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INITIAL BOUNDARY VALUE PROBLEM DESCRIBING A REAL EXPERIMENT RELATED TO THE SORET EFFECT

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Abstract. We focus on real experiments related to the Soret effect reported by Shimada-Sakai-Yamamoto-Watanabe [6] in which they arranged heat sources in a domain with complex structure to make temperature gradients. Our aims of this paper are to construct a mathematical model for their experiments and provide numerical solutions of the model by the finite volume method (FVM). Here, we note that a usual approximation way does not work well because of the complexity of the domain. Then, we have proposed a new approximation method in order to deal with the domain and discuss existence of weak solutions of the model and its approximation for numerical calculations.

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1 Introduction

As mentioned in Shimada-Sakai-Yamamoto-Watanabe [6], recently, local heating techniques are applied to several fields, for instance, medical therapy for tumor and molecular transport for DNA polymers in [5]. For development of the techniques, they focused on plasmon resonance and achieved to observed a temperature gradient by lighting nanometal (silver) particles arranged in a domain as shown in Figure 1.1. Moreover, due to private communications with Sakai and Shimada, Soret effects by plasmon resonance were observed in a mixed liquid in their experiments. We note that the Soret effect is well-known as a phenomenon on substance flow caused by temperature gradient in liquid. Thus, a main issue of the present paper is how to deal with the Soret effect on the domain with complex structure (Figure 1.1), numerically and theoretically.

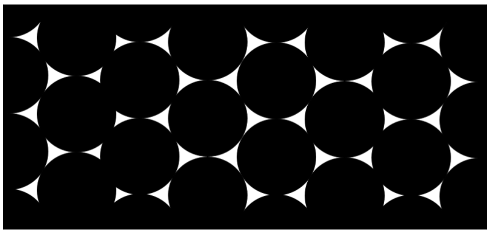

Figure 1.1: Domain structure

In [6], they also considered the following initial boundary value problem for the heat equation with boundary conditions and obtained numerical results: The problem is to find the temperature field θ on a domain $\mathbb{R}^2 \times (0, z_b) \subset \mathbb{R}^3$ for a given positive constant z_b satisfying

$$\begin{aligned} &C\theta_t = \text{ div } (\kappa\nabla\theta) + \theta_*\delta(z - z_h)s_p(x, y) \quad \text{ in } (0, T) \times \mathbb{R}^2 \times (0, z_b), \\ &\theta(t, x, y, z_b) = \theta_a, \ \theta(t, x, y, 0) = \theta_b \quad \text{ for } (t, x, y) \in (0, T) \times \mathbb{R}^2, \\ &\theta(0, x, y, z) = \theta_0(x, y, z) \quad \text{ for } (x, y, z) \in \mathbb{R}^2 \times (0, z_b), \end{aligned}$$

where $T > 0$, C and κ denote the heat capacity and the conductivity, respectively, θ_* is a given constant, δ is the delta function, s_p is a given periodic continuous function with respect to x and y, and θ_a, θ_b and θ_0 are given functions.

Thus, the diffusion of substance in the liquid was not considered in [6]. Therefore, we have proposed a new mathematical model describing the Soret effect by heating small metal (silver) particles in liquid. First, let $\Omega_1, \Omega_2 \subset \mathbb{R}^2$ be domains for liquid and metal (silver) regions, respectively, $\Omega = \Omega_1 \cup \Omega_2$, $\Omega_1 \cap \Omega_2 = \emptyset$ and $\Gamma = \partial\Omega_1 \backslash \partial\Omega$. In Figure 1.1 the black and white parts indicate liquid and metal regions, respectively. Here, in order to avoid difficulties concerned with mathematical and numerical analysis we reduce the dimension of the domain. Under consideration of the Soret and Dufour effects we have derived the following initial boundary value problem. Unknown functions of the problem are the temperature fields θ_1 and θ_2 in the liquid and metal regions, respectively, and the concentration u of some substance in the liquid. Also, θ_1, θ_2 and u satisfy

$$C_1\theta_{1t} = \text{div}(\kappa_1\nabla\theta_1 + d\theta_1\nabla u) + s_1(\theta_1) \quad \text{in } Q_1(T) := (0, T) \times \Omega_1, \tag{1.1}$$

