

A Conserved Phase-Field Model Based on Microconcentrations

Armel Judice Ntsokongo^{1*}, Narcisse Batangouna², Christian Tathy³

¹Faculté des Sciences et Techniques, Université Marien Ngouabi, Brazzaville, Republic of the Congo

²Institut Supérieur d'Architecture, Urbanisme, Batiment et Travaux Publics, Université Denis Sassou N'guesso, Kintele, Republic of the Congo

³Laboratoire de Mécanique, Énergétique et Ingénierie, Ecole Nationale Supérieure Polytechnique, Université Marien Ngouabi, Brazzaville, Republic of the Congo

Email: *armeljudice@gmail.com, banarcissess@yahoo.fr, christian.tathy@umng.cg

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Abstract

In this article, we consider the conserved phase-field model based on microconcentrations. In particular, we prove the well-posedness to this model and then prove the convergence of the solutions to those of the classical conserved phase-field model as a small parameter goes to zero, on finite time intervals. We also prove the existence of global attractor and we finally give some numerical simulations.

Keywords

Conserved Phase-Field Model, Microconcentrations, Neumann Boundary Conditions, Well-Posedness, Passage to the Limit, Global Attractor, Numerical Simulations

1. Introduction

In this paper, we are interested in the study of the following three equations:

$$\frac{\partial u}{\partial t} + \Delta^2 v - \Delta f(u) = -\Delta \theta, \quad (1.1)$$

$$u = v - \varepsilon \Delta v, \quad \varepsilon > 0, \quad (1.2)$$

$$\frac{\partial \theta}{\partial t} - \Delta \theta = -\frac{\partial u}{\partial t}, \quad (1.3)$$

where ε is expected to be small (it is related to the inverse of the penalty modulus), u is the order parameter, while v is the microconcentration and θ the (relative) temperature. Furthermore, here and below, we set all physical parame-

ters equal to one and we refer the interested reader to [1]-[12]. In particular, in the presence of the microconcentration, the total (Ginzburg-Landau type) free energy associated with the problem read (see [13]):

$$\Psi(u, v, \nabla v, \theta) = \int_{\Omega} \left(\frac{1}{2\varepsilon} (u-v)^2 + \frac{1}{2} |\nabla v|^2 + F(u) - \theta u - \frac{1}{2} \theta^2 \right) dx, \quad (1.4)$$

where the potential F is such that $F(s) = \int_0^s f(\tau) d\tau$, Ω is the domain occupied by the system (we assume here that it is a bounded and regular domain of \mathbb{R}^n , $n=1, 2$ or 3 , with boundary Γ), and the enthalpy

$$H = u + \theta. \quad (1.5)$$

As far as the evolution equations for the order parameter are concerned, one postulates the relaxation dynamics (with relaxation parameter set equal to one)

$$\frac{\partial u}{\partial t} = \Delta \frac{D\Psi}{Du}, \quad (1.6)$$

where Du denotes a variational derivative with respect to u , which yields (1.1) and (1.2). Then, we have the energy equation

$$\frac{\partial H}{\partial t} = -\operatorname{div} q, \quad (1.7)$$

where q is the heat flux. Assuming finally the usual Fourier law for heat conduction

$$q = -\nabla \theta, \quad (1.8)$$

we obtain (1.3).

The microconcentration model was used in [14] in an application to lithium-ion batteries, coupled with finite deformation elastoplasticity. The computational advantage of the microconcentration approach, compared to the standard classical conserved phase-field model, is that less regularity of shape functions is required for the concentration variables in a finite element setting [15].

Our aim in this paper is to prove the aforementioned convergence. We also prove the well-posedness to the conserved phase-field model based on microconcentrations and obtain error estimates on the difference of the solutions to this model and the classical conserved phase-field model, on finite time intervals. Finally, we prove the existence of global attractor and we give some numerical simulations.

2. Our Problem

We recall that we are interested in the following initial and boundary value problem:

$$\frac{\partial u}{\partial t} + \Delta^2 v - \Delta f(u) = -\Delta \theta, \quad (2.1)$$

$$u = v - \varepsilon \Delta v, \quad (2.2)$$

$$\frac{\partial \theta}{\partial t} - \Delta \theta = -\frac{\partial u}{\partial t}, \quad (2.3)$$

$$\frac{\partial u}{\partial \nu} = \frac{\partial v}{\partial \nu} = \frac{\partial \Delta v}{\partial \nu} = \frac{\partial \theta}{\partial \nu} = 0 \quad \text{on } \Gamma, \quad (2.4)$$

$$u|_{t=0} = u_0, \quad \theta|_{t=0} = \theta_0, \quad (2.5)$$

in a bounded and regular domain $\Omega \subset \mathbb{R}^n$, $n = 1, 2$ or 3 , with boundary Γ ; ν denotes the unit outer normal to Γ and $\frac{\partial \varphi}{\partial \nu} = \nabla \varphi \cdot \nu$ denotes the normal derivative on Γ . In particular, we assume, throughout this paper, that

$$0 < \varepsilon \leq \varepsilon_0 < 1. \quad (2.6)$$

As far as the nonlinear term is concerned, we make the following assumptions:

$$f \in C^2(\mathbb{R}), \quad f(0) = 0, \quad (2.7)$$

$$f' \geq -1. \quad (2.8)$$

$$F(s) \geq \frac{1}{8}s^4 - c_1, \quad c_1 \geq 0, \quad (2.9)$$

$$f(s)s \geq c_2 F(s) - c_3, \quad F(s) \geq -c_4, \quad c_2 > 0, \quad c_3, c_4 \geq 0, \quad s \in \mathbb{R}, \quad (2.10)$$

where $F(s) = \int_0^s f(\tau) d\tau$.

Remark 2.1. In particular, the usual cubic nonlinear term $f(s) = s^3 - s$ satisfied these assumptions and $F(s) = \frac{1}{4}s^4 - \frac{1}{2}s^2$.

3. Preliminaries and Notation

We introduce here our main assumptions, together with several mathematical tools which are needed in order to give a precise analytical statement of our results.

We denote by $\langle \varphi \rangle$ the spatial average of a function $\varphi \in L^1(\Omega)$,

$$\langle \varphi \rangle = \frac{1}{\text{Vol}(\Omega)} \int_{\Omega} \varphi(x) dx$$

and, for $\varphi \in H^{-1}(\Omega) = H^1(\Omega)'$,

$$\langle \varphi \rangle = \frac{1}{\text{Vol}(\Omega)} \langle \varphi, 1 \rangle_{H^{-1}(\Omega), H^1(\Omega)},$$

where $\langle \cdot, \cdot \rangle$ denotes the duality product. Furthermore, we set

$$\bar{\varphi} = \varphi - \langle \varphi \rangle,$$

where $\bar{\varphi}$ denotes the conjugate of φ .

