega)'$ and $H^1(\Omega)$.

1.2. **Known results**

In [1], the existence of weak solutions of problem (1.1)–(1.3) but with a constant solute diffusivity ($K_2 > 0$) is obtained *via* the introduction of a regularized problem approximating the degenerate thermal conductivity K_1 by a strictly positive, regular function followed by the derivation of suitable *a priori* estimates and the application of compactness arguments. More concretely, the following existence result was established in [1].

Theorem 1.2. *Let Ω be an open bounded domain of $\mathbb{R}^d$, $d = 2$ or 3, with smooth boundary Γ. Assume $\phi_0 \in H^{1+\gamma}(\Omega)$ with $1/2 < \gamma \leq 1$ such that $\frac{\partial\phi_0}{\partial\mathbf{n}} = 0$ on Γ, $\theta_0 \in L^2(\Omega)$ and $c_0 \in H^1(\Omega)$ such that $0 \leq c_0 \leq 1$ a.e. in $\overline{\Omega}$. Then, there exists (ϕ,θ,c) a weak solution of (1.1)–(1.3) (with $K_1 > 0$ a constant) in $(0,T)$.*

In addition, in [1] the authors say that the hypothesis $\phi_0 \in H^{1+\gamma}(\Omega)$ with $1/2 < \gamma \leq 1$ is not essential, and the result holds for $\phi_0 \in H^1(\Omega)$.

Scheid [12] proved the existence of weak solutions, by using a similar methodology to [1], for the following isothermal phase-field model of a binary alloy

$$\left\{\begin{array}{rcll} \alpha\varepsilon^2\phi_t - \varepsilon^2\Delta\phi & = & F_1(\phi) + cF_2(\phi) & \text{in } Q, \\ c_t & = & \nabla\cdot[D_1(\phi)(\nabla c + D_2(c,\phi)\nabla\phi)] & \text{in } Q, \end{array}\right. \tag{1.4}$$

which has a degenerate solute diffusivity $D_1(\phi) \geq 0$. The main difficulty of model (1.4) is the treatment of the nonlinear term involving $D_1(\phi)D_2(c,\phi)\nabla\phi$ in the concentration equation. Moreover, the maximum principle for the phase-field variable gives $-1 \leq \phi \leq 1$ under the assumptions that the above nonlinearities $F_1(\phi)$ and $F_2(\phi)$ vanish when $\phi = -1$ and $\phi = 1$.

Error estimates of nonlinear numerical schemes for isothermal phase-field models related to binary alloys are given in [10] for a model as (1.4), and, in [4], considering anisotropic diffusion for the phase-field equation and a more general right-hand side in the phase-field equation, changing the terms $F_1(\phi) + cF_2(\phi)$ considered in [10] by $S(c,\phi)$ being a bounded, Lipschitz function.

In [7], optimal error estimates are given for a fully discrete nonlinear numerical scheme of a more simplified phase-field model than (1.1) without the concentration (that is one material is only considered) and with constant thermal conductivity $K_1 > 0$, paying special attention on the dependency of the parameter ε. Stability estimates independent of ε are proved for k small enough with respect to ε, and α, β are constants depending on ε. It is also shown some error bounds depending only on a lower polynomial order for $1/\varepsilon$. Moreover, error estimates are used to establish the convergence of the fully discrete scheme to solutions of the sharp interface limits under different scaling hypotheses in its coefficients.

In [2], a time-discrete nonlinear scheme is proposed for a phase-field problem again without the concentration variable and replacing in the equation for the temperature the term $\frac{l}{2}\phi_t$ by the more general term $\frac{l}{2}f(\theta,\phi)_t$, where f is a generic function satisfying some adequate properties. Convergence of this semi-discrete in time scheme is proved, obtaining the existence and regularity of solutions for the limit problem.

1.3. Main results of the paper

In this work we will consider two numerical schemes in order to approximate problem (1.1) using continuous $\mathbb{P}_1$-finite elements for the tree variables (ϕ, θ, c). Since a maximum principle cannot be verified in general by the discrete concentration, we introduce a truncation operator on the L^2 projection onto $\mathbb{P}_0$, in order to guarantee a L^∞ bound for some terms in the discrete concentration equation. A similar idea of truncation, but without the L^2 projection onto $\mathbb{P}_0$, has been used in [8] for a $2D$ Navier-Stokes model with mass diffusion.

First of all, we will present in Section 2 the nonlinear numerical scheme (2.1)–(2.3) which will be unconditionally stable and convergent.

Theorem 1.3 (unconditionally stable, convergent nonlinear scheme)**.** *Assume*

$$\phi_0 \in H^1(\Omega), \quad \theta_0 \in L^2(\Omega) \quad \text{and} \quad c_0 \in L^2(\Omega) \quad \text{such that} \quad 0 \le c_0 \le 1 \quad \text{a.e. in } \overline{\Omega}.$$

Let Ω be such that the H^2-regularity for the Neumann problem (3.19) holds. Let $\mathcal{T}_h$ be a regular, quasi-uniform family of a polyhedral domain Ω. Then, there exists a convergent subsequence of functions $\phi_{h,k}, \theta_{h,k}$ and $c_{h,k}$ associated to scheme (2.1)–(2.3) (see Def. 3.5) towards a weak solution (ϕ, θ, c) of problem (1.1)–(1.3) in $(0, T)$, as $(h, k) \to 0$ in the following sense:

$$\theta_{h,k} \to \theta, \quad c_{h,k} \to c, \quad \text{in } L^\infty(0,T;L^2(\Omega))\text{-weak}*,$$

$$\phi_{h,k} \to \phi, \quad \text{in } L^\infty(0,T;H^1(\Omega))\text{-weak}*, \quad \text{and in } L^2(0,T;H^1(\Omega))\text{-strong}.$$

Second, we construct the linear numerical scheme (6.1)–(6.3) which will be conditionally stable and convergent.

Theorem 1.4 (conditionally stable, convergent linear scheme)**.** *Assume the assumptions of Theorem 1.3 and the constraint*

$$(S) \qquad \lim_{(h,k)\to 0} \frac{k}{h} = 0.$$

Then, there exists a convergent subsequence of functions $\phi_{h,k}$, $\theta_{h,k}$ and $c_{h,k}$ associated to scheme (6.1)–(6.3) (see Def. 3.5) towards a weak solution (ϕ, θ, c) of problem (1.1)–(1.3) in $(0, T)$, as $(h, k) \to 0$ in the same sense of Theorem 1.3.

At this point, it is well to point out that, in particular, the two previous theorems provide the existence of weak solutions of problem (1.1)–(1.3) under hypotheses on the data weaker than those imposed in [1] (see Thm. 1.2). To be more precise, the hypothesis on c_0 is relaxed from $c_0 \in H^1(\Omega)$ imposed in [1] to $c_0 \in L^2(\Omega)$ as was considered in [12]. Recall that in [12] the isothermal case is considered and in [1] there is not degeneration in the solute diffusivity.

Finally, assuming both the heat conductivity and solute diffusion coefficients are constants, error estimates of order $O(k + h)$ are shown towards a regular enough continuous solution to (1.1)–(1.3).

Theorem 1.5. *Under hypotheses of Theorem 1.3 (respectively Thm. 1.4), admitting that K_1, K_2 are two positive constants and that there exist a continuous solution (ϕ, θ, c) to (1.1)–(1.3) which verifies the regularity assumptions (7.2), then the discrete solution of scheme (2.1)–(2.3) (respectively (6.1)–(6.3)) satisfies for all $n < N$*

$$\|e_\phi^{n+1}\|^2_{H^1(\Omega)} + \frac{1}{4\varepsilon^2}\|e_\phi^{n+1}\|^4_{L^4(\Omega)} + C_V|e_\theta^{n+1}|^2 + |e_c^{n+1}|^2 + \alpha\, k \sum_{l=1}^{n} \left|\frac{e_\phi^{l+1} - e_\phi^{l}}{k}\right|^2$$
$$+ K_1\, k \sum_{l=1}^{n} |\nabla e_\theta^{l+1}|^2 + K_2 k \sum_{l=1}^{n} |\nabla e_c^{l+1}|^2 \le C\Big(h^2 + k^2\Big),$$

where C is a constant independent of h and k, and the errors are denoted by $e_\phi^{n+1} = \phi_h^{n+1} - \phi(t_{n+1})$, $e_\theta^{n+1} = \theta_h^{n+1} - \theta(t_{n+1})$ and $e_c^{n+1} = c_h^{n+1} - c(t_{n+1})$.

The rest of the paper is described as follows. In Section 2 the nonlinear scheme (2.1)–(2.3) is presented, obtaining its unconditionally stability in Section 3. In Section 4 some necessary compactness results are proved, passing to the limit in Section 5 and concluding the proof of Theorem 1.3. In addition, a conditionally stable and convergent linear scheme is studied in Section 6 giving an outline of the proof of Theorem 1.4. Finally, Section 7 is devoted to studying optimal error estimates for both schemes.

2. A nonlinear scheme

In what follows, let us consider a uniform partition $t_n = n\,k$ of the time interval $[0,T]$ with $k = T/N$ the time step, let $\Omega \subset \mathbb{R}^d$ ($d = 2$ or 3) be a domain with polyhedral boundary and $\mathcal{T}_h$ be a family of triangulations of Ω with $\overline{\Omega} = \bigcup_{K\in\mathcal{T}_h} K$. Here $h := \max_{K\in\mathcal{T}_h} h_K$ with h_K the diameter of K. Let X_h be the finite element subspace of $H^1(\Omega)$ furnished by globally continuous, piecewise linear functions, that is,

$$X_h = \{x_h \in C^0(\overline{\Omega})\colon x_h|_K \in \mathbb{P}_1(K), \quad \forall\, K \in \mathcal{T}_h,\}\cdot$$

A first idea to approximate equation $(1.1)_1$ is

$$\begin{cases} \alpha\left(\dfrac{\phi_h^{n+1}-\phi_h^n}{k}, x_h\right) + \left(\nabla\phi_h^{n+1}, \nabla x_h\right) + \dfrac{1}{2\varepsilon^2}\left((\phi_h^{n+1})^3, x_h\right) \\ = \dfrac{1}{2\varepsilon^2}\left(\phi_h^n, x_h\right) + \dfrac{\beta}{\varepsilon^2}\left(\theta_h^n - \theta_A c_h^n - \theta_B(1-c_h^n), x_h\right), \quad \forall\, x_h \in X_h. \end{cases}$$

But, we add $\left(\phi_h^{n+1}, x_h\right)$ to the left-hand side and $\left(\phi_h^n, x_h\right)$ to the right-hand side which will cancel each other in the limit as (h,k) go to zero. The reason why we introduce these terms is to get stability constants only of polynomial order with respect to ε avoiding exponential dependence. Concretely, since $\beta = O(\varepsilon)$, we will get stability constants depending on $1/\varepsilon$ (see Rem. 3.2 below).

Then we propose the following scheme to approximate problem (1.1)–(1.3):

Initialization: Let $(\phi_h^0, \theta_h^0, c_h^0) \in X_h \times X_h \times X_h$ be suitable approximations of (ϕ_0, θ_0, c_0).

Step $n+1$: Given $(\phi_h^n, \theta_h^n, c_h^n) \in X_h \times X_h \times X_h$.

Find $\phi_h^{n+1} \in X_h$ as a solution of the problem:

$$\begin{cases} \alpha\left(\dfrac{\phi_h^{n+1}-\phi_h^n}{k}, x_h\right) + \left(\nabla\phi_h^{n+1}, \nabla x_h\right) + \left(\phi_h^{n+1}, x_h\right) + \dfrac{1}{2\varepsilon^2}\left((\phi_h^{n+1})^3, x_h\right) \\ = \left(\dfrac{1}{2\varepsilon^2}+1\right)\left(\phi_h^n, x_h\right) + \dfrac{\beta}{\varepsilon^2}\left(\theta_h^n - \theta_A c_h^n - \theta_B(1-c_h^n), x_h\right), \quad \forall\, x_h \in X_h. \end{cases} \tag{2.1}$$

Find $\theta_h^{n+1} \in X_h$ and $c_h^{n+1} \in X_h$ as solutions of the decoupled variational problems:

$$C_V\left(\frac{\theta_h^{n+1}-\theta_h^n}{k}, x_h\right) + \left(K_1^h(\phi_h^{n+1})\nabla\theta_h^{n+1}, \nabla x_h\right) = -\frac{l}{2}\left(\frac{\phi_h^{n+1}-\phi_h^n}{k}, x_h\right), \quad \forall\, x_h \in X_h, \tag{2.2}$$

$$\begin{cases} \left(\dfrac{c_h^{n+1}-c_h^n}{k}, x_h\right) + \left(K_2^h(\phi_h^{n+1})\nabla c_h^{n+1}, \nabla x_h\right) \\ = -M\left(K_2^h(\phi_h^{n+1})[P_0 c_h^n]_T(1-[P_0 c_h^n]_T)\nabla\phi_h^n, \nabla x_h\right), \quad \forall\, x_h \in X_h. \end{cases} \tag{2.3}$$

Here $K_1^h = K_1 + g_1(h)$, $K_2^h = K_2 + g_2(h)$, where g_i are positive functions to be chosen later, and P_0 is the L^2 orthogonal projector onto X_h^0, where X_h^0 is the finite element space of piecewise constant functions, and $[\cdot]_T$ is a truncation operator defined from X_h^0 into X_h^0 as follows: Given $x_h \in X_h^0$, then $[x_h]_T \in X_h^0$ such that

$$\forall\, K \in \mathcal{T}_h, \quad [x_h]_T|_K = \begin{cases} x_h|_K & \text{if} \quad x_h|_K \in [0,1], \\ 0 & \text{if} \quad x_h|_K < 0, \\ 1 & \text{if} \quad x_h|_K > 1. \end{cases}$$

Since (2.2) and (2.3) are quadratic linear systems, it is easy to check the existence and uniqueness of solutions. On the other hand, (2.1) is a discrete nonlinear variational problem and its existence and uniqueness can be proved as follows: We define

$$J(\phi_h) = \frac{\alpha}{2\,k}\int_\Omega |\phi_h|^2 + \frac{1}{2}\int_\Omega \Big(|\nabla\phi_h|^2 + |\phi_h|^2\Big) + \frac{1}{8\varepsilon^2}\int_\Omega |\phi_h|^4 - \int_\Omega g\,\phi_h, \tag{2.4}$$

where $g = \dfrac{\alpha}{k}\phi_h^n + \Big(\dfrac{1}{2\varepsilon^2}+1\Big)\phi_h^n + \dfrac{\beta}{\varepsilon^2}\Big(\theta_h^n - \theta_A c_h^n - \theta_B(1-c_h^n)\Big)$. Clearly, J is a strictly convex functional on X_h, then the minimum problem $\min\limits_{\phi_h\in X_h} J(\phi_h)$ has a unique solution characterized by its Euler equation (2.1).

We will denote by C generic positive constants always independent of the discretization parameters h and k.