$$C_2\theta_{2t} = \mathrm{div}(\kappa_2\nabla\theta_2) + s_2(\theta_2) \quad \text{in } Q_2(T) := (0,T)\times\Omega_2, \tag{1.2}$$
$$u_t = \mathrm{div}(k\nabla u + bu\nabla\theta_1) \quad \text{in } Q_1(T), \tag{1.3}$$
$$(\kappa_1\nabla\theta_1 + d\theta_1\nabla u)\cdot\nu = 0 \quad \text{on } S(T) := (0,T)\times\partial\Omega, \tag{1.4}$$
$$\theta_1 = \theta_2,\ (\kappa_1\nabla\theta_1 + d\theta_1\nabla u)\cdot\nu_1 + \kappa_2\nabla\theta_2\cdot\nu_2 = 0 \quad \text{on } S_2(T) := (0,T)\times\partial\Gamma, \tag{1.5}$$
$$(k\nabla u + bu\nabla\theta_1)\cdot\nu_1 = 0 \quad \text{on } S_2(T), \tag{1.6}$$
$$(k\nabla u + bu\nabla\theta_1)\cdot\nu = 0 \quad \text{on } S(T), \tag{1.7}$$
$$\theta_i(0,\cdot) = \theta_{0i} \quad \text{on } \Omega_i,\ i = 1,2, \tag{1.8}$$
$$u(0,\cdot) = u_0 \quad \text{on } \Omega_1, \tag{1.9}$$

where ν, ν_1 and ν_2 are the outward unit normal vectors on $\partial\Omega, \partial\Omega_1\backslash\partial\Omega$ and Γ, respectively, $C_1, C_2 > 0$ are specific heats of mixed liquid, metals and $\kappa_1, \kappa_2 > 0$ are the thermal conductivities of mixed liquid, metals, $k > 0$ is the diffusion coefficient, b and d are the Soret and Dufour coefficients, respectively, and θ_{01}, θ_{02} and u_0 are initial functions. Moreover, $s_1, s_2 : \mathbb{R} \to \mathbb{R}$ are Lipschitz continuous functions corresponding to heat sources. Example of s_i $(i = 1, 2)$ is

$$s_i(\theta) = -a_i(\theta - \theta_{\mathrm{sub}}) + q_i,$$

where $a_i > 0$ is a positive constant, θ_{sub} is the temperature of the bottom of the experimental device, and q_i is the known heat quantity obtained by lighting metals. As in (1.1), we impose the Dufour effect in our system, namely, we suppose that the heat flux depends on the substance flow in the liquid region. The other feature of the system is that we consider the diffraction type of boundary conditions (1.5). This type of the boundary conditions is sometimes called a transmission type and already studied well, for example, see [2, 3].

When we try to get numerical solutions of the above system (1.1)–(1.9) by application of the finite volume method (FVM), it is not easy to treat the diffraction type of boundary conditions. More precisely, we must adopt extrapolation to approximate ∇u on $S_2(T)$, since u is not defined in $Q_2(T)$. It is known that the extrapolation gives us a bad approximation. In order to overcome this difficulty we introduce a dummy function u_2 of the concentration in $Q_2(T)$ in the following way: For $\varepsilon > 0$ we consider

$$C_1\theta_{1t} = \mathrm{div}(\kappa_1\nabla\theta_1 + d\theta_1\nabla u_1) + s_1(\theta_1) \quad \text{in } Q_1(T), \tag{1.10}$$
$$C_2\theta_{2t} = \mathrm{div}(\kappa_2\nabla\theta_2 + \varepsilon\nabla u_2) + s_2(\theta_1) \quad \text{in } Q_2(T), \tag{1.11}$$
$$u_{1t} = \mathrm{div}(k\nabla u_1 + bu_1\nabla\theta_1) \quad \text{in } Q_1(T), \tag{1.12}$$
$$u_{2t} = \varepsilon\mathrm{div}(\nabla u_2) \quad \text{in } Q_2(T), \tag{1.13}$$
$$(\kappa_1\nabla\theta_1 + d\theta_1\nabla u_1)\cdot\nu = 0 \quad \text{on } S(T), \tag{1.14}$$
$$\theta_1 = \theta_2,\ (\kappa_1\nabla\theta_1 + d\theta_1\nabla u)\cdot\nu_1 + (\kappa_2\nabla\theta_2 + \varepsilon\nabla u_2)\cdot\nu_2 = 0 \quad \text{on } S_2(T), \tag{1.15}$$
$$(k\nabla u_1 + bu_1\nabla\theta_1)\cdot\nu_1 + \varepsilon\nabla u_2 = 0 \quad \text{on } S_2(T), \tag{1.16}$$
$$(k\nabla u_1 + bu_1\nabla\theta_1)\cdot\nu = 0 \quad \text{on } S(T), \tag{1.17}$$
$$\theta_i(0,\cdot) = \theta_{0i} \text{ and } u_i(0,\cdot) = u_{0i} \quad \text{on } \Omega_i,\ i = 1,2, \tag{1.18}$$