We then set

$$\dot{H}^1(\Omega) = \{ \varphi \in H^1(\Omega), \langle \varphi \rangle = 0 \}$$

and

$$\dot{L}^2(\Omega) = \{ \varphi \in L^2(\Omega), \langle \varphi \rangle = 0 \}.$$

Integrating (2.1) over the spatial domain Ω , we have, owing to (2.4),

$$\frac{d}{dt} \langle u \rangle = 0. \quad (3.1)$$

Furthermore, integrating then (2.2) and (2.3) over Ω , we obtain resp.

$$\langle u \rangle = \langle v \rangle, \tag{3.2}$$

so that, also,

$$\frac{d}{dt} \langle v \rangle = 0 \tag{3.3}$$

and

$$\frac{d}{dt} \langle H \rangle = 0, \tag{3.4}$$

which also yields, owing to (3.1),

$$\frac{d}{dt} \langle \theta \rangle = 0. \tag{3.5}$$

We thus have the conservation of temperature, the conservation of mass, both for the order parameter u and the microconcentration v .

Let A be the operator defined by

$$\langle Au, \varphi \rangle_{H^{-1}(\Omega), H^1(\Omega)} = ((\nabla u, \nabla \varphi)), \quad \forall \varphi \in \dot{H}^1(\Omega),$$

where $((\cdot, \cdot))$ denotes the usual L^2 -scalar product, with associated norm $\|\cdot\|$, and the operator A is an unbounded linear, selfadjoint and positive operator with compact inverse and is an isomorphism from $\dot{H}^1(\Omega)$ onto its dual. Furthermore,

$$\mathcal{D}(A) = \left\{ \varphi \in H^2(\Omega) \cap \dot{H}^1(\Omega), \frac{\partial \varphi}{\partial \nu} = 0 \text{ on } \Gamma \right\}$$

and $Au = h, u \in \mathcal{D}(A), h \in \dot{L}^2(\Omega)$, is equivalent to

$$-\Delta u = h, \frac{\partial u}{\partial \nu} = 0 \text{ on } \Gamma.$$

We will thus write $-\Delta$ instead of A in what follows, meaning that we consider that this operator acts on functions with null spatial average; of course, it can also be defined on functions with nonvanishing spatial average. We refer the interested reader to, e.g., [16] for more details on this. Having this, we can rewrite, equivalently, (2.1) in the (weaker) form:

$$(-\Delta)^{-1} \frac{\partial u}{\partial t} - \Delta v + \overline{f(u)} = \theta - \langle \theta_0 \rangle, \tag{3.6}$$

noting that

$$\left\langle \frac{\partial u}{\partial t} \right\rangle = 0$$

and

$$\langle \theta \rangle = \langle \theta_0 \rangle, \quad \forall t \geq 0.$$

We only keep one boundary condition on v , namely

$$\frac{\partial v}{\partial \nu} = 0 \text{ on } \Gamma. \tag{3.7}$$

Remark 3.1. In particular, it follows from (2.1) to (2.3) that

$$\frac{\partial}{\partial t}(v - \varepsilon \Delta v) + \Delta^2 v - \Delta f(v - \varepsilon \Delta v) = -\Delta \theta, \quad (3.8)$$

$$\frac{\partial \theta}{\partial t} - \Delta \theta = -\frac{\partial}{\partial t}(v - \varepsilon \Delta v), \quad (3.9)$$

which we can rewrite in the following (at least formally) equivalent form:

$$\frac{\partial}{\partial t} \left((-\Delta)^{-1} \bar{v} + \varepsilon \bar{v} \right) - \Delta \bar{v} + \overline{f(\langle u_0 \rangle + \bar{v} - \varepsilon \Delta \bar{v})} = \bar{\theta}, \quad (3.10)$$

$$\frac{\partial \bar{\theta}}{\partial t} - \Delta \bar{\theta} = \frac{\partial}{\partial t} (\bar{v} + \varepsilon \bar{v}), \quad (3.11)$$

where $-\Delta$ denoting the minus Laplace operator with Neumann boundary conditions and acting on functions with null average. Also recall that

$$\langle u \rangle = \langle v \rangle = \langle u_0 \rangle, \quad \langle \theta \rangle = \langle \theta_0 \rangle, \quad \forall t \geq 0. \quad (3.12)$$

Alternatively, we can rewrite (2.2) in the equivalent form:

$$\langle u \rangle = \langle u_0 \rangle, \quad \bar{v} = (I - \varepsilon \Delta)^{-1} \bar{u}, \quad (3.13)$$

allowing us to rewrite (3.10)-(3.11) in the equivalent form:

$$(-\Delta)^{-1} \frac{\partial \bar{u}}{\partial t} - \Delta (I - \varepsilon \Delta)^{-1} \bar{u} + \overline{f(\langle u_0 \rangle + \bar{u})} = \bar{\theta}. \quad (3.14)$$

$$\frac{\partial \bar{\theta}}{\partial t} - \Delta \bar{\theta} = \frac{\partial \bar{u}}{\partial t}, \quad (3.15)$$

This shows that we can rewrite (2.1)-(2.4) as an equivalent problem for the sole unknown (u, v, θ) .

We set $\|\cdot\|_{-1} = \left\| (-\Delta)^{-\frac{1}{2}} \cdot \right\|$; $\|\cdot\|_{-1}$ is a norm on $\{v \in H^{-1}(\Omega), \langle v \rangle = 0\}$ which is equivalent to the usual $H^{-1}(\Omega)$ -norm. More generally, we denote by $\|\cdot\|_X$ the norm on the Banach space X .

Throughout this paper, the same letters c , c' and c'' denote (nonnegative or positive) constants which may vary from line to line, or even in a same line, and which are independent of ε (but may depend on ε_0).

4. Priori Estimates

In this section, we will establish a number of important inequalities that will be used later in the proof of the existence of the solution, the existence of global attractor and the convergence to the conserved phase-field model.

We assume that

$$\langle u_0 \rangle \leq M_1, \quad \langle \theta_0 \rangle \leq M_2 \quad (4.1)$$

for fixed positive constants M_1 and M_2 , which yields, owing to (3.12),

$$\langle u(t) \rangle = \langle v(t) \rangle \leq M_1, \quad \langle \theta(t) \rangle \leq M_2, \quad t \geq 0. \quad (4.2)$$

We start with the following proposition.