3. *A priori* estimates and weak convergences

Let us add and subtract the term $\dfrac{1}{2\varepsilon^2}\Big(\phi_h^{n+1}, x_h\Big)$ to the left-hand side of (2.1) in order to rewrite (2.1) with respect to the so-called Ginzburg-Landau function $f(\phi) = \dfrac{1}{2\varepsilon^2}\Big(\phi^2-1\Big)\phi$ which has the potential function $F(\phi) = \dfrac{1}{8\varepsilon^2}\Big(\phi^2-1\Big)^2$, that is, $f(\phi) = \nabla_\phi F(\phi)$. Then, (2.1) is rewritten as:

$$\begin{cases} \alpha\left(\dfrac{\phi_h^{n+1}-\phi_h^n}{k}, x_h\right) + \Big(\nabla\phi_h^{n+1}, \nabla x_h\Big) + \Big(\phi_h^{n+1}, x_h\Big) \\ +\Big(f(\phi_h^{n+1}), x_h\Big) + \dfrac{1}{2\varepsilon^2}\Big(\phi_h^{n+1}-\phi_h^n, x_h\Big) = \Big(\phi_h^n, x_h\Big) \\ +\dfrac{\beta}{\varepsilon^2}\Big(\theta_h^n - \theta_A c_h^n - \theta_B(1-c_h^n), x_h\Big) \quad \forall\, x_h \in X_h. \end{cases} \tag{3.1}$$

It is easy to check that if we select $\phi_h^0 = I_h\phi_0$, $\theta_h^0 = I_h\theta_0$ and $c_h^0 = I_h c_0$ as initial approximations, where I_h is an interpolation operator into X_h satisfying stability properties in the L^2, L^4 and H^1 norms, it follows that there exists a constant $C_2 > 0$ (independent of ε) such that

$$\frac{2C_V\beta}{l\varepsilon^2}|\theta_h^0|^2 + |c_h^0|^2 + 1 + \|\phi_h^0\|^2_{H^1(\Omega)} + \frac{1}{4\varepsilon^2}\int_\Omega (|\phi_h^0|^2-1)^2 \le \frac{C_2}{\varepsilon^2}. \tag{3.2}$$

For instance, this is true when I_h is the L^2-projector onto X_h, or I_h is the Clément or Scott-Zhang regularization operator.

Let us denote by $|\cdot|$ the $L^2(\Omega)$-norm and by $\|\cdot\|_{H^1(\Omega)}$ the $H^1(\Omega)$-norm. With such a notation we establish the following stability result.

Lemma 3.1. *Assume $\phi_0 \in H^1(\Omega)$, $\theta_0 \in L^2(\Omega)$ and $c_0 \in L^2(\Omega)$ such that $0 \le c_0 \le 1$ a.e. in $\overline{\Omega}$. Then, for each k such that $\dfrac{\beta k}{\varepsilon^2}$ is sufficiently small, the discrete solution of scheme (2.1)–(2.3) satisfies the following estimates:*

$$(\boldsymbol{i})\quad \max_{0\le n\le N} \|\phi_h^n\|^2_{H^1(\Omega)} \le C, \quad (\boldsymbol{ii})\quad \sum_{n=0}^{N-1} \|\phi_h^{n+1}-\phi_h^n\|^2_{H^1(\Omega)} \le C, \quad (\boldsymbol{iii})\quad k\sum_{n=0}^{N-1}\left|\frac{\phi_h^{n+1}-\phi_h^n}{k}\right|^2 \le C,$$

$$(\boldsymbol{iv})\quad \max_{0\le n\le N} |\theta_h^n|^2 \le C, \quad (\boldsymbol{v})\quad \sum_{n=0}^{N-1} |\theta_h^{n+1}-\theta_h^n|^2 \le C, \quad (\boldsymbol{vi})\quad k\sum_{n=0}^{N-1} |\sqrt{K_1^h(\phi_h^{n+1})}\nabla\theta_h^{n+1}|^2 \le C,$$

$$(\boldsymbol{vii})\quad \max_{0\le n\le N} |c_h^n|^2 \le C, \quad (\boldsymbol{viii})\quad \sum_{n=0}^{N-1} |c_h^{n+1}-c_h^n|^2 \le C, \quad (\boldsymbol{ix})\ k\sum_{n=0}^{N-1} |\sqrt{K_2^h(\phi_h^{n+1})}\nabla c_h^{n+1}|^2 \le C,$$

where $C>0$ depends on ε and the data (ϕ_0,θ_0,c_0) but is independent of (h,k).

Proof. Let $x_h = \dfrac{4\beta}{l\,\varepsilon^2}k\theta_h^{n+1}$ and $x_h = 2\,k\,c_h^{n+1}$ be test functions in (2.2) and (2.3), respectively. Now by using the identity $(a-b,2a) = |a|^2-|b|^2+|a-b|^2$ and bounding adequately the right-hand side, we have

$$\begin{aligned}
&\frac{2C_V\beta}{l\varepsilon^2}\Big(|\theta_h^{n+1}|^2-|\theta_h^n|^2+|\theta_h^{n+1}-\theta_h^n|^2\Big)+\frac{4\beta}{l\varepsilon^2}k|\sqrt{K_1^h(\phi_h^{n+1})}\nabla\theta_h^{n+1}|^2\\
&=-\frac{2\beta}{\varepsilon^2}k\left(\frac{\phi_h^{n+1}-\phi_h^n}{k},\theta_h^n+(\theta_h^{n+1}-\theta_h^n)\right)\\
&\le -\frac{2\beta}{\varepsilon^2}k\left(\frac{\phi_h^{n+1}-\phi_h^n}{k},\theta_h^n\right)+\frac{\alpha}{2}k\left|\frac{\phi_h^{n+1}-\phi_h^n}{k}\right|^2+\frac{2\beta^2}{\alpha\varepsilon^4}k|\theta_h^{n+1}-\theta_h^n|^2,
\end{aligned}\tag{3.3}$$

$$|c_h^{n+1}|^2-|c_h^n|^2+|c_h^{n+1}-c_h^n|^2+k|\sqrt{K_2^h(\phi_h^{n+1})}\nabla c_h^{n+1}|^2 \le C\,k|\nabla\phi_h^n|^2. \tag{3.4}$$

By choosing $\dfrac{\beta k}{\varepsilon^2}$ sufficiently small to control the last term on the right-hand side of (3.3), this inequality reduces to

$$\begin{aligned}
&\frac{2C_V\beta}{l\varepsilon^2}\Big(|\theta_h^{n+1}|^2-|\theta_h^n|^2+\frac{1}{2}|\theta_h^{n+1}-\theta_h^n|^2\Big)+\frac{4\beta}{l\varepsilon^2}k|\sqrt{K_1^h(\phi_h^{n+1})}\nabla\theta_h^{n+1}|^2 \le\\
&\qquad -\frac{2\beta}{\varepsilon^2}k\left(\frac{\phi_h^{n+1}-\phi_h^n}{k},\theta_h^n\right)+\frac{\alpha}{2}k\left|\frac{\phi_h^{n+1}-\phi_h^n}{k}\right|^2.
\end{aligned}\tag{3.5}$$

Next, take $x_h = 2\,k\dfrac{\phi_h^{n+1}-\phi_h^n}{k}$ as a test function in (2.1), it follows that

$$\begin{aligned}
&\alpha\,k\left|\frac{\phi_h^{n+1}-\phi_h^n}{k}\right|^2+\Big(\|\phi_h^{n+1}\|^2_{H^1(\Omega)}-\|\phi_h^n\|^2_{H^1(\Omega)}+\|\phi_h^{n+1}-\phi_h^n\|^2_{H^1(\Omega)}\Big)+2\Big(f(\phi_h^{n+1}),\phi_h^{n+1}-\phi_h^n\Big)\\
&\qquad+\frac{1}{\varepsilon^2}|\phi_h^{n+1}-\phi_h^n|^2 \le \frac{2\beta}{\varepsilon^2}k\left(\theta_h^n,\frac{\phi_h^{n+1}-\phi_h^n}{k}\right)+Ck|\phi_h^n|^2+C\frac{\beta^2}{\alpha\varepsilon^4}k(|c_h^n|^2+1),
\end{aligned}\tag{3.6}$$

where C is a constant independent of ε.

Now, using again the identity $(a-b,a)=\frac{1}{2}(|a|^2-|b|^2+|a-b|^2)$ twice, we can rewrite

$$\begin{aligned}2\Big(f(\phi_h^{n+1}),\phi_h^{n+1}-\phi_h^n\Big)&=\frac{1}{2\varepsilon^2}\int_\Omega\Big((\phi_h^{n+1})^2-1\Big)\Big((\phi_h^{n+1})^2-(\phi_h^n)^2+(\phi_h^{n+1}-\phi_h^n)^2\Big)\\&=2\int_\Omega\Big(F(\phi_h^{n+1})-F(\phi_h^n)+\frac{1}{8\varepsilon^2}((\phi_h^{n+1})^2-(\phi_h^n)^2)^2\Big)\\&\quad+\frac{1}{2\varepsilon^2}\int_\Omega\Big((\phi_h^{n+1})^2-1\Big)|\phi_h^{n+1}-\phi_h^n|^2.\end{aligned}\tag{3.7}$$

Note that the negative term on the right-hand side of (3.7) can be absorbed by the last term on the left-hand side of (3.6). This property can be summarized as

$$\frac{1}{2\varepsilon^2}\Big((\phi_h^{n+1})^3-\phi_h^n\Big)\Big(\phi_h^{n+1}-\phi_h^n\Big)\geq F(\phi_h^{n+1})-F(\phi_h^n)\tag{3.8}$$

which is an appropriate discrete version of the equality $f(\phi)\phi_t=F(\phi)_t$.

Next, if we add up (3.4), (3.5) and (3.6), the first term on the right hand side of (3.5) and (3.6) disappears, and we get

$$\begin{aligned}&\frac{2C_V\beta}{l\varepsilon^2}\Big(|\theta_h^{n+1}|^2-|\theta_h^n|^2+\frac{1}{2}|\theta_h^{n+1}-\theta_h^n|^2\Big)+\frac{4\beta}{l\varepsilon^2}k|\sqrt{K_1^h(\phi_h^{n+1})}\nabla\theta_h^{n+1}|^2\\&+(|c_h^{n+1}|^2+1)-(|c_h^n|^2+1)+|c_h^{n+1}-c_h^n|^2+k|\sqrt{K_2^h(\phi_h^{n+1})}\nabla c_h^{n+1}|^2\\&+\frac{\alpha}{2}k\left|\frac{\phi_h^{n+1}-\phi_h^n}{k}\right|^2+\Big(\|\phi_h^{n+1}\|^2_{H^1(\Omega)}-\|\phi_h^n\|^2_{H^1(\Omega)}+\|\phi_h^{n+1}-\phi_h^n\|^2_{H^1(\Omega)}\Big)\\&+2\int_\Omega\Big(F(\phi_h^{n+1})-F(\phi_h^n)\Big)\leq C\,k\|\phi_h^n\|^2_{H^1(\Omega)}+C\frac{\beta^2}{\alpha\varepsilon^4}k(|c_h^n|^2+1).\end{aligned}$$

Finally, by summing over n the discrete Gronwall lemma and the initial bound (3.2) provide the desired estimates, and this completes the proof. □

Remark 3.2. Since the initial estimates have order $O(\varepsilon^{-2})$, see (3.2), then the stability estimates obtained in Lemma 3.1 are of order $O(\varepsilon^{-2}\mathrm{e}^{C\beta^2\varepsilon^{-4}})$ for the variables $(\phi,\frac{\sqrt{\beta}}{\varepsilon}\theta,c)$. As β is of order $O(\varepsilon)$, the order reduces to $O(\varepsilon^{-2}\mathrm{e}^{C\varepsilon^{-2}})$. In particular, these estimates would be independent of ε if β were of order $O(\varepsilon^2)$ and considering an initial bound (3.2) independent of ε. Furthermore, if we truncate the discrete concentration c_h^n in (2.1) as made in (2.3), that is replacing $\frac{\beta}{\varepsilon^2}\Big(\theta_h^n-\theta_Ac_h^n-\theta_B(1-c_h^n),x_h\Big)$ by $\frac{\beta}{\varepsilon^2}\Big(\theta_h^n-\theta_A[P_0c_h^n]_T-\theta_B(1-[P_0c_h^n]_T),x_h\Big)$, this modified scheme has stability estimates of order $O(\varepsilon^{-2}+\beta^2\varepsilon^{-4})$.

Remark 3.3. Observe that in this nonlinear scheme, we have used a first-order semi-implicit approximation of the Ginzburg-Landau function $f(\phi)$, which provides a stationary problem to solve in each time step, identified with the critical point of a convex functional (see (2.4)). Moreover, this approximation verifies the property (3.8). For instance, if we use the first-order implicit approximation $f(\phi_h^{n+1})$, then the associated stationary problem (of Allen-Cahn type) is related to the critical points of a non-convex functional and the property (3.8) in not verified, because a negative term appears on the right-hand side. To be more concrete, it follows that

$$f(\phi_h^{n+1})\Big(\phi_h^{n+1}-\phi_h^n\Big)\geq F(\phi_h^{n+1})-F(\phi_h^n)-\frac{1}{4\varepsilon^2}(\phi_h^{n+1}-\phi_h^n)^2.$$

Consider the linear operator $L_h : X_h \to X_h$ defined as:

$$\Big(L_h\phi_h, x_h\Big) = \Big(\nabla\phi_h, \nabla x_h\Big) + \Big(\phi_h, x_h\Big) \quad \forall\, x_h \in X_h. \tag{3.9}$$

Then, the discrete phase-field equation (2.1) can be rewritten as:

$$\begin{cases} \Big(\dfrac{\phi_h^{n+1}-\phi_h^n}{k}, x_h\Big) + \dfrac{1}{\alpha}\Big(L_h\phi_h^{n+1}, x_h\Big) + \dfrac{1}{2\alpha\varepsilon^2}\Big((\phi_h^{n+1})^3, x_h\Big) \\ = \Big(\dfrac{1}{2\alpha\varepsilon^2}+\dfrac{1}{\alpha}\Big)\Big(\phi_h^n, x_h\Big) + \dfrac{\beta}{\alpha\varepsilon^2}\Big(\theta_h^n - \theta_A c_h^n - \theta_B(1-c_h^n), x_h\Big), \quad \forall\, x_h \in X_h. \end{cases} \tag{3.10}$$

Taking $x_h = L_h\phi_h^{n+1}$ as a test function in (3.10) and using the estimates of Lemma 3.1, the following result can be established.

Corollary 3.4. *Under the hypotheses of Lemma 3.1, it holds*

$$k\sum_{n=0}^{N-1} |L_h\phi_h^{n+1}|^2 \le C.$$

On the other hand, since $K_1(\cdot) \le b_1$ and $K_2(\cdot) \le b_2$, from (***vi***) and (***ix***) of Lemma 3.1 we also have

$$k\sum_{n=0}^{N-1} |K_1^h(\phi_h^{n+1})\nabla\theta_h^{n+1}|^2 \le C, \quad k\sum_{n=0}^{N-1} |K_2^h(\phi_h^{n+1})\nabla c_h^{n+1}|^2 \le C.$$

Definition 3.5. We define $\phi_{h,k}$ (respectively $\widehat{\phi}_{h,k}$) as the piecewise constant functions in time taking values ϕ_h^{n+1} on $(t_n, t_{n+1}]$ (respectively ϕ_h^n). Analogously, we define $\theta_{h,k}$, $\widehat{\theta}_{h,k}$, and $c_{h,k}$, $\widehat{c}_{h,k}$. Moreover, we define $\widetilde{\phi}_{h,k}$, $\widetilde{\theta}_{h,k}$, $\widetilde{c}_{h,k} \in C^0([0,T]; X_h)$ as the piecewise linear functions in time such that $\widetilde{\phi}_{h,k}(t_n) = \phi_h^n$, $\widetilde{\theta}_{h,k}(t_n) = \theta_h^n$, $\widetilde{c}_{h,k}(t_n) = c_h^n$, respectively.

An easy consequence of the previous definition, Lemma 3.1 and Corollary 3.4 is the following result.