where u_{0i} is a given initial function on Ω_i for each $i = 1, 2$.

One of main results of this paper is to show that our approximation method seems to be correct from numerical results (see Section 4).

The other main results are concerned with existence of solutions to our systems (1.1)–(1.9) and (1.10)–(1.18). Since we impose the Soret and Dufour effects, the cross diffusion terms appear in these two systems and its mathematical treatments are not easy. Hence, as a first step of theoretical parts in this research we suppose to neglect the Dufour effect. Namely, we get:

$$C_i\theta_{it} = \mathrm{div}(\kappa_i\nabla\theta_i) + s_i(\theta_i) \quad \text{in } Q_i(T),\ i = 1, 2, \tag{1.19}$$

$$u_t = \mathrm{div}(k\nabla u + bu\nabla\theta_1) \quad \text{in } Q_1(T), \tag{1.20}$$

$$\kappa_1\nabla\theta_1 \cdot \nu = 0 \quad \text{on } S(T),$$

$$\theta_1 = \theta_2,\ \kappa_1\nabla\theta_1 \cdot \nu_1 + \kappa_2\nabla\theta_2 \cdot \nu_2 = 0 \quad \text{on } S_2(T), \tag{1.21}$$

$$(k\nabla u + bu\nabla\theta_1) \cdot \nu_1 = 0 \quad \text{on } S_2(T), \tag{1.22}$$

$$(k\nabla u + bu\nabla\theta_1) \cdot \nu = 0 \quad \text{on } S(T), \tag{1.23}$$

$$\theta_i(0, \cdot) = \theta_{0i} \quad \text{on } \Omega_i,\ i = 1, 2,$$

$$u(0, \cdot) = u_0 \quad \text{on } \Omega_1. \tag{1.24}$$

Clearly, θ_1 and θ_2 are independent of u, namely, we can determine a pair of θ_1 and θ_2 as a solution of the initial boundary value problem for a semilinear equation (1.19) with the diffraction type of boundary condition (1.21). Hence, we assume that θ_1 and θ_2 are given functions in Sections 2 and 3. Accordingly, we will consider the system (1.20), (1.21), (1.22), (1.23) and (1.24).

From classical results on the diffraction problem, we note that we do not expect that $\theta \in L^2(0, T; H^2(\Omega))$, where $\theta = \chi_1\theta_1 + \chi_2\theta_2$ and χ_i is the characteristic function of Ω_i for each $i = 1, 2$. Hence, $\nabla\theta_1 \in L^\infty(0, T; L^2(\Omega_1)^2)$ is a reasonable assumption for θ_1 from the theory for the diffraction problem. Under this assumption, a mathematical treatment of the term bu appearing in (1.20) is still so hard since it is unbounded that we approximate this term by using a cut-off function σ_M for $M > 0$ and obtain the following problem

$$(\mathrm{P})_M : \quad \begin{cases} u_t = \mathrm{div}(k\nabla u + \sigma_M(u)\nabla\theta_1) \quad \text{in } Q_1(T), \\ (k\nabla u + \sigma_M(u)\nabla\theta_1) \cdot \nu_1 = 0 \quad \text{on } S_1(T), \\ (k\nabla u + \sigma_M(u)\nabla\theta_1) \cdot \nu = 0 \quad \text{on } S(T), \\ u(0, \cdot) = u_0 \quad \text{on } \Omega_1, \end{cases}$$

where

$$\sigma_M(u) = \begin{cases} bM \quad \text{for } u > M, \\ bu \quad \text{for } |u| \le M, \\ -bM \quad \text{for } u < -M. \end{cases}$$

From a physical point of view, the concentration u is a bounded function so that this approximation is not restrictive.