Proposition 4.1 *Any sufficiently regular solution to (2.1)-(2.5) satisfies the following estimates.*

$$\begin{aligned} & \|u(t)\|_{L^4(\Omega)}^2 + \|v(t)\|_{H^2(\Omega)}^2 + \|\theta(t)\|^2 \\ & \leq ce^{-c't} \left(\|u_0\|_{L^4(\Omega)}^2 + \|v_0\|_{H^2(\Omega)}^2 + \|\theta_0\|^2 \right) + c''_{M_1}, \quad c' > 0, t \geq 0 \end{aligned} \tag{4.3}$$

and

$$\begin{aligned} & \int_0^t \left(\left\| \frac{\partial u}{\partial t} \right\|_{-1}^2 + \|\theta\|_{H^1(\Omega)}^2 + \|v\|_{H^3(\Omega)}^2 \right) ds \\ & \leq ce^{-c't} \left(\|u_0\|_{L^4(\Omega)}^2 + \|v_0\|_{H^2(\Omega)}^2 + \|\theta_0\|^2 \right) + c''_{M_1}, \quad c' > 0, t \geq 0. \end{aligned} \tag{4.4}$$

Proof. The estimates below will be formal, but they can easily be justified within, e.g., a standard Galerkin scheme.

We multiply (3.6) by $\frac{\partial u}{\partial t}$ and have, integrating over Ω and by parts,

$$\left\| \frac{\partial u}{\partial t} \right\|_{-1}^2 - \left(\left(\Delta v, \frac{\partial u}{\partial t} \right) \right) + \frac{d}{dt} \int_{\Omega} F(u) dx = \left(\left(\theta, \frac{\partial u}{\partial t} \right) \right) - |\Omega| \langle \theta_0 \rangle \left\langle \frac{\partial u}{\partial t} \right\rangle.$$

Noting that, owing to (2.2),

$$\frac{\partial u}{\partial t} = \frac{\partial v}{\partial t} - \varepsilon \Delta \frac{\partial v}{\partial t} \tag{4.5}$$

and

$$\left\langle \frac{\partial u}{\partial t} \right\rangle = 0,$$

we thus deduce from the above that

$$\frac{d}{dt} \left(\|\nabla v\|^2 + \varepsilon \|\Delta v\|^2 + 2 \int_{\Omega} F(u) dx \right) + 2 \left\| \frac{\partial u}{\partial t} \right\|_{-1}^2 = 2 \left(\left(\theta, \frac{\partial u}{\partial t} \right) \right). \tag{4.6}$$

We then multiply (2.3) by θ to obtain

$$\frac{d}{dt} \|\theta\|^2 + 2 \|\nabla \theta\|^2 = -2 \left(\left(\theta, \frac{\partial u}{\partial t} \right) \right). \tag{4.7}$$

The sum of (4.6) and (4.7) gives, setting

$$E_1 = \|\nabla v\|^2 + \varepsilon \|\Delta v\|^2 + 2 \int_{\Omega} F(u) dx + \|\theta\|^2$$

the differential equality

$$\frac{dE_1}{dt} + 2 \left\| \frac{\partial u}{\partial t} \right\|_{-1}^2 + 2 \|\nabla \theta\|^2 = 0, \tag{4.8}$$

i.e., the decay of the total free energy.

We now multiply (3.6) by u and have, owing to (3.2), (2.10) and (4.2),

$$\frac{d}{dt} \|u\|_{-1}^2 + c \left(\|\nabla v\|^2 + \varepsilon \|\Delta v\|^2 + \int_{\Omega} F(u) dx \right) \leq \|\theta\|^2 + c'_{M_1}, \quad c > 0. \tag{4.9}$$

We next multiply (3.6) by $-\Delta u$ and find, owing to (2.8),

$$\frac{1}{2} \frac{d}{dt} \|u\|^2 + ((\Delta u, \Delta v)) \leq \frac{3}{2} \|\nabla u\|^2 + \frac{1}{2} \|\nabla \theta\|^2. \tag{4.10}$$

Noting that, owing to (2.2),

$$-\Delta v = \frac{1}{\varepsilon}(u - v),$$

we have

$$\begin{aligned} \frac{d}{dt} \|u\|^2 + \left(\frac{1}{\varepsilon} - 3\right) \|\nabla u\|^2 &\leq \|\nabla \theta\|^2 + \frac{2}{\varepsilon} ((\nabla u, \nabla v)) \\ &\leq \|\nabla \theta\|^2 + \left(\frac{1}{\varepsilon} - 1\right) \|\nabla u\|^2 + \frac{1}{\varepsilon(1-\varepsilon)} \|\nabla v\|^2 \end{aligned}$$

and we find

$$\frac{d}{dt} \|u\|^2 + \left(\frac{1}{\varepsilon} - 2\right) \|\nabla u\|^2 \leq \|\theta\|^2 + \frac{1}{\varepsilon(1-\varepsilon)} \|\nabla v\|^2, \quad (4.11)$$

which gives

$$\frac{d}{dt} (\varepsilon \|u\|^2) + (1 - 2\varepsilon_0) \|\nabla u\|^2 \leq \varepsilon_0 \|\theta\|^2 + \frac{1}{1-\varepsilon_0} \|\nabla v\|^2. \quad (4.12)$$

Writing now, in view of (2.2),

$$\Delta u = \Delta v - \varepsilon \Delta^2 v,$$

we deduce from (4.10) that

$$\frac{d}{dt} \|u\|^2 + \|\Delta v\|^2 + \|\nabla \Delta v\|^2 \leq 3 \|\nabla u\|^2 + \|\nabla \theta\|^2. \quad (4.13)$$

Summing (4.8), δ_1 times (4.9) and (4.13), where $\delta_1 > 0$ is small enough, we obtain, setting

$$E_2 = E_1 + \delta_1 \|u\|_{-1}^2 + \|u\|^2$$

an inequality of the form

$$\frac{dE_2}{dt} + c \left(E_2 + \left\| \frac{\partial u}{\partial t} \right\|_{-1}^2 + \|\theta\|_{H^1(\Omega)}^2 + \|v\|_{H^3(\Omega)}^2 \right) \leq c'_{M_1}, \quad (4.14)$$

where E_2 satisfies

$$E_2 \geq c \left(\|u\|_{L^4(\Omega)}^2 + \|v\|_{H^2(\Omega)}^2 + \|\theta\|^2 \right) - c'. \quad (4.15)$$

In particular, it follows from (4.14)-(4.15) and Gronwall's lemma the dissipative estimate (4.3) and (4.4), where

$$v_0 = (I - \varepsilon \Delta)^{-1} u_0.$$

Remark 4.1. When $\varepsilon = 0$, then we have $v = u$ and (4.8) reads

$$\frac{dE_1}{dt} + 2 \left\| \frac{\partial u}{\partial t} \right\|_{-1}^2 + 2 \|\nabla \theta\|^2 = 0, \quad (4.16)$$

where

$$E_1 = \|\nabla u\|^2 + 2 \int_{\Omega} F(u) dx + \|\theta\|^2,$$

which is precisely the energy decay for the classical conserved phase-field model

(see [17]).