Lemma 3.6. *Under the hypotheses of Lemma 3.1, the following estimates hold:*

$$\{\theta_{h,k}\}_{h,k},\ \{\widehat{\theta}_{h,k}\}_{h,k},\ \{\widetilde{\theta}_{h,k}\}_{h,k} \quad \textit{is bounded in} \quad L^\infty(0,T;L^2(\Omega)), \tag{3.11}$$

$$\{c_{h,k}\}_{h,k},\ \{\widehat{c}_{h,k}\}_{h,k},\ \{\widetilde{c}_{h,k}\}_{h,k} \quad \textit{is bounded in} \quad L^\infty(0,T;L^2(\Omega)), \tag{3.12}$$

$$\{\phi_{h,k}\}_{h,k},\ \{\widehat{\phi}_{h,k}\}_{h,k},\ \{\widetilde{\phi}_{h,k}\}_{h,k} \quad \textit{is bounded in} \quad L^\infty(0,T;H^1(\Omega)), \tag{3.13}$$

$$\{K_1^h(\phi_{h,k})\nabla\theta_{h,k}\}_{h,k} \quad \textit{is bounded in} \quad L^2(0,T;L^2(\Omega)), \tag{3.14}$$

$$\{K_2^h(\phi_{h,k})\nabla c_{h,k}\}_{h,k} \quad \textit{is bounded in} \quad L^2(0,T;L^2(\Omega)), \tag{3.15}$$

$$\left\{\frac{\mathrm{d}}{\mathrm{d}t}\widetilde{\phi}_{h,k}\right\}_{h,k} \quad \textit{is bounded in} \quad L^2(0,T;L^2(\Omega)). \tag{3.16}$$

$$\{L_h\phi_{h,k}\}_{h,k} \quad \textit{is bounded in} \quad L^2(0,T;L^2(\Omega)). \tag{3.17}$$

In addition, there exist a subsequence of (h,k) (denoted in the same way) and limit functions ϕ, θ, c, w, J_1 and J_2 verifying the following weak convergences as $(h,k)\to 0$:

$$\theta_{h,k}\to\theta,\quad \widehat{\theta}_{h,k}\to\theta,\quad \widetilde{\theta}_{h,k}\to\theta\quad \textit{in } L^\infty(0,T;L^2(\Omega))\textit{-weak*},$$

$$c_{h,k}\to c,\quad \widehat{c}_{h,k}\to c,\quad \widetilde{c}_{h,k}\to c\quad \textit{in } L^\infty(0,T;L^2(\Omega))\textit{-weak*},$$
$$\phi_{h,k}\to\phi,\quad \widehat{\phi}_{h,k}\to\phi,\quad \widetilde{\phi}_{h,k}\to\phi\quad \textit{in } L^\infty(0,T;H^1(\Omega))\textit{-weak*},$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\widetilde{\phi}_{h,k}\to\frac{\mathrm{d}}{\mathrm{d}t}\phi\quad \textit{in } L^2(0,T;L^2(\Omega))\textit{-weak},$$
$$L_h\phi_{h,k}\to w\quad \textit{in } L^2(0,T;L^2(\Omega))\textit{-weak},$$
$$K_1^h(\phi_{h,k})\nabla\theta_{h,k}\to J_1\quad \textit{in } L^2(0,T;L^2(\Omega))\textit{-weak},$$
$$K_2^h(\phi_{h,k})\nabla c_{h,k}\to J_2\quad \textit{in } L^2(0,T;L^2(\Omega))\textit{-weak}.$$

So far, neither the $H^2(\Omega)$-regularity for the Neumann problem (3.19) nor the quasi-uniform property of the triangulation $\mathcal{T}_h$ of Ω has not been necessary to impose. Now, imposing these hypotheses, the next corollary provides a "discrete interpolation" inequality which plays an important role in getting a compactness result (see the proof of Prop. 4.3) that we will use to pass to the limit in (2.3) (respectively, in (6.3) for the linear scheme).

Corollary 3.7. *Under the hypotheses of Theorem 1.3, it follows that*

$$\|\phi_h^{n+1}\|_{W^{1,3}(\Omega)}\le C|\phi_h^{n+1}|^{1/2}|L_h\phi_h^{n+1}|^{1/2}\tag{3.18}$$

where $C>0$ is independent of h and k.

Proof. Let $\phi(h)\in H^2(\Omega)$ be the solution to the problem

$$-\Delta\phi(h)+\phi(h)=L_h\phi_h^{n+1}\text{ in }\Omega,\quad \frac{\partial\phi(h)}{\partial\boldsymbol{n}}=0\text{ on }\Gamma.\tag{3.19}$$

We now suppose that problem (3.19) has the regularity property $\|\phi(h)\|_{H^2(\Omega)}\le C|L_h\phi_h^{n+1}|$ (such a condition holds if, for instance, Ω is a convex polygon). From (3.9) and (3.19), we have

$$\Big(\nabla\phi(h)-\nabla\phi_h^{n+1},\nabla x_h\Big)+\Big(\phi(h)-\phi_h^{n+1},x_h\Big)=0\quad\forall x_h\in X_h;$$

hence ϕ_h^{n+1} can be interpreted as the H^1-projection of $\phi(h)$ onto X_h. Then, the estimate $\|\phi_h^{n+1}\|_{W^{1,3}(\Omega)}\le C\|\phi(h)\|_{W^{1,3}(\Omega)}$ holds for a constant $C>0$ independent of h (see [3], Chap. 8, and [11]). Thus,

$$\|\phi_h^{n+1}\|^2_{W^{1,3}(\Omega)}\le C\|\phi(h)\|_{H^1(\Omega)}\|\phi(h)\|_{H^2(\Omega)}\le C\|\phi(h)\|_{H^1(\Omega)}|L_h\phi_h^{n+1}|.$$

Therefore, it remains to bound $\|\phi(h)\|_{H^1(\Omega)}\le C\|\phi_h^{n+1}\|_{H^1(\Omega)}$ in order to obtain (3.18). Indeed, we write

$$\|\phi(h)\|_{H^1(\Omega)}\le\|\phi(h)-\phi_h^{n+1}\|_{H^1(\Omega)}+\|\phi_h^{n+1}\|_{H^1(\Omega)}\le C\,h|L_h\phi_h^{n+1}|+\|\phi_h^{n+1}\|_{H^1(\Omega)},$$

where in the last bound we have used that $\|\phi(h)-\phi_h^{n+1}\|_{H^1(\Omega)}\le C\,h\|\phi(h)\|_{H^2(\Omega)}$. Finally, the estimate $|L_h\phi_h^{n+1}|\le C\frac{1}{h}\|\phi_h^{n+1}\|_{H^1(\Omega)}$ can be deduced by taking $\phi_h=\phi_h^{n+1}$ and $x_h=L_h\phi_h^{n+1}$ in (3.9) and using the inverse inequality $\|L_h\phi_h^{n+1}\|_{H^1(\Omega)}\le C\frac{1}{h}|L_h\phi_h^{n+1}|$ (here the quasi-uniform property of the triangulation is used). □

A straightforward application of (3.18) shows that

$$\{\phi_{h,k}\}_{h,k}\text{ is bounded in }L^4(0,T;W^{1,3}(\Omega)).\tag{3.20}$$

4. Strong convergences

Let us show some compactness results in order to identify firstly $w = -\Delta\phi + \phi$, $J_1 = \nabla(K_1(\phi)\theta) - \theta\nabla K_1(\phi)$ and $J_2 = \nabla(K_2(\phi)\theta) - \theta\nabla K_2(\phi)$ and then to pass to the limit as $(h,k) \to 0$.

4.1. **Compactness for phase-field sequences**

First of all, since $\{\widetilde{\phi}_{h,k}\}_{h,k}$ is bounded in $L^\infty(0,T,H^1(\Omega))$ and $\left\{\frac{\mathrm{d}}{\mathrm{d}t}\widetilde{\phi}_{h,k}\right\}_{h,k}$ is bounded in $L^2(0,T;L^2(\Omega))$, a compactness theorem of Aubin-Lions type [13] provides

$$\widetilde{\phi}_{h,k} \to \phi \quad \text{in } C(0,T;L^p(\Omega)) \text{ strongly as } (h,k) \to 0,$$

with $p < 6$. Moreover, owing to Lemma 3.1

$$\|\widetilde{\phi}_{h,k} - \phi_{h,k}\|^2_{L^2(0,T;L^2(\Omega))} \le \|\widehat{\phi}_{h,k} - \phi_{h,k}\|^2_{L^2(0,T;L^2(\Omega))} = k\sum_{n=0}^{N-1} |\phi_h^{n+1} - \phi_h^n|^2 \le C\,k.$$

Therefore, $\phi_{h,k} \to \phi$, $\widehat{\phi}_{h,k} \to \phi$ in $L^2(0,T;L^2(\Omega))$ strongly as $(h,k) \to 0$. As $\{\phi\}_{h,k}$ and $\{\widehat{\phi}\}_{h,k}$ are bounded in $L^\infty(0,T;H^1(\Omega))$, Sobolev's imbedding gives us the strong convergences

$$\phi_{h,k}, \widehat{\phi}_{h,k} \to \phi \quad \text{in } L^q(0,T;L^p(\Omega)) \text{ strongly as } (h,k) \to 0,$$

with $q < \infty$ and $p < 6$.

To prove the compactness of $\{\phi_{h,k}\}_{h,k}$ in $L^2(0,T;H^1(\Omega))$ we firstly must identify $w = -\Delta\phi + \phi$. Indeed, we consider $\eta \in C_c^\infty(Q)$ and choose $\eta_h^n \in X_h$ a suitable approximation of $\eta(t_n)$ such that $\eta_{h,k} \to \eta$ in $L^2(0,T;H^1(\Omega))$ strongly as $(h,k) \to 0$ (here $\eta_{h,k}$ is defined by η_h^n as in Def. 3.5). Then, setting $\phi_h = \phi_h^{n+1}$ and $x_h = \eta_h^{n+1}$ in the definition of L_h (3.9), multiplying by k and summing over n and tending $(h,k) \to 0$, one sees that

$$\int_Q \Big(\nabla\phi, \nabla\eta\Big) + \Big(\phi, \eta\Big) \leftarrow \int_Q \Big(\nabla\phi_{h,k}, \nabla\eta_{h,k}\Big) + \Big(\phi_{h,k}, \eta_{h,k}\Big) = \int_Q \Big(L_h\phi_{h,k}, \eta_{h,k}\Big) \to \int_Q \Big(w, \eta\Big).$$

Therefore, it is clear that $w = -\Delta\phi + \phi$ in $L^2(\Omega)$. Next, taking $\eta \in C^\infty(Q)$ and proceeding in the same manner, we recover the boundary condition $\dfrac{\partial\phi}{\partial \boldsymbol{n}} = 0$ on Σ.

Now, we continue to get the compactness of $\{\phi_{h,k}\}_{h,k}$ in $L^2(0,T;H^1(\Omega))$. Considering $\phi_h = \phi_h^{n+1}$ and $x_h = \phi_h^{n+1}$ in (3.9), multiplying by k and summing over n, this results

$$\int_0^T \|\phi_{h,k}\|^2_{H^1(\Omega)} = \int_0^T \Big(L_h\phi_{h,k}, \phi_{h,k}\Big) \longrightarrow \int_0^T \Big(-\Delta\phi + \phi, \phi\Big) = \int_0^T \|\phi\|^2_{H^1(\Omega)} \quad \text{as } (h,k) \to 0,$$

because of $\phi_{h,k} \to \phi$ strongly in $L^2(0,T;L^2(\Omega))$ and $\{L_h\phi_{h,k}\}_{h,k} \to -\Delta\phi + \phi$ weakly in $L^2(0,T;L^2(\Omega)$.

Therefore, one can obtain the convergence $\|\phi_{h,k}\|_{L^2(0,T;H^1(\Omega))} \to \|\phi\|_{L^2(0,T;H^1(\Omega))}$ as $(h,k) \to 0$. Consequently, since $\phi_{h,k} \to \phi$ weakly* in $L^2(0,T;H^1(\Omega))$, one has

$$\|\phi_{h,k} - \phi\|_{L^2(0,T;H^1(\Omega))} \to 0 \text{ as } (h,k) \to 0.$$

4.2. Compactness for temperature and concentration sequences

Lemma 4.1. *The following estimates hold*

$$\int_0^T \left\| \frac{\mathrm{d}}{\mathrm{d}t}\widetilde{\theta}_{h,k}(t) \right\|^2_{H^1(\Omega)'} \mathrm{d}t \le C, \tag{4.1}$$

$$\int_0^T \left\| \frac{\mathrm{d}}{\mathrm{d}t}\widetilde{c}_{h,k}(t) \right\|^2_{H^1(\Omega)'} \mathrm{d}t \le C, \tag{4.2}$$

where $C > 0$ is independent of (h, k).

Proof. Let P_h be the orthogonal projector from $L^2(\Omega)$ onto X_h. Let $x \in H^1(\Omega)$. Then, by taking $x_h = P_h x$ as a test function in (2.2), we obtain

$$C_V \left(\frac{\theta_h^{n+1} - \theta_h^n}{k}, x \right) \le C|K_1^h(\phi_h^{n+1})\nabla\theta_h^{n+1}|\, \|x\|_{H^1(\Omega)} + \frac{l}{2}\left| \frac{\phi_h^{n+1} - \phi_h^n}{k} \right| |x|, \tag{4.3}$$

where we have used the following stability properties of the L^2-projector, $|P_h x| \le |x|$ and $\|P_h x\|_{H^1} \le C\,\|x\|_{H^1}$ (the stability in the H^1-norm can be obtained by means of a duality argument and comparing with the H^1-projector). Taking into account that $\dfrac{\mathrm{d}}{\mathrm{d}t}\widetilde{\theta}_{h,k}(t) = \dfrac{\theta_h^{n+1} - \theta_h^n}{k}$ for each $t \in (t_n, t_{n+1})$, multiplying (4.3) by k, and adding up over n, estimate (4.1) is proved.

In a analogous way, one can be proved estimate (4.2). □

As a consequence of Lemmas 3.6 and 4.1, one can use a compactness result [13] obtaining the following strong convergences as $(h, k) \to 0$:

$$\widetilde{\theta}_{h,k} \to \theta \quad \text{strongly in } L^2(0,T;H^1(\Omega)'),$$

$$\widetilde{c}_{h,k} \to c \quad \text{strongly in } L^2(0,T;H^1(\Omega)'). \tag{4.4}$$

In fact, due to Lemma 3.1, we also have that $\widehat{\theta}_{h,k}, \theta_{h,k} \to \theta$ strongly in $L^2(0,T;H^1(\Omega)')$ (analogously $\widehat{c}_{h,k}, \widetilde{c}_{h,k} \to c$ strongly in $L^2(0,T;H^1(\Omega)')$ as $(h,k) \to 0$), since

$$\begin{aligned} \|\widetilde{\theta}_{h,k} - \theta_{h,k}\|^2_{L^2(0,T;H^1(\Omega)')} &\le \|\theta_{h,k} - \widehat{\theta}_{h,k}\|^2_{L^2(0,T;H^1(\Omega)')} \\ &\le C\,\|\widehat{\theta}_{h,k} - \theta_{k,h}\|^2_{L^2(0,T;L^2(\Omega))} = C\,k\sum_{n=0}^{N-1} |\theta_h^{n+1} - \theta_h^n|^2 \le C\,k. \end{aligned}$$

To be able to pass to the limit in the nonlinear term of (2.3) we have to prove that the sequence $\{K_2^h(\phi_{h,k})[P_0 c_{h,k}]_T(1 - [P_0 c_{h,k}]_T)\}_{h,k}$ is weakly convergent to a certain limit which has to be identified later on.

First of all, we prove that $P_0 c_{h,k} - c_{h,k}$ tends to zero as (h,k) tend to zero under a certain condition for the auxiliary function $g_2(h)$ which defines K_2^h.

Proposition 4.2. *If the function $g_2(h)$ given in Section 2 satisfies the condition $h/\sqrt{g_2(h)} \to 0$ as $h \to 0$, then the following convergence holds*

$$\|P_0\widehat{c}_{h,k} - \widehat{c}_{h,k}\|_{L^2(0,T;L^2(\Omega))} \to 0 \qquad \textit{as } (h,k) \to 0. \tag{4.5}$$

Proof. By using the fact that $K_2^h(\cdot) \ge g_2(h)$ and estimate (***ix***) of Lemma 3.1, we get

$$k\sum_{n=0}^{N-1} |\nabla c_h^{n+1}|^2 \le \frac{C}{g_2(h)}. \tag{4.6}$$

By combining (4.6) and the error interpolation $|P_0 c_h^n - c_h^n| \leq C\, h|\nabla c_h^n|$ applied for each $n \geq 1$, we see that

$$\begin{aligned} \|P_0\widehat{c}_{h,k} - \widehat{c}_{h,k}\|^2_{L^2(0,T;L^2(\Omega))} &\leq k|P_0 c_h^0 - c_h^0|^2 + C\, h^2\, \|\nabla c_{h,k}\|^2_{L^2(0,T;L^2(\Omega))} \\ &\leq k|P_0 c_h^0 - c_h^0|^2 + C\frac{h^2}{g_2(h)}, \end{aligned}$$

hence $\|P_0\widehat{c}_{h,k} - \widehat{c}_{h,k}\|^2_{L^2(0,T;L^2(\Omega))} \to 0$ as $(h,k) \to 0$. □

Finally, the following compactness result is established for the coefficients $K_2^h(\phi_{h,k})[P_0\widehat{c}_{h,k}]_T(1 - [P_0\widehat{c}_{h,k}]_T)$ which will achieve by using the fact that $[P_0\widehat{c}_{h,k}(\boldsymbol{x},t)]_T = T_0^1(P_0\widehat{c}_{h,k}(\boldsymbol{x},t))$ *a.e.* $(\boldsymbol{x},t) \in Q$ owing to $P_0 c_{h,k}$ is a piecewise constant function, where T_0^1 is the pointwise truncation operator defined as

$$T_0^1 c(\boldsymbol{x},t) = \begin{cases} c(\boldsymbol{x},t) & \text{if} \quad c(\boldsymbol{x},t) \in [0,1], \\ 0 & \text{if} \quad c(\boldsymbol{x},t) < 0, \\ 1 & \text{if} \quad c(\boldsymbol{x},t) > 1. \end{cases}$$

This compactness is not clear if we truncate $c_{h,k}$ by nodes, as was made in [8] for a nondegenerate mass diffusion Navier-Stokes model.

Proposition 4.3. *The following convergence as $(h,k) \to 0$ holds, for each $p < \infty$:*

$$K_2^h(\phi_{h,k})[P_0\widehat{c}_{h,k}]_T(1 - [P_0\widehat{c}_{h,k}]_T) \to K_2(\phi)T_0^1 c(1 - T_0^1 c) \quad \textit{in } L^p(Q)\textit{-strong.} \tag{4.7}$$

Proof. First of all, we prove that $K_2^h(\phi_{h,k})c_{h,k} \to K_2(\phi)c$ strongly in $L^2(0,T;L^{3/2}(\Omega))$ as $(h,k) \to 0$. To this end, we define $\widetilde{\varphi}_{h,k}$ as the piecewise linear, globally continuous in time function taking the value $K_2^h(\phi_h^{n+1})c_h^{n+1}$ at the time $t = t_{n+1}$. Our task now is to obtain an estimate in the $(W^{1,s})'$-norm for the time derivative of $\widetilde{\varphi}_{h,k}$, with $s > 3$. Indeed, for $t \in (t_n, t_{n+1})$,

$$\frac{\mathrm{d}}{\mathrm{d}t}\widetilde{\varphi}_{h,k}(t) = \frac{K_2^h(\phi_h^{n+1})c_h^{n+1} - K_2^h(\phi_h^n)c_h^n}{k} = K_2^h(\phi_h^{n+1})\frac{c_h^{n+1} - c_h^n}{k} + c_h^n\frac{K_2^h(\phi_h^{n+1}) - K_2^h(\phi_h^n)}{k}.$$

By the mean value theorem, the last term can be written as

$$c_h^n\frac{K_2^h(\phi_h^{n+1}) - K_2^h(\phi_h^n)}{k} = c_h^n\,(K_2^h)'(\xi_h^{n+1})\frac{\phi_h^{n+1} - \phi_h^n}{k},$$

where $\xi_h^{n+1} \in (\min\{\phi_h^n, \phi_h^{n+1}\}, \max\{\phi_h^n, \phi_h^{n+1}\})$. Therefore,

$$\frac{\mathrm{d}}{\mathrm{d}t}\widetilde{\varphi}_{h,k} = K_2^h(\phi_{h,k})\frac{\mathrm{d}}{\mathrm{d}t}\widetilde{c}_{h,k} + (K_2^h)'(\xi_{h,k})\widehat{c}_{h,k}\frac{\mathrm{d}}{\mathrm{d}t}\widetilde{\phi}_{h,k}.$$

We know that $\{K_2^h(\phi_{h,k})\frac{\mathrm{d}}{\mathrm{d}t}\widetilde{c}_{h,k}\}_{h,k}$ is bounded in $L^2(0,T;(W^{1,s}(\Omega))')$ with $s > 3$ (owing to $\{K_2^h(\phi_{h,k})\}_{h,k}$ is bounded in $L^\infty(0,T;H^1(\Omega))$ and (4.2)) and $\{(K_2^h)'(\xi_{h,k})\widehat{c}_{h,k}\frac{\mathrm{d}}{\mathrm{d}t}\widetilde{\phi}_{h,k}\}_{h,k}$ is bounded in $L^2(0,T;L^1(\Omega))$ (owing to $\{(K_2^h)'(\xi_{h,k})\}_{h,k}$ is bounded in $L^\infty(Q)$, (3.12) and (3.16)); hence $\{\frac{\mathrm{d}}{\mathrm{d}t}\widetilde{\varphi}_{h,k}\}_{h,k}$ is bounded in $L^1(0,T;(W^{1,s}(\Omega))')$, with $s > 3$. On the other hand, by using (3.12), (3.15) and the estimate of $\{\phi_{h,k}\}_{h,k}$ in $L^4(0,T;W^{1,4})$ given in (3.20), it is not hard to check that $\{\widetilde{\varphi}_{h,k}\}_{h,k}$ is bounded in $L^2(0,T;W^{1,6/5}(\Omega))$ (by assuming $K_2(\phi_h^0)c_h^0$ is bounded in $W^{1,6/5}(\Omega)$, which can be obtained as a consequence of inverse estimates and a constraint between h and k).

Therefore, by a compactness result [13], there exists $\chi \in L^2(0,T;L^p(\Omega))$ with $p < 2$, such that

$$\widetilde{\varphi}_{h,k} \to \chi \text{ in } L^2(0,T;L^p(\Omega)), \quad \text{as } (h,k) \to 0. \tag{4.8}$$

In turn, $\varphi_{h,k} := K_2^h(\phi_{h,k})c_{h,k}$ tends strongly to χ in $L^2(0,T;L^{3/2}(\Omega))$, since the difference $R_{h,k} := \widetilde{\varphi}_{h,k}(t) - \varphi_{h,k}(t)$ tends to zero strongly in $L^2(0,T;L^{3/2}(\Omega))$. Indeed, we may write for $t \in (t_n, t_{n+1})$

$$R_{h,k}(t) := \frac{t - t_{n+1}}{k}\Big((K_2^h)'(\xi_h^{n+1})(\phi_h^{n+1} - \phi_h^n)c_h^{n+1} + K_2^h(\phi_h^n)(c_h^{n+1} - c_h^n)\Big),$$

with ξ_h^{n+1} being as before. It thus follows that

$$\begin{aligned} \|R_{h,k}\|_{L^2(0,T;L^{3/2}(\Omega))} &\leq \left(C\,k\sum_{n=0}^{N-1}\|c_h^{n+1} - c_h^n\|^2_{L^2(\Omega)}\right)^{1/2} + \left(C\,k\sum_{n=0}^{N-1}\|\phi_h^{n+1} - \phi_h^{n+1}\|^2_{H^1(\Omega)}\right)^{1/2} \\ &\leq C\,k^{1/2} \to 0, \end{aligned}$$

due to estimates (***ii***) and (***viii***) of Lemma 3.1. Then, as announced we have

$$\varphi_{h,k} \to \chi \text{ in } L^2(0,T;L^{3/2}(\Omega)), \quad \text{as } (h,k) \to 0. \tag{4.9}$$

To identify $\chi = K_2(\phi)c$, we see that since K_2 is a globally Lipschitz continuous function on $\mathbb{R}$ and $\phi_{h,k}$ converges to ϕ in $L^2(0;T;H^1(\Omega))$, then (see [9], Thm. 16.7)

$$K_2(\phi_{h,k}) \to K_2(\phi) \quad \text{strongly in } L^2(0,T;H^1(\Omega)). \tag{4.10}$$

Thus, $K_2^h(\phi_{h,k})c_{h,k}$ converges weakly to $K_2(\phi)c$ in $L^2(0,T;L^{3/2}(\Omega))$ by taking into account that $g_2(h)c_{h,k}$ converges strongly to 0 in $L^\infty(0,T;L^2(\Omega))$ as $(h,k) \to 0$. Therefore, we can identify $\chi = K_2(\phi)c$ and

$$\varphi_{h,k} = K_2^h(\phi_{h,k})c_{h,k} \to K_2(\phi)c \quad \text{strongly in } L^2(0,T;L^{3/2}(\Omega)) \text{ as } (h,k) \to 0.$$

As a consequence, by using estimate (***viii***) of Lemma 3.1, we have

$$K_2^h(\phi_{h,k})\widehat{c}_{h,k} \to K_2(\phi)c \quad \text{strongly in } L^2(0,T;L^{3/2}(\Omega)), \text{ as } (h,k) \to 0. \tag{4.11}$$

From (4.10), we get $K_2(\phi_{h,k}(\boldsymbol{x},t)) \to K_2(\phi(\boldsymbol{x},t))$ *a.e.* $(\boldsymbol{x},t) \in Q$. In particular, one has

$$K_2^h(\phi_{h,k}(\boldsymbol{x},t)) \to K_2(\phi(\boldsymbol{x},t)) \text{ a.e. } (\boldsymbol{x},t) \in Q. \tag{4.12}$$

If we define $\widetilde{Q} = \{(\boldsymbol{x},t) \in Q\colon K_2(\phi(\boldsymbol{x},t)) > 0\}$, since $K_2^h(\phi_{h,k}(\boldsymbol{x},t)) > 0$ for all $(\boldsymbol{x},t)$, it is easy to prove that

$$\widehat{c}_{h,k}(\boldsymbol{x},t) \to c(\boldsymbol{x},t) \text{ a.e. } (\boldsymbol{x},t) \in \widetilde{Q} \tag{4.13}$$

from (4.11) and the pointwise convergence (4.12).

Once we have achieved the pointwise convergence of $\widehat{c}_{h,k}$ to the limit c, let us see the pointwise convergence

$$[P_0\widehat{c}_{h,k}(\boldsymbol{x},t)]_T \to T_0^1 c(\boldsymbol{x},t) \text{ a.e. } (\boldsymbol{x},t) \in \widetilde{Q}. \tag{4.14}$$

Indeed, this convergence follows from the inequality

$$|[P_0\widehat{c}_{h,k}(\boldsymbol{x},t)]_T - T_0^1 c(\boldsymbol{x},t)| = |T_0^1(P_0\widehat{c}_{h,k}(\boldsymbol{x},t)) - T_0^1 c(\boldsymbol{x},t)| \leq |P_0\widehat{c}_{h,k}(\boldsymbol{x},t) - c(\boldsymbol{x},t)| \text{ a.e. } (\boldsymbol{x},t) \in Q,$$

the triangular inequality and the pointwise convergence as a consequence of (4.5).

Finally,

$$K_2^h(\phi_{h,k}(\boldsymbol{x},t))[P_0\widehat{c}_{h,k}]_T \to K_2(\phi(\boldsymbol{x},t))T_0^1 c(\boldsymbol{x},t) \text{ a.e. } (\boldsymbol{x},t) \in Q$$

holds from (4.12), (4.14), and $K_2^h(\phi_{h,k}(\boldsymbol{x},t))$ converges to 0 a.e. in $Q\backslash\widetilde{Q}$. In particular,

$$K_2^h(\phi_{h,k}(\boldsymbol{x},t))[P_0\widehat{c}_{h,k}]_T^2 \to K_2(\phi(\boldsymbol{x},t))T_0^1 c(\boldsymbol{x},t)^2 \ a.e.\ (\boldsymbol{x},t)\in Q.$$

Then, (4.7) holds as a consequence of the dominated convergence theorem, and the proof of Proposition 4.3 is finished. □

Remark 4.4. In the case of a nondegenerate solute diffusivity K_2 we may prove firstly that $\widehat{c}_{h,k}\to c$ strongly in $L^2(0,T;L^2(\Omega))$ by a compactness result, then this convergence is extended to $P_0\widehat{c}_{h,k}\to c$ strongly in $L^2(0,T;L^2(\Omega))$ from Proposition 4.3, and finally we may establish $[\widehat{P}_0 c_{h,k}]_T\to T_0^1 c$ strongly in $L^2(0,T;L^2(\Omega))$ as an application of the dominated convergence theorem.

Now, we want to identify $J_1=\nabla(K_1(\phi)\theta)-\theta\nabla K_1(\phi)$ (and $J_2=\nabla(K_2(\phi)c)-c\nabla K_2(\phi)$). Indeed, analogue to (4.10) we have

$$K_1(\phi_{h,k})\to K_1(\phi)\quad \text{strongly in } L^2(0,T;H^1(\Omega)). \tag{4.15}$$

On the other hand, using the fact that $\theta_{h,k}\to\theta$ weakly* in $L^\infty(0,T;L^2(\Omega))$ and (4.15), the following weak convergences hold:

$$\theta_{h,k}\nabla K_1(\phi_{h,k})\to\theta\nabla K_1(\phi)\quad \text{weakly in } L^2(0;T;L^1(\Omega)), \tag{4.16}$$

$$\theta_{h,k}K_1(\phi_{h,k})\to\theta K_1(\phi)\quad \text{weakly in } L^2(0;T;L^{3/2}(\Omega)). \tag{4.17}$$

Now, using the regularity $K_1(\phi_{h,k})\in L^\infty(0,T;H^1(\Omega))$ and $\theta_{h,k}\in L^2(0,T;H^1(\Omega))$ (because of $0<g_1(h)\le K_1^h(\cdot)$) and the Sobolev product $\|\varphi\psi\|_{W^{1,3/2}(\Omega)}\le C\|\varphi\|_{H^1(\Omega)}\|\psi\|_{H^1(\Omega)}$ for all $\varphi,\psi\in H^1(\Omega)$, we get

$$K_1(\phi_{h,k})\theta_{h,k}\in L^2(0,T;W^{1,3/2}(\Omega))$$

and, in particular,

$$\nabla(K_1(\phi_{h,k})\theta_{h,k})=K_1(\phi_{h,k})\nabla\theta_{h,k}+\theta_{h,k}\nabla K_1(\phi_{h,k}). \tag{4.18}$$

Therefore, in view of the convergences (4.16), (4.17) and the identity (4.18), one arrives at

$$K_1(\phi_{h,k})\nabla\theta_{h,k}\to\nabla(K_1(\phi)\theta)-\theta\nabla K_1(\phi)\quad \text{in } L^2(0,T;W^{-1,3/2-\varepsilon}(\Omega)) \tag{4.19}$$

with $1/2>\varepsilon>0$.