5. Well-Posedness and Semigroup

In this section we consider that $\varepsilon > 0$ is fixed. We have the following.

Theorem 5.1. *Let $T > 0$ be given. We assume that (2.6) holds, $(u_0, \theta_0) \in H^1(\Omega) \times L^2(\Omega)$ and $\varepsilon u_0 \in H^2(\Omega)$. Then, (2.1)-(2.5) possesses a unique weak solution (u, θ) such that*

$$\begin{aligned} u &\in L^\infty(\mathbb{R}^+; L^4(\Omega)) \cap L^2(0, T; H^1(\Omega)), \\ \frac{\partial u}{\partial t} &\in L^2(0, T; H^{-1}(\Omega)), \\ v &\in L^\infty(\mathbb{R}^+; H^2(\Omega)) \cap L^2(0, T; H^3(\Omega)), \\ \frac{\partial v}{\partial t} &\in L^2(0, T; H^1(\Omega)) \end{aligned}$$

and

$$\theta \in L^\infty(\mathbb{R}^+; L^2(\Omega)) \cap L^2(0, T; H^1(\Omega)).$$

Furthermore, $u \in C([0, T]; L^4(\Omega)_w)$, $v \in C([0, T]; H^2(\Omega))$ and $\theta \in C([0, T]; L^2(\Omega))$ where the index w denotes the weak topology.

Proof. Existence: The proof of existence, as well as of further regularity, is based on the above a priori estimates and a proper Galerkin scheme. Furthermore, the continuity results follow from the Lions-Magenes theorem and the Strauss lemma (see, e.g., [18] for details).

We can note that (3.10)-(3.11) is associated with the following weak formulation:

Find $(u, v, \theta): [0, T] \rightarrow \dot{H}^1(\Omega)^3$, such that

$$\begin{aligned} \frac{d}{dt} \left(((-\Delta)^{-1} \bar{v} + \varepsilon \bar{v}, \varphi) \right) + ((\nabla \bar{v}, \nabla \varphi)) + \left((f(\langle u_0 \rangle + \bar{v} - \varepsilon \Delta \bar{v}), \varphi) \right) \\ = ((\bar{\theta}, \varphi)) \text{ in } \mathcal{D}'(\Omega), \end{aligned} \tag{5.1}$$

$$\frac{d}{dt} \left((\bar{\theta}, \varphi) \right) + ((\nabla \bar{\theta}, \nabla \varphi)) = -\frac{d}{dt} \left((\bar{v} - \varepsilon \Delta \bar{v}, \varphi) \right) \text{ in } \mathcal{D}'(\Omega), \tag{5.2}$$

$$\forall \varphi \in \dot{H}^1(\Omega),$$

$$\bar{v}|_{t=0} = \bar{v}_0, \quad \bar{\theta}|_{t=0} = \bar{\theta}_0. \tag{5.3}$$

Let $(e_i)_{i \in \mathbb{N}}$ be eigenvectors of the minus Laplace operator associated with Neumann boundary conditions; these eigenvectors are associated with the eigenvalues $0 < \lambda_1 \leq \lambda_2 \leq \dots$,

$$-\Delta e_i = \lambda_i e_i$$

and acting on functions with null spatial average. We assume that the e_i s are orthonormal in $\dot{L}^2(\Omega)$ and orthogonal in $\dot{H}^1(\Omega)$.

We set for $m \in \mathbb{N}$,

$$V_m = \text{Span}\{e_1, \dots, e_m\}.$$

Actually, here, the only difficulty is to prove the existence of a local in time solution to an approximated problem. To do so, keeping the same notation as in the previous section, we consider the following approximated problem, for $m \in \mathbb{N}$ given:

Find $(u_m, v_m, \theta_m) : [0, T] \rightarrow V_m^3$, such that

$$\begin{aligned} \frac{d}{dt} \left(((-\Delta)^{-1} \bar{v}_m + \varepsilon \bar{v}_m, \varphi) \right) + ((\nabla \bar{v}_m, \nabla \varphi)) + \left((f(\langle u_0 \rangle + \bar{v}_m - \varepsilon \Delta \bar{v}_m), \varphi) \right) \\ = ((\bar{\theta}_m, \varphi)) \text{ in } \mathcal{D}'(\Omega), \end{aligned} \tag{5.4}$$

$$\frac{d}{dt} \left((\bar{\theta}_m, \varphi) \right) + ((\nabla \bar{\theta}_m, \nabla \varphi)) = -\frac{d}{dt} \left((\bar{v}_m - \varepsilon \Delta \bar{v}_m, \varphi) \right) \text{ in } \mathcal{D}'(\Omega), \tag{5.5}$$

$$\forall \varphi \in V_m,$$

$$\bar{v}_m|_{t=0} = \bar{v}_{0,m}, \quad \bar{\theta}_m|_{t=0} = \bar{\theta}_{0,m}, \tag{5.6}$$

where

$$\bar{u}_{0,m} = \bar{v}_{0,m} - \varepsilon \bar{v}_{0,m}, \tag{5.7}$$

$$\bar{u}_{0,m} = P_m \bar{u}_0, \quad \bar{\theta}_{0,m} = P_m \bar{\theta}_0 \tag{5.8}$$

P_m being the orthogonal projector onto V_m (for the $L^2(\Omega)$ -norm).

The existence of a local in time solution to (5.4)-(5.8) then follows from the Cauchy-Lipschitz theorem. Having this, we can pass to the limit in a standard way, owing to the above a priori estimates (which also hold at the approximated level) and standard Aubin-Lions compactness results, and deduce the existence of a solution.

Uniqueness: Let (u_1, v_1, θ_1) and (u_2, v_2, θ_2) be two solutions with initial data $(u_{0,1}, \theta_{0,1})$ and $(u_{0,2}, \theta_{0,2})$, respectively, such that $|\langle u_{0,i} \rangle| \leq M_1$ and $|\langle \theta_{0,i} \rangle| \leq M_2, \quad i = 1, 2$. We set

$$(u, v, \theta) = (u_1, v_1, \theta_1) - (u_2, v_2, \theta_2)$$

and have

$$(-\Delta)^{-1} \frac{\partial u}{\partial t} - \Delta v + \overline{f(u_1) - f(u_2)} = \theta, \tag{5.9}$$

$$u = v - \varepsilon \Delta v, \tag{5.10}$$

$$\frac{\partial \theta}{\partial t} - \Delta \theta = -\frac{\partial u}{\partial t}, \tag{5.11}$$

$$\langle u \rangle = \langle v \rangle = \langle \theta \rangle = 0, \quad t \geq 0, \tag{5.12}$$

$$\frac{\partial v}{\partial \nu} = \frac{\partial \theta}{\partial \nu} = 0 \text{ on } \Gamma, \tag{5.13}$$

$$u|_{t=0} = u_0, \quad \theta|_{t=0} = \theta_0. \tag{5.14}$$

We multiply (5.9) by u and have, owing to (2.8),

$$\frac{1}{2} \frac{d}{dt} \|u\|_{-1}^2 + ((-\Delta v, u)) \leq \frac{3}{2} \|u\|^2 + \frac{1}{2} \|\theta\|^2. \tag{5.15}$$