Next, recalling the definition of $K_1^h=g_1(h)+K_1$, we write

$$K_1^h(\phi_{h,k})\nabla\theta_{h,k}=g_1(h)\nabla\theta_{h,k}+K_1(\phi_{h,k})\nabla\theta_{h,k}. \tag{4.20}$$

Now, taking into account that $\|g_1(h)^{1/2}\nabla\theta_{h,k}\|_{L^2(Q)}\le\|\sqrt{K_1^h(\phi_{h,k})}\nabla\theta_{h,k}\|_{L^2(Q)}\le C$ with $C>0$ independent of (k,h), one obtains

$$g_1(h)\nabla\theta_{h,k}\to 0\quad \text{in } L^2(Q)$$

that jointly with (4.19) and (4.20) gives us

$$K_1^h(\phi_{h,k})\nabla\theta_{h,k}\to\nabla(K_1(\phi)\theta)-\theta\nabla K_1(\phi)\quad \text{in } L^2(0,T;W^{-1,3/2-\varepsilon}(\Omega)).$$

Finally, this convergence and the weak convergence to J_1 given in Lemma 3.6 conclude the identification $J_1=\nabla(K_1(\phi)\theta)-\theta\nabla K_1(\phi)$.

5. Passing to the limit

In order to pass to the limit in the discrete concentration equation, we will use the following result, which is easy to prove because equation (5.1) satisfies the maximum principle:

Lemma 5.1. *The following two systems are equivalent:*

$$c_t = \nabla \cdot (K_2(\phi)[\nabla c + M\, T_0^1 c(1 - T_0^1 c)\nabla \phi]) \quad \text{in } Q, \tag{5.1}$$

and

$$0 \le c \le 1, \quad c_t = \nabla \cdot (K_2(\phi)[\nabla c + M\, c(1-c)\nabla \phi]) \quad \text{in } Q.$$

To pass to the limit in scheme (2.1)–(2.3), we rewrite the scheme as follows: Taking $x_h = \eta_h^{n+1} \in X_h$ a suitable approximation at time t_{n+1} of any function $\eta \in C^0([0,T]; C_c^\infty(\Omega))$ such that $\eta(T) = 0$ (clearly $\eta_h^N = 0$) as a test function in (2.1), (2.2) and (2.3), multiplying by k, summing over n and denoting the function $\eta_{h,k}$ similarly to Definition 3.5, one arrives at

$$\begin{cases} \alpha\varepsilon^2 \displaystyle\int_0^T \left(\frac{\mathrm{d}}{\mathrm{d}t}\widetilde{\phi}_{h,k}, \eta_{h,k}\right) + \varepsilon^2 \int_0^T \left(\nabla\phi_{h,k}, \nabla\eta_{h,k}\right) + \varepsilon^2 \int_0^T \left(\phi_{h,k} - \widehat{\phi}_{h,k}, \eta_{h,k}\right) \\ +\dfrac{1}{2}\displaystyle\int_0^T \left((\phi_{h,k})^3 - \widehat{\phi}_{h,k}, \eta_{h,k}\right) - \beta \int_0^T \left(\widehat{\theta}_{h,k} - \theta_A \widehat{c}_{h,k} - \theta_B(1 - \widehat{c}_{h,k}), \eta_{h,k}\right) = 0, \end{cases}$$

$$C_V \int_0^T \left(\frac{\mathrm{d}}{\mathrm{d}t}\widetilde{\theta}_{h,k}, \eta_{h,k}\right) + \frac{l}{2}\int_0^T \left(\frac{\mathrm{d}}{\mathrm{d}t}\widetilde{\phi}_{h,k}, \eta_{h,k}\right) + \int_0^T \left(K_1^h(\phi_{h,k})\nabla\theta_{h,k}, \nabla\eta_{h,k}\right) = 0,$$

$$\begin{cases} \displaystyle\int_0^T \left(\frac{\mathrm{d}}{\mathrm{d}t}\widetilde{c}_{h,k}, \eta_{h,k}\right) + \int_0^T \left(K_2^h(\phi_{h,k})\nabla c_{h,k}, \nabla\eta_{h,k}\right) \\ + M \displaystyle\int_0^T \left(K_2^h(\phi_{h,k})[P_0\widehat{c}_{h,k}]_T(1 - [P_0\widehat{c}_{h,k}]_T)\nabla\widehat{\phi}_{h,k}, \nabla\eta_{h,k}\right) = 0. \end{cases} \tag{5.2}$$

By applying all the convergences already obtained, there are no additional difficulties in passing to the limit obtaining that (ϕ, θ, c) is a weak solution of (1.1). In particular, taking $(h,k) \to 0$ in the discrete equation for the concentration c and using (4.7), we arrive at the limit equation (5.1); hence $0 \le c \le 1$ and $T_0^1 c = c$. Finally, the discrete phase-field equation is verified pointwise in Q thanks to the strong regularity of ϕ. The proof of Theorem 1.3 is finished.

Remark 5.2. As mentioned in Remark 3.2, taking $[P_0 c_h^n]$ instead of c_h^n in the discrete equation for the phase field variable (2.1) provides better stability estimates with respect to ε. Nevertheless we find that there is a limit function $\vartheta \in L^\infty(0,T; L^2(\Omega))$ such that $[P_0 c_h^n]$ tends to ϑ weakly* in $L^\infty(0,T; L^2(\Omega))$, but it is not clear how to identify ϑ with the limit function c. By using (4.14) and that $0 \le c \le 1$ *a.e.* Q (owing to the limit in (5.2) can be taken as before), we can only deduce that $\vartheta = c$ *a.e.* in $\widetilde{Q}$, $\widetilde{Q}$ being defined in the proof of Proposition 4.3.

6. A conditionally stable, convergent linear scheme

In this section we study a more explicit scheme, where the nonlinear discrete approximation (2.1) of $(1.1)_1$ is considered completely in the previous step time, resulting a linear (and decoupled) scheme. Contrary to the previous nonlinear scheme, now to obtain stability we will impose a constraint on the discrete parameters.

Recall the definition of the Ginzburg-Landau function $f(\phi) = \dfrac{1}{2\varepsilon^2}(\phi^2 - 1)\phi$ associated to the potential function $F(\phi) = \dfrac{1}{8\varepsilon^2}(\phi^2 - 1)^2$. We propose the following linear scheme:

Initialization: Let $(\phi_h^0, \theta_h^0, c_h^0) \in X_h \times X_h \times X_h$ be suitable approximations of (ϕ_0, θ_0, c_0).
Step $n+1$: Given $(\phi_h^n, \theta_h^n, c_h^n) \in X_h \times X_h \times X_h$.

Find $\phi_h^{n+1} \in X_h$ as a solution of the problem:

$$\alpha\left(\frac{\phi_h^{n+1}-\phi_h^n}{k}, x_h\right) + \left(\nabla\phi_h^{n+1}, \nabla x_h\right) + \left(\phi_h^{n+1}, x_h\right) = -\Big(f(\phi_h^n), x_h\Big) + \Big(\phi_h^n, x_h\Big) + \frac{\beta}{\varepsilon^2}\Big(\theta_h^n - \theta_A c_h^n - \theta_B(1-c_h^n), x_h\Big), \quad \forall\, x_h \in X_h. \tag{6.1}$$

Find $\theta_h^{n+1} \in X_h$ and $c_h^{n+1} \in X_h$ as solutions of the decoupled variational problems:

$$C_V\left(\frac{\theta_h^{n+1}-\theta_h^n}{k}, x_h\right) + \Big(K_1^h(\phi_h^{n+1})\nabla\theta_h^{n+1}, \nabla x_h\Big) = -\frac{l}{2}\left(\frac{\phi_h^{n+1}-\phi_h^n}{k}, x_h\right), \quad \forall\, x_h \in X_h, \tag{6.2}$$

$$\begin{cases} \left(\dfrac{c_h^{n+1}-c_h^n}{k}, x_h\right) + \Big(K_2^h(\phi_h^{n+1})\nabla c_h^{n+1}, \nabla x_h\Big) \\ = -M\Big(K_2^h(\phi_h^{n+1})[P_0 c_h^n]_T(1-[P_0 c_h^n]_T)\nabla\phi_h^n, \nabla x_h\Big), \quad \forall\, x_h \in X_h. \end{cases} \tag{6.3}$$

The conditional stability of scheme (6.1)–(6.3) will be obtained by induction on the time step n. First of all, we establish the following result which provides a basic recursive inequality.

Lemma 6.1. *Assume the constraint:*

$$(S) \qquad \lim_{(h,k)\to 0} k/h = 0.$$

If there exists a constant $C_d > 0$ (independent of h, k and n, but dependent on ε) such that

$$\|\phi_h^n\|^2_{H^1(\Omega)} + \frac{2C_V\beta}{l\varepsilon^2}|\theta_h^n|^2 + |c_h^n|^2 + 1 \le C_d, \tag{6.4}$$

then the following inequalities hold for (h,k) sufficiently small (independent of n),

$$\begin{cases} \Big(\|\phi_h^{n+1}\|^2_{H^1(\Omega)} - \|\phi_h^n\|^2_{H^1(\Omega)} + \|\phi_h^{n+1}-\phi_h^n\|^2_{H^1(\Omega)}\Big) \\ + \dfrac{2C_V\beta}{l\varepsilon^2}\Big(|\theta_h^{n+1}|^2 - |\theta_h^n|^2 + \dfrac{1}{2}|\theta_h^{n+1}-\theta_h^n|^2\Big) \\ + 2\displaystyle\int_\Omega \Big(F(\phi_h^{n+1}) - F(\phi_h^n) + \dfrac{1}{8\varepsilon^2}((\phi_h^{n+1})^2 - (\phi_h^n)^2)^2\Big) \\ + \dfrac{\alpha}{2}\,k\left|\dfrac{\phi_h^{n+1}-\phi_h^n}{k}\right|^2 + \dfrac{2\beta}{l\varepsilon^2}k\Big|\sqrt{K_1^h(\phi_h^{n+1})}\nabla\theta_h^{n+1}\Big|^2 \\ \le R_1\, k|\phi_h^n|^2 + R_2\,\dfrac{\beta^2}{\varepsilon^4}k(|c_h^n|^2+1), \end{cases} \tag{6.5}$$

$$|c_h^{n+1}|^2 - |c_h^n|^2 + |c_h^{n+1}-c_h^n|^2 + k\Big|\sqrt{K_2^h(\phi_h^{n+1})}\nabla c_h^{n+1}\Big|^2 \le R_1\, k|\nabla\phi_h^n|^2, \tag{6.6}$$

where R_1 and R_2 are positive constants independent of h, k, n, and ε.

Proof. Firstly, we consider $x_h = 2k\dfrac{\phi_h^{n+1}-\phi_h^n}{k}$ in (6.1) and bound the right-hand side

$$\frac{3}{2}\alpha k\left|\frac{\phi_h^{n+1}-\phi_h^n}{k}\right|^2 + \Big(\|\phi_h^{n+1}\|^2_{H^1(\Omega)} - \|\phi_h^n\|^2_{H^1(\Omega)} + \|\phi_h^{n+1}-\phi_h^n\|^2_{H^1(\Omega)}\Big) + 2\Big(f(\phi_h^n), \phi_h^{n+1}-\phi_h^n\Big) \le \frac{2\beta}{\varepsilon^2}k\left(\theta_h^n, \frac{\phi_h^{n+1}-\phi_h^n}{k}\right) + \frac{C}{\alpha}k|\phi_h^n|^2 + C\,\frac{\beta^2}{\alpha\varepsilon^4}k(|c_h^n|^2+1). \tag{6.7}$$

Now, we handle the last term on the left-hand side of (6.7) as follows:

$$2\Big(\phi_h^{n+1}-\phi_h^n, f(\phi_h^n)\Big) = \frac{1}{\varepsilon^2}\Big(\phi_h^{n+1}-\phi_h^n, ((\phi_h^{n+1})^2-1)\phi_h^n\Big) + \frac{1}{\varepsilon^2}\Big(\phi_h^{n+1}-\phi_h^n, ((\phi_h^n)^2-(\phi_h^{n+1})^2)\phi_h^n\Big) := I_1 - I_2.$$

Next, we continue rewriting I_1 as follows:

$$\begin{aligned} I_1 &= \frac{1}{2\varepsilon^2}\int_\Omega ((\phi_h^{n+1})^2-1)((\phi_h^{n+1})^2-(\phi_h^n)^2-(\phi_h^{n+1}-\phi_h^n)^2) \\ &= \frac{1}{4\varepsilon^2}\int_\Omega \Big(((\phi_h^{n+1})^2-1)^2-((\phi_h^n)^2-1)^2+((\phi_h^{n+1})^2-(\phi_h^n)^2)^2\Big) \\ &\quad + \frac{k^2}{2\varepsilon^2}\int_\Omega (1-(\phi_h^{n+1})^2)\left|\frac{\phi_h^{n+1}-\phi_h^n}{k}\right|^2. \end{aligned} \tag{6.8}$$

The term I_2 is bounded as

$$I_2 \le C\frac{1}{\varepsilon^2}\,k^2\|\phi_h^n\|^2_{L^\infty(\Omega)}\left|\frac{\phi_h^{n+1}-\phi_h^n}{k}\right|^2 + \frac{1}{8\varepsilon^2}\int_\Omega ((\phi_h^{n+1})^2-(\phi_h^n)^2)^2.$$

Therefore, we get from (6.7) and the previous computations

$$\begin{aligned} &\frac{3}{2}\alpha\, k\left|\frac{\phi_h^{n+1}-\phi_h^n}{k}\right|^2 + \Big(\|\phi_h^{n+1}\|^2_{H^1(\Omega)} - \|\phi_h^n\|^2_{H^1(\Omega)} + \|\phi_h^{n+1}-\phi_h^n\|^2_{H^1(\Omega)}\Big) \\ &\quad + 2\int_\Omega \Big(F(\phi_h^{n+1}) - F(\phi_h^n) + \frac{1}{8\varepsilon^2}((\phi_h^{n+1})^2-(\phi_h^n)^2)^2\Big) + \frac{k^2}{2\varepsilon^2}\left|\frac{\phi_h^{n+1}-\phi_h^n}{k}\right|^2 \\ &\le \frac{2\beta}{\varepsilon^2}k\left(\theta_h^n, \frac{\phi_h^{n+1}-\phi_h^n}{k}\right) + \frac{C}{\alpha}\,k|\phi_h^n|^2 + C\,\frac{\beta^2}{\varepsilon^4\alpha}k(|c_h^n|^2+1) \\ &\quad + C\frac{1}{\varepsilon^2\alpha}\,k\Big(\|\phi_h^n\|^2_{L^\infty(\Omega)} + \|\phi_h^{n+1}\|^2_{L^\infty(\Omega)}\Big)k\left|\frac{\phi_h^{n+1}-\phi_h^n}{k}\right|^2 \\ &\le \frac{2\beta}{\varepsilon^2}k\left(\theta_h^n, \frac{\phi_h^{n+1}-\phi_h^n}{k}\right) + \frac{C}{\alpha}\,k|\phi_h^n|^2 + C\,\frac{\beta^2}{\varepsilon^4}k(|c_h^n|^2+1) \\ &\quad + C\frac{1}{\varepsilon^2}\frac{k}{h}\Big(\|\phi_h^n\|^2_{H^1(\Omega)} + \|\phi_h^{n+1}\|^2_{H^1(\Omega)}\Big)k\left|\frac{\phi_h^{n+1}-\phi_h^n}{k}\right|^2, \end{aligned} \tag{6.9}$$

where in the last line the inverse estimate $\|x_h\|_{L^\infty(\Omega)} \le C\,h^{-1/2}\|x_h\|_{H^1(\Omega)}$ has been used.

Now we are looking for the bound $\|\phi_h^{n+1}\|_{H^1(\Omega)} \le C_1$ where $C_1 > 0$ depends on the constant C_d of hypothesis (6.4) but it will be independent of n. It will be carried out by bounding $\|\phi_h^{n+1}\|_{H^1(\Omega)}$ in terms of $\|\phi_h^n\|_{H^1(\Omega)}$, $|\theta_h^n|$ and $|c_h^n|$ and using hypothesis (6.4). Indeed, taking again $x_h = 2k\dfrac{\phi_h^{n+1}-\phi_h^n}{k}$ as a test function in (6.1),

but now bounding directly the term depending on $f(\phi_h^n)$ on the right-hand side, we get

$$\begin{aligned}\alpha\, k\left|\frac{\phi_h^{n+1}-\phi_h^n}{k}\right|^2 &+ \Big(\|\phi_h^{n+1}\|^2_{H^1(\Omega)} - \|\phi_h^n\|^2_{H^1(\Omega)} + \|\phi_h^{n+1}-\phi_h^n\|^2_{H^1(\Omega)}\Big) \le C\frac{\beta^2}{\varepsilon^4\alpha}\, k|\theta_h^n|^2\\ &+ \frac{C}{\alpha}k|\phi_h^n|^2 + C\frac{\beta^2}{\varepsilon^4\alpha}\, k(|c_h^n|^2+1) + C\, k\,|f(\phi_h^n)|^2\\ &\le C\frac{\beta^2}{\varepsilon^4\alpha}\, k|\theta_h^n|^2 + \frac{C}{\alpha}k|\phi_h^n|^2 + C\frac{\beta^2}{\varepsilon^4\alpha}\, k(|c_h^n|^2+1)\\ &+ C\frac{1}{\varepsilon^4}\, k\|\phi_h^n\|^6_{H^1(\Omega)} + C\frac{1}{\varepsilon^4}\, k\|\phi_h^n\|^2_{H^1(\Omega)}.\end{aligned}$$

In particular, by using hypothesis (6.4), the previous inequality says us

$$\|\phi_h^{n+1}\|^2_{H^1(\Omega)} \le \|\phi_h^n\|^2_{H^1(\Omega)} + C\, k\Big(\frac{C_d\beta}{\varepsilon^2} + C_d + \frac{C_d\beta^2}{\varepsilon^4} + \frac{C_d^3}{\varepsilon^4} + \frac{C_d}{\varepsilon^4}\Big) \le \|\phi_h^n\|^2_{H^1(\Omega)} + C_1(\varepsilon)\, k$$

with $C_1(\varepsilon)$ independent of h, k and n.

Thus, by using the previous estimate in (6.9) and again hypothesis (6.4), we get

$$\begin{aligned}&\frac{3}{2}\alpha\, k\left|\frac{\phi_h^{n+1}-\phi_h^n}{k}\right|^2 + \Big(\|\phi_h^{n+1}\|^2_{H^1(\Omega)} - \|\phi_h^n\|^2_{H^1(\Omega)} + \|\phi_h^{n+1}-\phi_h^n\|^2_{H^1(\Omega)}\Big)\\ &\quad + 2\int_\Omega\Big(F(\phi_h^{n+1}) - F(\phi_h^n) + \frac{1}{8\varepsilon^2}((\phi_h^{n+1})^2-(\phi_h^n)^2)^2\Big)\\ &\le \frac{2\beta}{\varepsilon^2}k\left(\theta_h^n, \frac{\phi_h^{n+1}-\phi_h^n}{k}\right) + \frac{C}{\alpha}k|\phi_h^n|^2 + C\,\frac{\beta^2}{\alpha\varepsilon^4}k(|c_h^n|^2+1) + C\frac{k}{h}\frac{1}{\varepsilon^2}\Big(C_d + C_1(\varepsilon)\, k\Big)k\left|\frac{\phi_h^{n+1}-\phi_h^n}{k}\right|^2.\end{aligned}$$

By taking into account the constraint (S), in particular $\lim\limits_{(h,k)\to 0}\frac{k}{h}\frac{1}{\varepsilon^2}\Big(C_d + C_1(\varepsilon)\, k\Big) = 0$, so for any (h,k) small enough such that $C\frac{k}{h}\frac{1}{\varepsilon^2}\Big(C_d + C_1(\varepsilon)\, k\Big) \le \frac{1}{2}\alpha$, the last term on the right-hand side can be absorbed, and remains

$$\begin{aligned}\alpha\, k\left|\frac{\phi_h^{n+1}-\phi_h^n}{k}\right|^2 &+ \Big(\|\phi_h^{n+1}\|^2_{H^1(\Omega)} - \|\phi_h^n\|^2_{H^1(\Omega)} + \|\phi_h^{n+1}-\phi_h^n\|^2_{H^1(\Omega)}\Big) + 2\int_\Omega\Big(F(\phi_h^{n+1}) - F(\phi_h^n)\\ &+ \frac{1}{8\varepsilon^2}((\phi_h^{n+1})^2-(\phi_h^n)^2)^2\Big) \le \frac{2\beta}{\varepsilon^2}k\left(\theta_h^n, \frac{\phi_h^{n+1}-\phi_h^n}{k}\right) + \frac{C}{\alpha}k|\phi_h^n|^2 + C\,\frac{\beta^2}{\alpha\varepsilon^4}k(|c_h^n|^2+1).\end{aligned} \tag{6.10}$$

On the other hand, take $x_h = \frac{4\beta}{l\varepsilon^2}k\theta_h^{n+1}$ in (6.2) to arrive at inequality (3.5), that is

$$\begin{aligned}&\frac{2C_V\beta}{l\varepsilon^2}\Big(|\theta_h^{n+1}|^2 - |\theta_h^n|^2 + \frac{1}{2}|\theta_h^{n+1}-\theta_h^n|^2\Big) + \frac{4\beta}{l\varepsilon^2}k|\sqrt{K_1^h(\phi_h^{n+1})}\nabla\theta_h^{n+1}|^2 \le\\ &\qquad - \frac{2\beta}{\varepsilon^2}k\left(\frac{\phi_h^{n+1}-\phi_h^n}{k}, \theta_h^n\right) + \frac{\alpha}{2}k\left|\frac{\phi_h^{n+1}-\phi_h^n}{k}\right|^2.\end{aligned} \tag{6.11}$$

Consequently, it suffices to add up (6.11) and (6.10) to get (6.5).

Finally, inequality (6.6) is easily obtained by testing (6.3) by c_h^{n+1} and bounding adequately as in the proof of Lemma 3.1. □

On the other hand, we turn our attention to the initial bound (3.2) which in particular verifies hypothesis (6.4) imposed in Lemma 6.1. It is very important in order to guarantee a correct induction argument.

Now, we are in position to give the following stability result.

Lemma 6.2. *Under the hypotheses of Lemma 6.1, the discrete solution of scheme (6.1)–(6.3) satisfies the following estimates:*

$$(\boldsymbol{i})\ \max_{0\le n\le N}\|\phi_h^n\|^2_{H^1(\Omega)}\le C,\quad (\boldsymbol{ii})\ \sum_{n=0}^{N-1}\|\phi_h^{n+1}-\phi_h^n\|^2_{H^1(\Omega)}\le C,\quad (\boldsymbol{iii})\ k\sum_{n=0}^{N-1}\left|\frac{\phi_h^{n+1}-\phi_h^n}{k}\right|^2\le C,$$

$$(\boldsymbol{iv})\ \max_{0\le n\le N}|\theta_h^n|^2\le C,\quad (\boldsymbol{v})\ \sum_{n=0}^{N-1}|\theta_h^{n+1}-\theta_h^n|^2\le C,\quad (\boldsymbol{vi})\ k\sum_{n=0}^{N-1}|\sqrt{K_1^h(\phi_h^{n+1})}\nabla\theta_h^{n+1}|^2\le C,$$

$$(\boldsymbol{vii})\ \max_{0\le n\le N}|c_h^n|^2\le C,\quad (\boldsymbol{viii})\ \sum_{n=0}^{N-1}|c_h^{n+1}-c_h^n|^2\le C,\quad (\boldsymbol{ix})\ k\sum_{n=0}^{N-1}|\sqrt{K_2^h(\phi_h^{n+1})}\nabla c_h^{n+1}|^2\le C,$$

where $C>0$ is independent of (h,k) and depends on the data (ϕ_0,θ_0,c_0), α,β and ε.

Proof. Obviously, if we let (6.5) and (6.6) hold for $n=0,...,N-1$, we get all the statements of this lemma by adding (6.5) and (6.6) and applying the discrete Gronwall lemma. Therefore, it suffices to prove that (6.5) and (6.6) hold for $n=0,...,N-1$.

Let us consider $C_d=\mathrm{e}^{(R_1+\frac{\beta^2}{\varepsilon^4}R_2)\,T}C_2/\varepsilon^2$ with $C_2>0$ given in (3.2) and R_1,R_2 given in Lemma 6.1. As the initial approximations hold hypothesis (6.4) for $n=0$, inequalities (6.5) and (6.6) are satisfied for $n=0$.

The final induction step can be easily seen by assuming that inequalities (6.5) and (6.6) hold for $l=0,...,n-1$. Then, adding up (6.5) and (6.6) from 0 to $n-1$, one has

$$\frac{2C_V\beta}{l\varepsilon^2}|\theta_h^n|^2+|c_h^n|^2+1+\|\phi_h^n\|^2_{H^1(\Omega)}+2\int_\Omega F(\phi_h^n)\le\frac{2C_V\beta}{l\varepsilon^2}|\theta_h^0|^2+|c_h^0|^2+1+\|\phi_h^0\|^2_{H^1(\Omega)}$$
$$+2\int_\Omega F(\phi_h^0)+k\sum_{l=0}^{n-1}\Big(R_1\|\phi_h^l\|^2_{H^1}+R_2\frac{\beta^2}{\varepsilon^4}(|c_h^l|^2+1)\Big).$$

Now, the discrete Gronwall lemma and (3.2) yield

$$\frac{2C_V\beta}{l\varepsilon^2}|\theta_h^n|^2+|c_h^n|^2+1+\|\phi_h^n\|^2_{H^1(\Omega)}+2\int_\Omega F(\phi_h^n)\le\mathrm{e}^{(R_1+\frac{\beta^2}{\varepsilon^4}R_2)(n-1)\,k}\Big(\frac{2C_V\beta}{l\varepsilon^2}|\theta_h^0|^2+|c_h^0|^2$$
$$+1+\|\phi_h^0\|^2_{H^1(\Omega)}+2\int_\Omega F(\phi_h^0)\Big)\le\mathrm{e}^{(R_1+\frac{\beta^2}{\varepsilon^4}R_2)\,T}C_2/\varepsilon^2:=C_d.$$

Then, we find that hypothesis (6.4) is satisfied. Therefore, in view of Lemma 6.1, inequalities (6.5) and (6.6) hold. □

Note that the stability estimates obtained in Lemma 6.2 are of order $O((1/\varepsilon^2)\mathrm{e}^{(\beta^2/\varepsilon^4)})$ for the variable $(\phi,\frac{\sqrt{\beta}}{\varepsilon}\theta,c)$ as in the nonlinear scheme, but now an adequate constraint for (h,k) small enough (depending exponentially on $1/\varepsilon$) is necessary (recall that in the nonlinear scheme, only $\frac{\beta k}{\varepsilon^2}$ small enough was imposed).

To finish the proof of Theorem 1.4 it is necessary to prove the convergence of the linear scheme (6.1)–(6.3). But, as the argument for this is similar to that developed for the nonlinear scheme (2.1)–(2.3), it is left to the reader. □

7. Error estimates for the non-degenerate case

In this section we deal with the error analysis of both linear and nonlinear scheme. The presence of the truncation operator applied to the piecewise constant operator P_0 makes nonstandard this error analysis and this particular truncation is responsible of order $O(h)$ in error estimates, although higher-order finite elements were considered.

In order to be able to guarantee a sufficient regular solution of problem (1.1)–(1.3) we assume the non-degenerate case. For simplicity, we assume that K_1 and K_2 are positive constants, providing in particular standard Neumann boundary conditions in (1.2).

Let $\{\mathcal{T}_h\}$, $0 < h \leq 1$, be a regular, quasi-uniform family of subdivisions of a polyhedral domain $\Omega \subset \mathbb{R}^m$, $m = 2$ or 3, whose boundary Γ is such that the problem

$$-\Delta u + u = f \text{ in } \Omega, \quad \frac{\partial u}{\partial \boldsymbol{n}} = 0 \text{ on } \Gamma \tag{7.1}$$

holds the stability property $\|u\|_{H^2(\Omega)} \leq |f|$, for each $f \in L^2(\Omega)$. Recall that, both previous hypotheses are also assumed in Theorem 1.3 to prove the convergence.

Define the global error $e_\phi^n = \phi_h^n - \phi(t_n)$, $e_\theta^n = \theta_h^n - \theta(t_n)$, and $e_c^n = c_h^n - c(t_n)$. These errors are decomposed into a discrete error $e_{\cdot,d}$, and an interpolation error $e_{\cdot,i}$ as follows

$$\begin{aligned} e_{\phi,d}^n &= \phi_h^n - P_h^1\phi(t_n), \quad & e_{\phi,i}^n &= P_h^1\phi(t_n) - \phi(t_n), \\ e_{\theta,d}^n &= \theta_h^n - P_h^0\theta(t_n), \quad & e_{\theta,i}^n &= P_h^0\theta(t_n) - \theta(t_n), \\ e_{c,d}^n &= c_h^n - P_h^0 c(t_n), \quad & e_{c,i}^n &= P_h^0 c(t_n) - c(t_n), \end{aligned}$$

where $P_h^1 : H^1 \to X_h$ is the H^1-projection operator defined as

$$\left(\psi - P_h^1\psi, x_h\right) + \left(\nabla\psi - \nabla P_h^1\psi, \nabla x_h\right) = 0 \quad \forall x_h \in X_h,$$

and $P_h^0 : L^2 \to X_h$ is the L^2-projection operator defined as

$$\left(\psi - P_h^0\psi, x_h\right) = 0 \quad \forall x_h \in X_h.$$

Finally, let us recall some approximation properties of P_h^1 and P_h^0 to be used later on (see [6], Prop. 1.134, p. 73):

$$\begin{aligned} \|\psi - P_h^0\psi\|_{H^1(\Omega)} &\leq C\,h\|\psi\|_{H^2(\Omega)}, \quad & \|\psi - P_h^1\psi\|_{H^1(\Omega)} &\leq C\,h\|\psi\|_{H^2(\Omega)}, \\ |\psi - P_0\psi| &\leq C\,h\|\psi\|_{H^1(\Omega)}, \quad & |\psi - P_h^1\psi| &\leq C\,h\|\psi\|_{H^1(\Omega)}. \end{aligned}$$

In particular, from the last inequality, one has

$$k\,|\delta_t\psi(t_{n+1}) - \delta_t P_h^1\psi(t_{n+1})|^2 \leq Ch^2 \int_{t_n}^{t_{n+1}} \|\psi_t\|_{H^1(\Omega)}^2,$$

where we use δ_t to denote the discrete backward Euler time derivative, that is

$$\delta_t\psi(t_{n+1}) = \frac{\psi(t_{n+1}) - \psi(t_n)}{k}.$$

Note that, for the H^1-interpolation error of P_h^0, a quasi-uniform family of finite elements must be assumed and, for the L^2-interpolation error of P_h^1, a duality argument is required where the elliptic H^2-regularity for the Elliptic-Neumann problem (7.1) is imposed.