Next, multiplying (5.11) by $(-\Delta)^{-1}(u + \theta)$, we find

$$\frac{d}{dt} \|u + \theta\|_{-1}^2 + \|\theta\|^2 \leq \|u\|^2. \tag{5.16}$$

Summing finally δ_2 times (5.15) and (5.16), where $\delta_2 > 0$ is small enough, we find

$$\frac{d}{dt} (\delta_2 \|u\|_{-1}^2 + \|u + \theta\|_{-1}^2) + \delta_2 ((-\Delta v, u)) + (1 - \delta_2) \|\theta\|^2 \leq (3\delta_2 + 1) \|u\|^2, \tag{5.17}$$

where

$$1 - \delta_2 > 0.$$

Note that it follows from (5.10) that

$$((-\Delta v, u)) = \|\nabla v\|^2 + \varepsilon \|\Delta v\|^2$$

and

$$\|u\|^2 = \|v\|^2 + 2\varepsilon \|\nabla v\|^2 + \varepsilon^2 \|\Delta v\|^2.$$

We thus deduce that

$$\begin{aligned} & \frac{d}{dt} (\delta_2 \|u\|_{-1}^2 + \|u + \theta\|_{-1}^2) + \delta_2 (\|\nabla v\|^2 + \varepsilon \|\Delta v\|^2) + (1 - \delta_2) \|\theta\|^2 \\ & \leq (3\delta_2 + 1) (\|v\|^2 + 2\varepsilon \|\nabla v\|^2 + \varepsilon^2 \|\Delta v\|^2) \end{aligned}$$

and (2.6) yields, employing the Poincar-Wirtinger inequality,

$$\frac{d}{dt} (\delta_2 \|u\|_{-1}^2 + \|u + \theta\|_{-1}^2) + (1 - \varepsilon_0) \varepsilon \delta_2 \|\Delta v\|^2 + (1 - \delta_2) \|\theta\|^2 \leq c \|\nabla v\|^2. \tag{5.18}$$

Writing next

$$\|u\|_{-1}^2 = \left\| (-\Delta)^{\frac{1}{2}} (v - \varepsilon \Delta v) u \right\|_{-1}^2 = \|v\|_{-1}^2 + 2\varepsilon \|v\|^2 + \varepsilon^2 \|\nabla v\|^2,$$

it follows that, setting

$$E_3 = \delta_2 \|u\|_{-1}^2 + \|u + \theta\|_{-1}^2$$

an inequality of the form

$$\frac{dE_3}{dt} \leq \frac{c}{\varepsilon^2} E_3, \tag{5.19}$$

E_3 satisfies

$$E_3 \geq c' (\|u\|_{-1}^2 + \|\theta\|_{-1}^2), \quad c' > 0. \tag{5.20}$$

It follows from (5.19), (5.20) and Gronwall's lemma that

$$\|u(t)\|_{-1}^2 + \|\theta(t)\|_{-1}^2 \leq c' \exp\left(\frac{c}{\varepsilon^2} t\right) (\|u_0\|_{-1}^2 + \|\theta_0\|_{-1}^2), \quad t \geq 0, \tag{5.21}$$

finally yields the continuous (with respect to the $H^{-1}(\Omega)^2$ -norm) dependence on the initial data, as well as the uniqueness, for (u, v, θ) .

This yields uniform in time estimates (*i.e.*, on \mathbb{R}^+) on the solutions, as well as the dissipativity of the corresponding solution operators, we set

$$\Phi = H^1(\Omega) \times L^2(\Omega).$$

We have the continuous (with respect to the semigroup

$$S_\varepsilon(t): \Phi \rightarrow \Phi, (u_0, \theta_0) \mapsto (u^\varepsilon(t), \theta^\varepsilon(t)), t \geq 0, \varepsilon \in (0, \varepsilon_0]$$

(i.e., $S_\varepsilon(0) = I$ (identity operator) and $S_\varepsilon(t+s) = S_\varepsilon(t) \circ S_\varepsilon(s), t, s \geq 0$). We then deduce from (4.3) the following theorem.

Theorem 5.2. *The semigroup $S_\varepsilon(t)$ is dissipative in Φ , i.e., there exists a bounded set $\mathcal{B}_0 \subset \Phi$ (called absorbing set) such that, for every bounded set $\mathcal{B} \subset \Phi$, there exists $t_0 = t_0(\mathcal{B}) \geq 0$ such that $t \geq t_0$ implies $S_\varepsilon(t)\mathcal{B} \subset \mathcal{B}_0$.*

We thus deduce from standard results the following theorem.

Theorem 5.3. *The semigroup $S_\varepsilon(t)$ possesses the connected global attractor \mathcal{A}_ε such that \mathcal{A}_ε is compact in Φ , verifying:*

1. \mathcal{A}_ε is invariant, i.e., $S_\varepsilon(t)\mathcal{A}_\varepsilon = \mathcal{A}_\varepsilon, \forall t \geq 0$;
2. \mathcal{A}_ε attracts all bounded sets of initial data in the following sense:

$$\forall B \subset \Phi \text{ bounded, } \text{dist}(S_\varepsilon(t)B, \mathcal{A}_\varepsilon) \rightarrow 0 \text{ as } t \rightarrow +\infty,$$

where dist denotes the Hausdorff semi-distance between sets defined by

$$\text{dist}(A, B) = \sup_{a \in A} \inf_{b \in B} \|a - b\|_\Phi$$

(we refer the reader to, e.g., [18] for more details.)

The next step would be to study the existence of finite-dimensional attractors for $t \geq 0, \varepsilon \in (0, \varepsilon_0]$, and their stability with respect to ε , as well as their convergence to (proper $S_\varepsilon(t)$ liftings of) those corresponding to $S_\varepsilon(t)$ as $\varepsilon \rightarrow 0^+$. In particular, one interesting and important problem would be to construct a robust (i.e., both upper and lower semicontinuous as $\varepsilon \rightarrow 0^+$) family of exponential attractors, meaning that the dynamics of the original and limit problems are close in some proper sense. This will be addressed elsewhere. We also refer the interested reader to, e.g., [19] for discussions on such objects.