Throughout the section we assume a regular solution of (1.1)–(1.3). Concretely, one assumes

$$\begin{aligned}
&\phi \in L^\infty(0,T;W^{1,\infty}(\Omega)) \cap L^2(0,T;H^2(\Omega)),\ \phi_t \in L^2(0,T;H^1(\Omega)),\ \phi_{tt} \in L^2(0,T;L^2(\Omega)),\\
&\theta \in L^\infty(0,T;H^1(\Omega)) \cap L^2(0,T,H^2(\Omega)),\ \theta_t \in L^2(0,T;L^2(\Omega)),\ \theta_{tt} \in L^2(0,T;H^1(\Omega)'),\\
&c \in L^\infty(0,T;H^1(\Omega)) \cap L^2(0,T,H^2(\Omega)),\ c_t \in L^2(0,T;L^2(\Omega)),\ c_{tt} \in L^2(0,T;H^1(\Omega)').
\end{aligned} \tag{7.2}$$

7.1. Error estimates for the nonlinear scheme

We now state our error estimates for the fully discrete nonlinear scheme (2.1)–(2.3). If we compare the exact problem with the scheme and use the equality $a^3 - b^3 = (a-b)^3 + 3\,a\,b(a-b)$, then the error equations are given by

$$\begin{cases}
\alpha\left(\delta_t e^{n+1}_{\phi,d}, x_h\right) + \left(\nabla e^{n+1}_{\phi,d}, \nabla x_h\right) + \left(e^{n+1}_{\phi,d}, x_h\right) + \dfrac{1}{2\varepsilon^2}\left((e^{n+1}_{\phi,d})^3, x_h\right)\\
= -\alpha\left(\delta_t e^{n+1}_{\phi,i}, x_h\right) - \dfrac{1}{2\varepsilon^2}\left((e^{n+1}_{\phi,i})^3, x_h\right) - \dfrac{3}{2\varepsilon^2}\left(P^1_h(\phi(t_{n+1}))\phi(t_{n+1})e^{n+1}_{\phi,i}, x_h\right)\\
\quad -\dfrac{3}{2\varepsilon^2}\left(\phi^{n+1}_h P^1_h(\phi(t_{n+1}))e^{n+1}_{\phi,d}, x_h\right) + \dfrac{1}{2\varepsilon^2}\left(e^n_{\phi,d} + e^n_{\phi,i}, x_h\right)\\
\quad +\left(e^n_{\phi,d} + e^n_{\phi,i}, x_h\right) + \dfrac{\beta}{\varepsilon^2}\left(e^n_{\theta,d}, x_h\right) - \dfrac{\beta}{\varepsilon^2}(\theta_A + \theta_B)\left(e^n_{c,d}, x_h\right) + \left(R^{n+1}_\phi, x_h\right),
\end{cases} \tag{7.3}$$

$$\begin{cases}
C_V\left(\delta_t e^{n+1}_{\theta,d}, x_h\right) + K_1\left(\nabla e^{n+1}_{\theta,d}, \nabla x_h\right)\\
= -K_1\left(\nabla e^{n+1}_{\theta,i}, \nabla x_h\right) - \dfrac{l}{2}\left(\delta_t e^{n+1}_\phi, x_h\right) + \left(R^{n+1}_\theta, x_h\right),
\end{cases} \tag{7.4}$$

$$\begin{cases}
\left(\delta_t e^{n+1}_{c,d}, x_h\right) + K_2\left(\nabla e^{n+1}_{c,d}, \nabla x_h\right) = -K_2\left(\nabla e^{n+1}_{c,i}, \nabla x_h\right)\\
- M\,K_2\left([P_0 c^n_h]_T(1 - [P_0 c^n_h]_T)\nabla e^n_\phi, \nabla x_h\right)\\
- M\,K_2\left((1 - [P_0 c^n_h]_T)e^n_{c_T}\nabla\phi(t_n), \nabla x_h\right)\\
+ M\,K_2\left(c(t_n)e^n_{c_T}\nabla\phi(t_n), \nabla x_h\right) + \left(R^{n+1}_c, x_h\right),
\end{cases} \tag{7.5}$$

where $\delta_t e^{n+1} = (e^{n+1} - e^n)/k$, $e^n_{c_T} = [P_0 c^n_h]_T - c(t_n)$ and

$$\begin{aligned}
R^{n+1}_\phi &= \frac{\alpha}{k}\int_{t_n}^{t_{n+1}} (t_n - t)\phi_{tt}(t)\mathrm{d}t + \left(\frac{1}{2\varepsilon^2} + 1\right)\int_{t_n}^{t_{n+1}} \phi_t(t)\mathrm{d}t\\
&\quad + \frac{\beta}{\varepsilon^2}\int_{t_n}^{t_{n+1}} \theta_t(t)\mathrm{d}t + \frac{\beta}{\varepsilon^2}(\theta_A + \theta_B)\int_{t_n}^{t_{n+1}} c_t(t)\mathrm{d}t,\\
R^{n+1}_\theta &= \frac{C_V}{k}\int_{t_n}^{t_n} (t_n - t)\theta_{tt}(t)\mathrm{d}t - \frac{l}{2k}\int_{t_n}^{t_{n+1}} (t_n - t)\phi_{tt}(t)\mathrm{d}t,
\end{aligned} \tag{7.6}$$

$$\begin{aligned}
R^{n+1}_c &= \frac{1}{k}\int_{t_n}^{t_{n+1}} (t_n - t)c_{tt}(t)\mathrm{d}t + \nabla\cdot\left(\left(1 - c(t_{n+1})\right)c(t_{n+1})\left(\int_{t_n}^{t_{n+1}} \nabla\phi_t(t)\right)\right.\\
&\quad \left. + \left(1 - (c(t_n) + c(t_{n+1})\right)\left(\int_{t_n}^{t_{n+1}} c_t(t)\right)\nabla\phi(t_n)\right).
\end{aligned}$$

Theorem 7.1. *Under the assumptions of Theorem 1.3, if the solution (ϕ,θ,c) of (1.1)–(1.3) satisfies that $(\phi(t),\theta(t),c(t)) \in H^2(\Omega)^3$ for all $t \in [0,T]$ and the regularity given in (7.2), then the following error estimates hold for k small enough:*

$$\max_{0\le n\le N}\left(\|e^{n+1}_\phi\|^2_{H^1(\Omega)} + |e^{n+1}_\theta|^2 + |e^{n+1}_c|^2\right) + k\sum_{n=0}^{N-1}\left(|\delta_t e^{n+1}_\phi|^2 + |\nabla e^{n+1}_\theta|^2 + |\nabla e^{n+1}_c|^2\right) \le C\left(h^2 + k^2\right), \tag{7.7}$$

where the constant $C > 0$ depends on the exact solution, but is independent of (h, k).

Proof. Set $x_h = 2k\delta_t e_{\phi,d}^{n+1} \in X_h$ as a test function in (7.3), and using the equalities

$$a^3(a-b) = \frac{1}{2}a^2(a^2 - b^2 + (a-b)^2) = \frac{1}{4}(a^4 - b^4 + (a^2-b^2)^2) + \frac{1}{2}a^2(a-b)^2$$

for $a = e_\phi^{n+1}$ and $b = e_\phi^n$, we get

$$\begin{cases} \alpha 2k\left|\delta_t e_{\phi,d}^{n+1}\right|^2 + \left(\|e_{\phi,d}^{n+1}\|_{H^1(\Omega)}^2 - \|e_{\phi,d}^n\|_{H^1(\Omega)}^2 + \|e_{\phi,d}^{n+1} - e_{\phi,d}^n\|_{H^1(\Omega)}^2\right) \\ \quad + \dfrac{1}{4\varepsilon^2}\left(\|e_{\phi,d}^{n+1}\|_{L^4(\Omega)}^4 - \|e_{\phi,d}^n\|_{L^4(\Omega)}^4 + |(e_{\phi,d}^{n+1})^2 - (e_{\phi,d}^n)^2|^2 + 2|(e_{\phi,d}^{n+1})(e_{\phi,d}^{n+1} - e_{\phi,d}^n)|^2\right) \\ = -\alpha 2k\left(\delta_t e_{\phi,i}^{n+1}, \delta_t e_{\phi,d}^{n+1}\right) - \dfrac{1}{\varepsilon^2}k\left((e_{\phi,i}^{n+1})^3, \delta_t e_{\phi,d}^{n+1}\right) \\ \quad - \dfrac{3}{\varepsilon^2}k\left(P_h^1(\phi(t_{n+1}))\phi(t_{n+1})e_{\phi,i}^{n+1}, \delta_t e_{\phi,d}^{n+1}\right) - \dfrac{3}{\varepsilon^2}k\left(\phi_h^{n+1}P_h^1(\phi(t_{n+1}))e_{\phi,d}^{n+1}, \delta_t e_{\phi,d}^{n+1}\right) \\ \quad + \dfrac{1}{\varepsilon^2}k\left(e_{\phi,d}^n + e_{\phi,i}^n, \delta_t e_{\phi,d}^{n+1}\right) + 2k\left(e_{\phi,d}^n + e_{\phi,i}^n, \delta_t e_{\phi,d}^{n+1}\right) \\ \quad + 2\dfrac{\beta}{\varepsilon^2}k\left(e_{\theta,d}^n, \delta_t e_{\phi,d}^{n+1}\right) - 2\dfrac{\beta}{\varepsilon^2}(\theta_A + \theta_B)k\left(e_{c,d}^n, \delta_t e_{\phi,d}^{n+1}\right) + 2k\left(R_\phi^{n+1}, \delta_t e_{\phi,d}^{n+1}\right) := \displaystyle\sum_{i=1}^{9} I_i. \end{cases} \tag{7.8}$$

Now, we must bound each term on the right-hand side of (7.8). We just focus on the terms I_2, I_3 and I_4:

$$\begin{aligned} I_2 &\le C_\lambda \tfrac{1}{\varepsilon^4\alpha}k\|e_{\phi,i}^{n+1}\|_{L^6(\Omega)}^6 + \lambda\, k\, \alpha|\delta_t e_{\phi,d}^{n+1}|^2 \le C_\lambda \tfrac{1}{\varepsilon^4\alpha}\, k\, h^6\|\phi(t_{n+1})\|_{H^2(\Omega)}^6 + \lambda\, k\, \alpha|\delta_t e_{\phi,d}^{n+1}|^2, \\ I_3 &\le \frac{3}{\varepsilon^2}\, k\|P_h^1(\phi(t_{n+1}))\|_{L^6(\Omega)}\|\phi(t_{n+1})\|_{L^6(\Omega)}\|e_{\phi,i}^{n+1}\|_{L^6(\Omega)}|\delta_t e_{\phi,d}^{n+1}| \\ &\le C_\lambda \frac{1}{\varepsilon^4\alpha}\, k\|\phi(t_{n+1})\|_{H^1(\Omega)}^4\|e_{\phi,i}^{n+1}\|_{H^1(\Omega)}^2 + \lambda\, k\, \alpha|\delta_t e_{\phi,d}^{n+1}|^2 \\ &\le C_\lambda \frac{1}{\varepsilon^4\alpha}\, k\, h^2\|\phi(t_{n+1})\|_{H^1(\Omega)}^4\|\phi(t_{n+1})\|_{H^2(\Omega)}^2 + \lambda\, k\, \alpha|\delta_t e_{\phi,d}^{n+1}|^2, \\ I_4 &\le \frac{3}{\varepsilon^2}\, k\|\phi_h^{n+1}\|_{L^6(\Omega)}\|P_h^1(\phi(t_{n+1}))\|_{L^6(\Omega)}\|e_{\phi,d}^{n+1}\|_{L^6(\Omega)}|\delta_t e_{\phi,d}^{n+1}| \\ &\le C_\lambda\, \frac{1}{\varepsilon^4\alpha}\, k\|\phi(t_{n+1})\|_{H^1(\Omega)}^2\|e_{\phi,d}^{n+1}\|_{H^1(\Omega)}^2 + \lambda\, k\, \alpha|\delta_t e_{\phi,d}^{n+1}|^2. \end{aligned}$$

In the last line, the stability estimate $\|\phi_h^{n+1}\|_{L^6(\Omega)} \le C$ given in Lemma 3.1 has been applied. Note that the previous inequalities hold for any $\lambda > 0$ and $C_\lambda > 0$ are different constants of order $O(1/\lambda)$. Finally, the constants C_λ bounding I_2 and I_3 are independent of ε, but the constant C_λ related to I_4 depends on ε *via* the bound of Lemma 3.1.

The remainder of the terms can be bounded more easily. Thus, by choosing λ small enough, we get

$$\begin{cases} \alpha\, k\left|\delta_t e_{\phi,d}^{n+1}\right|^2 + \left(\|e_{\phi,d}^{n+1}\|_{H^1(\Omega)}^2 - \|e_{\phi,d}^n\|_{H^1(\Omega)}^2 + \|e_{\phi,d}^{n+1} - e_{\phi,d}^n\|_{H^1(\Omega)}^2\right) \\ \quad + \dfrac{1}{4\varepsilon^2}\left(\|e_{\phi,d}^{n+1}\|_{L^4(\Omega)}^4 - \|e_{\phi,d}^n\|_{L^4(\Omega)}^4 + |(e_{\phi,d}^{n+1})^2 - (e_{\phi,d}^n)^2|^2 + 2|e_{\phi,d}^{n+1}(e_{\phi,d}^{n+1} - e_{\phi,d}^n)|^2\right) \\ \le C\, k\, h^2\left(h^4\|\phi(t_{n+1})\|_{H^2(\Omega)}^6 + \|\phi(t_{n+1})\|_{H^1(\Omega)}^4\|\phi(t_{n+1})\|_{H^2(\Omega)}^2 + \|\phi(t_n)\|_{H^1(\Omega)}^2\right) \\ \quad + C\, k\dfrac{1}{\varepsilon^4\alpha}\left(\beta^2|e_{c,d}^n|^2 + \beta^2 C_V|e_{\theta,d}^n|^2 + \|e_{\phi,d}^n\|_{H^1(\Omega)}^2 + \|\phi(t_{n+1})\|_{H^1(\Omega)}^2\|e_{\phi,d}^{n+1}\|_{H^1(\Omega)}^2\right) \\ \quad + C\, h^2\displaystyle\int_{t_n}^{t_{n+1}}\|\phi_t(s)\|_{H^1(\Omega)}^2 + C\, k^2\int_{t_n}^{t_{n+1}}\left(|\phi_t(s)|^2 + |\theta_t(s)|^2 + |c_t(s)|^2 + |\phi_{tt}(s)|^2\right)\mathrm{d}s, \end{cases} \tag{7.9}$$

where $C > 0$ are different constants independent of (h, k) and independent of the exact solution (ϕ, θ, c).