6. Convergence to the Classical Conserved Phase-Field Model

Our aim in this section is to pass to the limit in (2.1)-(2.5) as ε goes to 0^+ . Note that the limit problem for $\varepsilon = 0$ corresponds to the classical conserved phase-field model,

$$\frac{\partial u^0}{\partial t} + \Delta^2 v^0 - \Delta f(u^0) = -\Delta \theta^0, \quad (6.1)$$

$$u^0 = v^0, \quad (6.2)$$

$$\frac{\partial \theta^0}{\partial t} - \Delta \theta^0 = -\frac{\partial u^0}{\partial t}, \quad (6.3)$$

$$\frac{\partial u^0}{\partial \nu} = \frac{\partial v^0}{\partial \nu} = \frac{\partial \Delta v^0}{\partial \nu} = \frac{\partial \theta^0}{\partial \nu} = 0 \text{ on } \Gamma, \quad (6.4)$$

$$u^0|_{t=0} = u_0, \theta^0|_{t=0} = \theta_0. \quad (6.5)$$

To do so, we first need to derive estimates on the solutions to (2.1)-(2.5) which

are independent of ε (we consider here strong solutions as given in Theorem 5.1). We thus consider the initial and boundary value problem

$$\frac{\partial u^\varepsilon}{\partial t} + \Delta^2 v^\varepsilon - \Delta f(u^\varepsilon) = -\Delta \theta^\varepsilon, \tag{6.6}$$

$$u^\varepsilon = v^\varepsilon - \varepsilon \Delta v^\varepsilon, \tag{6.7}$$

$$\frac{\partial \theta^\varepsilon}{\partial t} - \Delta \theta^\varepsilon = -\frac{\partial u^\varepsilon}{\partial t}, \tag{6.8}$$

$$\frac{\partial u^\varepsilon}{\partial \nu} = \frac{\partial v^\varepsilon}{\partial \nu} = \frac{\partial \Delta v^\varepsilon}{\partial \nu} = \frac{\partial \theta^\varepsilon}{\partial \nu} = 0 \text{ on } \Gamma, \tag{6.9}$$

$$u^\varepsilon|_{t=0} = u_0, \theta^\varepsilon|_{t=0} = \theta_0, \tag{6.10}$$

Repeating, for (6.6)-(6.10), the estimates leading to (4.14), we obtain

$$\frac{dE_2^\varepsilon}{dt} + c \left(E_2^\varepsilon + \left\| \frac{\partial u^\varepsilon}{\partial t} \right\|_{-1}^2 + \|\theta^\varepsilon\|_{H^1(\Omega)}^2 + \|v^\varepsilon\|_{H^3(\Omega)}^2 \right) \leq c', \tag{6.11}$$

where

$$E_2^\varepsilon = E_1^\varepsilon + \delta_1 \|u^\varepsilon\|_{-1}^2 + \|u^\varepsilon\|^2$$

and

$$E_1^\varepsilon = \|\nabla v^\varepsilon\|^2 + \varepsilon \|\Delta v^\varepsilon\|^2 + 2 \int_\Omega F(u^\varepsilon) dx + \|\theta^\varepsilon\|^2. \tag{6.12}$$

We can now prove the following.

Theorem 6.1. *We assume that the assumptions of Theorem 5.1 hold. Then, the sequence of solutions $(u^\varepsilon, v^\varepsilon, \theta^\varepsilon)$ to (6.6)-(6.10) converges to a solution to (6.1)-(6.5) on finite time intervals $[0, T]$, $T > 0$, as $\varepsilon \rightarrow 0^+$.*

Proof. It follows from the uniform (with respect to ε) a priori estimates derived and standard Aubin-Lions compactness results that, at least for a subsequence that we do not relabel, there exist (u^0, v^0, θ^0) and χ such that, in particular,

$$u^\varepsilon \rightharpoonup u^0 \text{ in } L^\infty(0, T; L^4(\Omega)) \text{ weak-}\star, \text{ in } L^2(0, T; H^1(\Omega)) \text{ weakly and a.e.,}$$

$$\frac{\partial u^\varepsilon}{\partial t} \rightharpoonup \frac{\partial u^0}{\partial t} \text{ in } L^2(0, T; H^{-1}(\Omega)) \text{ weakly}$$

$$v^\varepsilon \rightharpoonup v^0 \text{ in } L^\infty(0, T; H^1(\Omega)) \text{ weak-}\star \text{ and } L^2(0, T; H^2(\Omega)) \text{ weakly,}$$

$$\varepsilon^{\frac{1}{2}} v^\varepsilon \rightharpoonup \chi \text{ in } L^\infty(0, T; H^2(\Omega)) \text{ weak-}\star \text{ and } L^2(0, T; H^3(\Omega)) \text{ weakly}$$

and

$$\theta^\varepsilon \rightharpoonup \theta^0 \text{ in } L^\infty(0, T; L^2(\Omega)) \text{ weak-}\star \text{ and } L^2(0, T; H^1(\Omega)) \text{ weakly.}$$

For a proper u , which implies that

$$f(u^\varepsilon) \rightarrow f(u^0) \text{ a.e. and } f(u^\varepsilon) \text{ is bounded in } L^{\frac{4}{3}}((\Omega) \times (0, T)).$$

Therefore, $f(u^\varepsilon) \rightarrow f(u^0)$ in $L^{\frac{4}{3}}((\Omega) \times (0, T))$ weakly, which is sufficient to

pass to the limit in the weak formulation.

Having this, it is now standard to pass to the limit in (6.6)-(6.10) to find, at the limit,

$$\frac{d}{dt}((u^0, \varphi)) + ((\Delta u^0, \Delta \varphi)) + ((\nabla f(u^0), \nabla \varphi)) = 0 \text{ in } \mathcal{D}'(\Omega), \tag{6.13}$$

$$\frac{d}{dt}((\theta^0, \varphi)) + ((\nabla \theta^0, \nabla \varphi)) = -\frac{d}{dt}((u^0, \varphi)) \text{ in } \mathcal{D}'(\Omega), \tag{6.14}$$

$$u^0|_{t=0} = u_0, \theta^0|_{t=0} = \theta_0 \tag{6.15}$$

i.e., (u^0, θ^0) is solution to the classical conserved phase-field model.

Noting finally that the solution to the classical conserved phase-field model (6.1)-(6.5) is unique, we see that the whole sequence $(u^\varepsilon, v^\varepsilon, \theta^\varepsilon)$ converges.

We can also derive error estimates and prove the following.

Theorem 6.2. *Under the assumptions of Theorem 6.1, then, $\forall T > 0$,*

$$\|u^\varepsilon - u^0\|_{-1}^2 + \|\theta^\varepsilon - \theta^0\|_{-1}^2 \leq c(\varepsilon, T) e^{cT} (\|u_0\|_{L^4(\Omega)}^2 + \|v_0\|_{H^2(\Omega)}^2 + \|\theta_0\|^2).$$

Proof. We set $(u, v, \theta) = (u^\varepsilon, v^\varepsilon, \theta^\varepsilon) - (u_0, v_0, \theta_0)$. Note that

$$\langle u \rangle = \langle v \rangle = \langle \theta \rangle = 0, \quad t \geq 0. \tag{6.16}$$

Furthermore, (u, v, θ) solves

$$(-\Delta)^{-1} \frac{\partial u}{\partial t} - \Delta v + \overline{f(u^\varepsilon)} - \overline{f(u^0)} = \theta, \tag{6.17}$$

$$u = v - \varepsilon \Delta v \tag{6.18}$$

$$\frac{\partial \theta}{\partial t} - \Delta \theta = \frac{\partial u}{\partial t} \tag{6.19}$$

$$\frac{\partial v}{\partial \nu} = \frac{\partial \theta}{\partial \nu} = 0 \text{ on } \Gamma, \tag{6.20}$$

$$u|_{t=0} = u_0, \theta|_{t=0} = \theta_0. \tag{6.21}$$

Multiplying (6.17) by u , we obtain, owing to (2.8),

$$\frac{d}{dt} \|u\|_{-1}^2 - 2((u, \Delta v)) \leq 3\|u\|^2 + \|\theta\|^2. \tag{6.22}$$

Note that, employing the interpolation inequality

$$\|u\|^2 \leq \|u\|_{-1} \|\nabla u\|$$

we can write, owing to (6.18),

$$\|u\|^2 \leq \|u\|_{-1} \|\nabla u\| + \|u\|_{-1} \|\nabla \Delta v^\varepsilon\|. \tag{6.23}$$

Moreover, employing again (6.18), we can see that

$$-2((u, \Delta v)) = 2\|\nabla v\|^2 - 2\varepsilon((\nabla v, \nabla \Delta v^\varepsilon)). \tag{6.24}$$

It thus follows from (6.22) to (6.24) that

$$\frac{d}{dt} \|u\|_{-1}^2 + 2\|\nabla v\|^2 \leq 3\|u\|_{-1} \|\nabla u\| + 3\|u\|_{-1} \|\nabla \Delta v^\varepsilon\| + 2\|\nabla v\| \|\nabla \Delta v^\varepsilon\| + \|\theta\|^2,$$

which yields, employing Young’s inequality,

$$\frac{d}{dt} \|u\|_{-1}^2 + \|\nabla v\|^2 \leq c \left(\|u\|_{-1}^2 + \varepsilon^2 \|\nabla \Delta v^\varepsilon\|^2 + \|\theta\|^2 \right). \tag{6.25}$$

Let us next multiply (6.19) by $(-\Delta)^{-1}(u + \theta)$ to obtain

$$\frac{d}{dt} \|u + \theta\|_{-1}^2 + \|\theta\|^2 \leq \|u\|^2. \tag{6.26}$$

Summing (6.25) and ε^2 times (6.26), we find

$$\frac{d}{dt} \left(\|u\|_{-1}^2 + \varepsilon^2 \|u + \theta\|_{-1}^2 \right) \leq c \left(\|u\|_{-1}^2 + \varepsilon^2 \|\nabla \Delta v^\varepsilon\|^2 + \varepsilon^2 \|u\|^2 \right), \quad c > 0, \tag{6.27}$$

where

$$\|u\|_{-1}^2 + \varepsilon^2 \|u + \theta\|_{-1}^2 \geq c \left(\|u\|_{-1}^2 + \|\theta\|_{-1}^2 \right). \tag{6.28}$$

Applying Gronwall’s lemma to (6.27), owing to (6.28) leads to

$$\|u(t)\|_{-1}^2 + \|\theta(t)\|_{-1}^2 \leq c\varepsilon^2 (1+T) e^{cT} \int_0^T \left(\|\nabla \Delta v^\varepsilon\|^2 + \|u\|^2 \right)(s) ds.$$

Integrating next (6.11) over $(0, T)$, we find

$$\int_0^T \left(\|\nabla \Delta v^\varepsilon\|^2 + \|u\|^2 \right)(s) ds \leq c \left(\|u_0\|_{L^4(\Omega)}^2 + \|v_0\|_{H^2(\Omega)}^2 + \|\theta_0\|^2 \right),$$

which finishes the proof.

Remark 6.1. According to (2.2), the error estimate on (u, θ) implies the error estimate on v .

7. Numerical Simulations

As far as the numerical simulations are concerned, we use a P1-finite element for the space discretization, together with a semi-implicit Euler time discretization (i.e., implicit for the linear terms and explicit for the nonlinear ones). The numerical simulations are performed with the software Freefem++ [20]. In the simulations below, we set $\Omega = (0,1) \times (0,1)$ and we choose $f(s) = s^3 - s$. The triangulation \mathcal{T}_h is obtained by dividing Ω into 100×100 rectangles and by dividing each rectangle along the same diagonal. We set

$$V_0^h = \left\{ v^h \in C^0(\bar{\Omega}); v^h|_T \text{ is affine } \forall T \in \mathcal{T}_h; \frac{\partial v^h}{\partial \nu} = 0 \text{ on } \Gamma \right\}.$$

The time step is taken as $\delta t = 0.001$.

In order to simulate a spinodal decomposition, the initial data u_0^h is taken as the projection onto V_0^h of a randomly distributed function between 0.5 and 0.7. The solution $u_h(\cdot, n\delta t) \in V_0^h$ is denoted by u_h^n .

The full discretization scheme of (2.1)-(2.4) reads: Then, for $n \geq 0$, we look for $(u_h^{n+1}, w_h^{n+1}, v_h^{n+1}, \theta_h^{n+1}) \in V^h \times V^h \times V^h \times V^h$ such that:

$$\begin{cases} \frac{1}{\delta t}((u_h^{n+1}, \phi)) + ((\nabla w_h^{n+1}, \nabla \phi)) - ((\nabla \theta_h^{n+1}, \nabla \phi)) = \frac{1}{\delta t}((u_h^n, \phi)), \\ ((w_h^{n+1}, \psi)) - ((\nabla v_h^{n+1}, \nabla \psi)) = -((f(u_h^n), \psi)), \\ ((u_h^{n+1}, \tau)) - ((v_h^{n+1}, \tau)) - \varepsilon((\nabla v_h^{n+1}, \nabla \tau)) = 0, \\ \frac{1}{\delta t}((u_h^{n+1}, \phi)) + \frac{1}{\delta t}((\theta_h^{n+1}, \phi)) + ((\nabla \theta_h^{n+1}, \nabla \phi)) = \frac{1}{\delta t}((\theta_h^n, \phi)) + \frac{1}{\delta t}((u_h^n, \phi)), \end{cases} \quad (7.1)$$

for all $\phi, \psi, \tau, \varphi \in V_h^0$.

Figure 1 corresponding to the fixed parameter $\varepsilon = 0.05$, show the evolution of θ_h , first part of the numerical solution $(u_h^n, v_h^n, \theta_h^n)$ to (7.1), at different times $t = 0.05$ ($n = 50$), $t = 0.1$ ($n = 100$).