We now test (7.4) with $2ke_{\theta,d}^{n+1}$ and bound the right-hand side

$$\begin{cases} C_V\Big(|e_{\theta,d}^{n+1}|^2-|e_{\theta,d}^{n}|^2+|e_{\theta,d}^{n+1}-e_{\theta,d}^{n}|^2\Big)+2K_1\,k|\nabla e_{\theta,d}^{n+1}|^2 \\ =-2K_1\,k\Big(\nabla e_{\theta,i}^{n+1},\nabla e_{\theta,d}^{n+1}\Big)-l\,k\,\Big(\delta_t e_{\phi,d}^{n+1}+\delta_t e_{\phi,i}^{n+1},e_{\theta,d}^{n+1}\Big)+2\,k\Big(R_\theta^{n+1},e_{\theta,d}^{n+1}\Big) \\ \le C\,k\,h^2\|\theta(t_{n+1})\|_{H^2(\Omega)}^2+K_1k|\nabla e_{\theta,d}^{n+1}|^2+C\,h^2\displaystyle\int_{t_n}^{t_{n+1}}\|\phi_t(s)\|_{H^1(\Omega)}^2\mathrm{d}s \\ \quad+\dfrac{\alpha}{2}k|\delta_t e_{\phi,d}^{n+1}|^2+C\,C_V\,k\,|e_{\theta,d}^{n+1}|^2+C\,k^2\displaystyle\int_{t_n}^{t_{n+1}}(\|\theta_{tt}(s)\|_{H^1(\Omega)'}^2+\|\phi_{tt}(s)\|_{H^1(\Omega)'}^2)\mathrm{d}s. \end{cases} \tag{7.10}$$

Let us now take $x_h=2ke_{c,d}^{n+1}$ as a test function into (7.5),

$$\begin{cases} |e_{c,d}^{n+1}|^2-|e_{c,d}^{n}|^2+|e_{c,d}^{n+1}-e_{c,d}^{n}|^2+2K_2\,k|\nabla e_{c,d}^{n+1}|^2 \\ =-\,2K_2k\Big(\nabla e_{c,i}^{n+1},\nabla e_{c,d}^{n+1}\Big)-2M\,K_2k\Big([P_0c_h^n]_T(1-[P_0c_h^n]_T)\nabla(e_{\phi,d}^n+e_{\phi,i}^n),\nabla e_{c,d}^{n+1}\Big) \\ \quad-\,2M\,K_2k\Big((1-[P_0c_h^n]_T)e_{c_T}^n\,\nabla\phi(t_n),\nabla e_{c,d}^{n+1}\Big) \\ \quad+\,2M\,K_2k\Big(c(t_n)e_{c_T}^n\,\nabla\phi(t_n),\nabla e_{c,d}^{n+1}\Big)+2k\Big(R_c^{n+1},e_{c,d}^{n+1}\Big). \end{cases}$$

We firstly bound the truncated error

$$\begin{aligned} |e_{c_T}^n|^2 &= |[P_0c_h^n]_T-P_0c(t_n)+P_0c(t_n)-c(t_n)|^2 \\ &\le C\Big(|[P_0c_h^n]_T-P_0c(t_n)|^2+|P_0c(t_n)-c(t_n)|^2\Big) \\ &\le C\Big(|P_0c_h^n-P_0c(t_n)|^2+h^2|\nabla c(t_n)|^2\Big) \\ &\le C\Big(|e_{c,d}^n|^2+|e_{c,i}^n|^2+h^2|\nabla c(t_n)|^2\Big) \\ &\le C\Big(|e_{c,d}^n|^2+h^2\|c(t_n)\|_{H^1(\Omega)}^2\Big), \end{aligned} \tag{7.11}$$

where in the last line we have used the stability property $|P_0\psi|\le|\psi|$. Note that the interpolation error $|P_0c(t_n)-c(t_n)|$ appearing in (7.11) is only of order $O(h)$, independent of the finite element approximation.

By virtue of (7.11), we bound

$$\begin{cases} |e_{c,d}^{n+1}|^2-|e_{c,d}^{n}|^2+|e_{c,d}^{n+1}-e_{c,d}^{n}|^2+K_2\,k|\nabla e_{c,d}^{n+1}|^2 \\ \le C\,k\,h^2\|c(t_{n+1})\|_{H^2(\Omega)}^2+C\,k|\nabla e_{\phi,d}^n|^2+C\,k\,h^2\|\nabla\phi(t_n)\|_{L^\infty(\Omega)}^2\|c(t_n)\|_{H^1(\Omega)}^2 \\ \quad+C\;k\,h^2\|\phi(t_n)\|_{H^2(\Omega)}^2+C\,k\|\nabla\phi(t_n)\|_{L^\infty(\Omega)}^2|e_{c,d}^n|^2 \\ \quad+C\,k^2\displaystyle\int_{t_n}^{t_{n+1}}|\nabla\phi_t(s)|^2\mathrm{d}s \\ \quad+C\,k^2\|\nabla\phi(t_{n+1})\|_{L^\infty}^2\displaystyle\int_{t_n}^{t_{n+1}}|c_t(s)|^2\mathrm{d}s+C\,k^2\int_{t_n}^{t_{n+1}}\|c_{tt}(s)\|_{H^1(\Omega)'}^2\mathrm{d}s. \end{cases} \tag{7.12}$$

Again, $C>0$ are different constants independent of (h,k) and independent of the exact solution (ϕ,θ,c).

By adding (7.9), (7.10) and (7.12) and applying the generalized discrete Gronwall lemma, we establish the following estimate for all $n < N$ and for k small enough:

$$\|e_{\phi,d}^{n+1}\|_{H^1(\Omega)}^2 + \frac{1}{4\varepsilon^2}\|e_{\phi,d}^{n+1}\|_{L^4(\Omega)}^4 + C_V|e_{\theta,d}^{n+1}|^2 + |e_{c,d}^{n+1}|^2 + \alpha\, k\sum_{l=0}^{n}\left|\delta_t e_{\phi,d}^{l+1}\right|^2 + K_1\, k\sum_{l=0}^{n}|\nabla e_{\theta,d}^{l+1}|^2 + K_2 k\sum_{l=0}^{n}|\nabla e_{c,d}^{l+1}|^2 \le \exp(C_1 T)\Big(C_2 h^2 + C_3 k^2\Big), \quad (7.13)$$

where

$$C_1 = \frac{C\left(1 + \|\phi\|_{L^2(0,T;W^{1,\infty}(\Omega))}^2\right)}{1 - C\,k\,\max\{1, \|\phi\|_{L^\infty(0,T;H^1(\Omega))}^2\}}$$

$$\begin{aligned} C_2 \;=\; & C\Big(\|\phi\|_{L^\infty(0,T;H^1(\Omega))}^4\|\phi\|_{L^2(0,T;H^2(\Omega))}^2 + \|\phi\|_{L^2(0,T;H^2(\Omega))}^2 \\ & + \|\phi_t\|_{L^2(0,T;H^1(\Omega))}^2 + \|\theta\|_{L^2(0,T;H^2(\Omega))}^2 \\ & + \|\phi\|_{L^2(0,T;W^{1,\infty}(\Omega))}^2\|c\|_{L^\infty(0,T;H^1(\Omega))}^2 + \|c\|_{L^2(0,T;H^2(\Omega))}^2\Big), \end{aligned}$$

and

$$\begin{aligned} C_3 \;=\; & C\Big(\|\phi_t\|_{L^2(0,T;L^2(\Omega))}^2 + \|\theta_t\|_{L^2(0,T;L^2(\Omega))}^2 + \|c_t\|_{L^2(0,T;L^2(\Omega))}^2 + \|\phi_{tt}\|_{L^2(0,T;L^2(\Omega))}^2 \\ & + \|\theta_{tt}\|_{L^2(0;T;H^1(\Omega)')}^2 + \|\phi_{tt}\|_{L^2(0,T;H^1(\Omega)')}^2 + \|\phi_t\|_{L^2(0,T;H^1(\Omega))}^2 \\ & + \|\phi\|_{L^\infty(0,T;W^{1,\infty}(\Omega))}^2\|c_t\|_{L^2(0,T;L^2(\Omega))}^2 \mathrm{d}s + \|c_{tt}\|_{L^2(0,T;H^1(\Omega)')}^2\Big), \end{aligned}$$

with $C > 0$ independent of (h, k) and independent of the exact solution (ϕ, θ, c).

The same estimates are obtained for the total errors by using the interpolation errors; hence (7.7) can be deduced. □

Remark 7.2. Observe that, to obtain error estimates in the previous theorem, the monotony property (analogous to (3.8))

$$\frac{1}{2\varepsilon^2}((e_{\phi,d}^{n+1})^3 - e_{\phi,d}^n)(e_{\phi,d}^{n+1} - e_{\phi,d}^n) \ge F(e_{\phi,d}^{n+1}) - F(e_{\phi,d}^n)$$

is not used, because the corresponding initial term is

$$\int_\Omega F(e_{\phi,d}^0) = \frac{1}{8\varepsilon^2}\int_\Omega((e_{\phi,d}^0)^2 - 1)^2 = O\left(\frac{1}{\varepsilon^2}\right)\cdot$$

Therefore, by using this property, the error estimates of order $O(k + h)$ does not hold, because in this case the final bound remains of order $O(k + h + 1/\varepsilon^2)$.

7.2. Error estimates for the linear scheme

As the derivation of the error equations for θ_h^{n+1} and c_h^{n+1} is exactly the same as in the previous nonlinear scheme, we only treat in this section the error equation for ϕ_h^{n+1}, which is given by

$$\begin{cases} \alpha\left(\delta_t e_{\phi,d}^{n+1}, x_h\right) + \left(\nabla e_{\phi,d}^{n+1}, \nabla x_h\right) + \left(e_{\phi,d}^{n+1}, x_h\right) + \dfrac{1}{2\varepsilon^2}\left((e_{\phi,d}^n)^3, x_h\right) \\ = -\,\alpha\left(\delta_t e_{\phi,i}^{n+1}, x_h\right) - \dfrac{1}{2\varepsilon^2}\left((e_{\phi,i}^n)^3, x_h\right) - \dfrac{3}{2\varepsilon^2}\left(P_h^1(\phi(t_n))\phi(t_n)e_{\phi,i}^n, x_h\right) \\ \quad - \dfrac{3}{2\varepsilon^2}\left(\phi_h^n P_h^1(\phi(t_n))e_{\phi,d}^n, x_h\right) + \dfrac{1}{2\varepsilon^2}\left(e_{\phi,d}^n + e_{\phi,i}^n, x_h\right) \\ \quad + \left(e_{\phi,d}^n + e_{\phi,i}^n, x_h\right) + \dfrac{\beta}{\varepsilon^2}\left(e_{\theta,d}^n - (\theta_A + \theta_B)e_{c,d}^n, x_h\right) + \left(R_\phi^{n+1} + S_\phi^{n+1}, x_h\right) \end{cases} \quad (7.14)$$

where R_ϕ^{n+1} is as above and

$$S_\phi^{n+1} = -\frac{1}{2\varepsilon^2}(\phi(t_{n+1})^3 - \phi(t_n)^3) = -\frac{3}{2\varepsilon^2}\int_{t_n}^{t_{n+1}} \phi(s)^2\phi_t(s)\,\mathrm{d}s.$$

Again, we take $x_h = 2k\delta_t e_{\phi,d}^{n+1}$ as a test function in (7.14), and all computations work as for the nonlinear scheme, except the explicit term. Now, by using the equalities

$$\begin{aligned} b^3(a-b) &= [ba^2 + b(b^2-a^2)](a-b) = \frac{1}{2}a^2(a^2-b^2-(a-b)^2) + b(b^2-a^2)(a-b) \\ &= \frac{1}{4}(a^4 - b^4 + (a^2-b^2)^2) - \frac{1}{2}a^2(a-b)^2 + b(b^2-a^2)(a-b) \end{aligned}$$

for $a = e_{\phi,d}^{n+1}$ and $b = e_{\phi,d}^n$, we get

$$\begin{aligned} \frac{k}{\varepsilon^2}\Big((e_{\phi,d}^n)^3, \delta_t e_{\phi,d}^{n+1}\Big) &= \frac{1}{4\varepsilon^2}\Big(\|e_{\phi,d}^{n+1}\|_{L^4(\Omega)}^4 - \|e_{\phi,d}^n\|_{L^4(\Omega)}^4 + |(e_{\phi,d}^{n+1})^2 - (e_{\phi,d}^n)^2|^2\Big) \\ &\quad - \frac{1}{2\varepsilon^2}|e_{\phi,d}^{n+1}(e_{\phi,d}^{n+1} - e_{\phi,d}^n)|^2 + \frac{k}{\varepsilon^2}\Big(e_{\phi,d}^n[(e_{\phi,d}^n)^2 - (e_{\phi,d}^{n+1})^2], \delta_t e_{\phi,d}^{n+1}\Big). \end{aligned}$$

Applying the inverse inequality $\|e_{\phi,d}^{n+1}\|_{L^\infty(\Omega)}^2 \le (C/h)\|e_{\phi,d}^{n+1}\|_{H^1(\Omega)}^2$ and the stability estimates of the (linear) scheme $\|\phi_h^n\|_{H^1(\Omega)} \le C$ given in Lemma 6.2, we can bound the last two terms as follows

$$\begin{aligned} \frac{1}{2\varepsilon^2}|e_{\phi,d}^{n+1}(e_{\phi,d}^{n+1} - e_{\phi,d}^n)|^2 &\le \frac{1}{2\varepsilon^2}k^2\|e_{\phi,d}^{n+1}\|_{L^\infty(\Omega)}^2|\delta_t e_{\phi,d}^{n+1}|^2 \\ &\le C_\varepsilon\frac{k^2}{h}\|e_{\phi,d}^{n+1}\|_{H^1(\Omega)}^2|\delta_t e_{\phi,d}^{n+1}|^2 \le C_\varepsilon\frac{k}{h}k|\delta_t e_{\phi,d}^{n+1}|^2, \end{aligned}$$

$$\begin{aligned} \frac{k}{\varepsilon^2}\Big(e_{\phi,d}^n[(e_{\phi,d}^n)^2 - (e_{\phi,d}^{n+1})^2], \delta_t e_{\phi,d}^{n+1}\Big) &\le C_\varepsilon\, k^2\|e_{\phi,d}^n\|_{L^\infty(\Omega)}^2\left|\delta_t e_{\phi,d}^{n+1}\right|^2 + \frac{1}{8\varepsilon^2}|(e_{\phi,d}^n)^2 - (e_{\phi,d}^{n+1})^2|^2 \\ &\le C_\varepsilon\frac{k}{h}\,k|\delta_t e_{\phi,d}^{n+1}|^2 + \frac{1}{8\varepsilon^2}|(e_{\phi,d}^n)^2 - (e_{\phi,d}^{n+1})^2|^2. \end{aligned}$$

Therefore, proceeding as in the nonlinear scheme, we get the same error estimates (7.7) by using the constraint (S) $k/h \to 0$. Notice that this time we need not make an induction argument thanks to the stability estimates provided by Lemma 6.2.

Remark 7.3. All the above error estimates hold for the modified scheme where the term c_h^n in (2.1) (respectively, in (6.1)) is replaced by $[P_0 c_h^n]_T$. To this end, we have to take into account estimate (7.11). We have already seen in Remark 3.2 that this type of more truncated schemes has stability constants depending on $1/\varepsilon$ only of polynomial form.

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