Figure 2 and **Figure 3** correspond to the numerical solution θ_h at time $t = 0.1$ ($n = 100$), for different values of ε : $\varepsilon = 0.1$, $\varepsilon = 0.01$, $\varepsilon = 0.001$, $\varepsilon = 0$. It illustrates the fact that, as ε tends to 0, the solution (u_h, θ_h) tends to the solution of the classical conserved phase-field model (corresponding to the trivial case $\varepsilon = 0$).

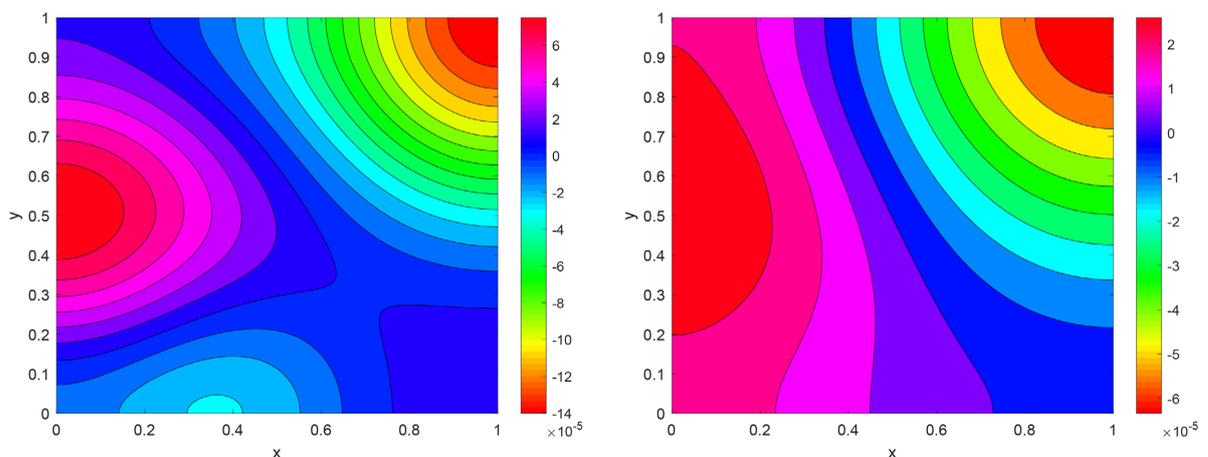


Figure 1. θ_h with $\varepsilon = 0.05$; at time $t = 0.05$ (left), $t = 0.1$ (right).

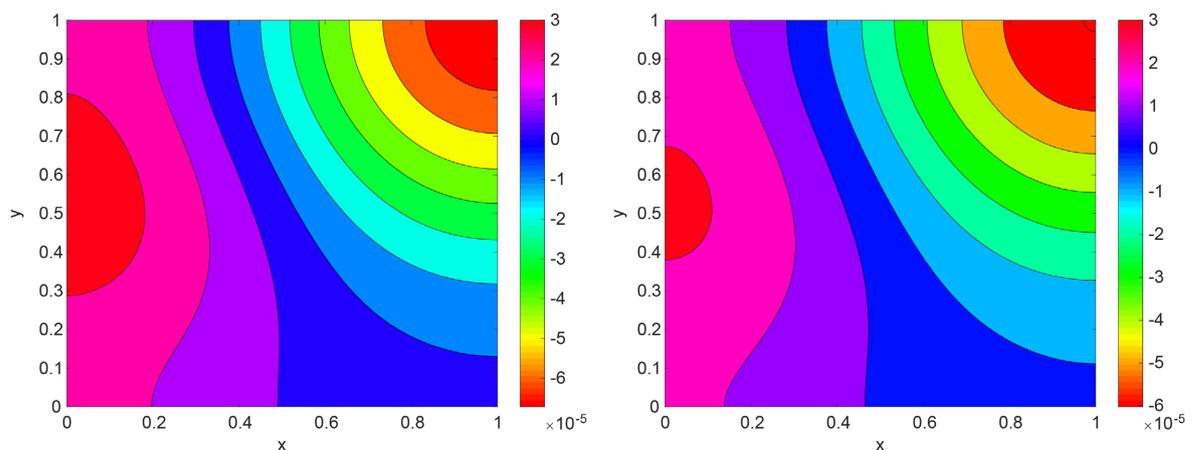


Figure 2. θ_h at time $t = 0.1$; when $\varepsilon = 0.1$ (left), $\varepsilon = 0.01$ (right).

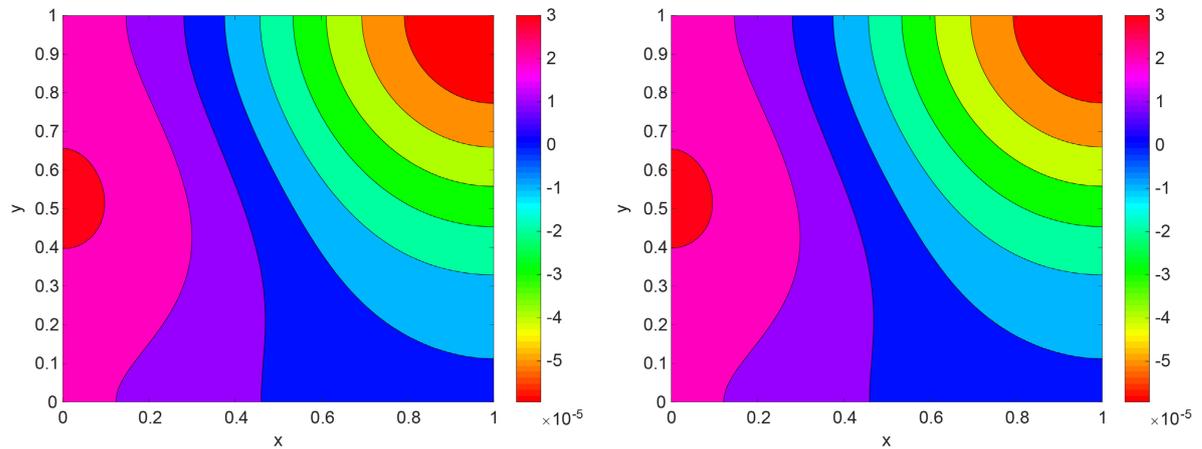


Figure 3. θ_h at time $t=0.1$; when $\varepsilon=0.001$ (left), $\varepsilon=0$ (right).

8. Conclusion

In this article, we proposed a conserved phase-field model based on microconcentrations. In particular, we proved the existence and uniqueness of solutions, as well as the convergence to the classical conserved phase-field model and the existence of the global attractor. Furthermore, we obtained some numerical simulations.

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Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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