Similarly, for each $\varepsilon > 0$ we can derive the following problem $(\mathrm{P})_M(\varepsilon)$ from (1.10)–

(1.18):

$$(\mathrm{P})_M(\varepsilon): \quad \begin{cases} u^\varepsilon_{1t} = \mathrm{div}(k\nabla u^\varepsilon_1 + bu^\varepsilon_1\nabla\theta_1) \quad \text{in } Q_1(T), \\ u^\varepsilon_{2t} = \varepsilon \mathrm{div}\nabla u^\varepsilon_2 \quad \text{in } Q_2(T), \\ u^\varepsilon_1 = u^\varepsilon_2,\ (k\nabla u^\varepsilon_1 + bu^\varepsilon_1\nabla\theta_1)\cdot\nu_1 + \varepsilon\nabla u^\varepsilon_2\cdot\nu_2 = 0 \text{ on } S_2(T), \\ (k\nabla u^\varepsilon_1 + bu^\varepsilon_1\nabla\theta_1)\cdot\nu = 0 \quad \text{on } S(T), \\ u^\varepsilon_1(0,\cdot) = u_0 \quad \text{on } \Omega_1, u^\varepsilon_2(0,\cdot) = u_0 \quad \text{on } \Omega_2. \end{cases}$$

Here, we remark that by lack of regularity for θ_1 we could not prove uniqueness of solutions to $(\mathrm{P})_M$ and $(\mathrm{P})_M(\varepsilon)$, even if θ_1 is given. Accordingly, we also do not obtain a convergence result for solutions of $(\mathrm{P})_M(\varepsilon)$, when ε tends to 0. In future works we will try to establish uniqueness and convergence by applying results concerned with high regularity of θ_1 discussed in [2]. Moreover, we may treat the system (1.20), (1.21), (1.22), (1.23) and (1.24) without the cut-off function in this case.

In Section 2 of this paper, we give assumptions and main mathematical results, and shall prove existence of solutions of $(\mathrm{P})_M$ and $(\mathrm{P})_M(\varepsilon)$ in Section 3. In the final section we provide numerical results.

2 Main results

Notation. We use the spaces $H_1 := L^2(\Omega_1)$, $H := L^2(\Omega)$, $V_1 := W^{1,2}(\Omega_1)$, $V := W^{1,2}(\Omega)$, with respective standard norms, for instance $|\cdot|_{H_1}$, $|\cdot|_{V_1}$. Moreover, V_1^* and V^* denote the dual spaces of V_1 and V, respectively and the pairing between V_1 and V_1^* by $\langle\cdot,\cdot\rangle_{V_1^*}$. Also, for $u \in H_1$ we can write

$$\langle u, \eta\rangle_{V_1^*} = \int_{\Omega_1} u\eta\, dx \quad \text{for all } \eta \in V_1.$$

Furthermore, we define an inner product of V_1 by

$$(u,v)_{V_1} := k\int_{\Omega_1} \nabla u\cdot\nabla v\, dx + \left(\int_{\Omega_1} u\, dx\right)\left(\int_{\Omega_1} v\, dx\right) \quad \text{for all } u, v \in V_1. \tag{2.1}$$

Let $F : V_1 \to V_1^*$ be the duality mapping, namely,

$$\langle Fu, v\rangle_{V_1^*} = (u,v)_{V_1} \text{ and } |Fu|_{V_1^*} = |u|_{V_1} \quad \text{for } u, v \in V_1.$$

Then, we can define the inner product of V_1^* by

$$(u,v)_{V_1^*} := \langle u, F^{-1}v\rangle \quad \text{for } u, v \in V_1^*. \tag{2.2}$$

Definition 2.1. For $M > 0$ a function $u : [0,T] \to H_1$ is called a weak solution of $(\mathrm{P})_M$ on $[0,T]$ if

$$u \in L^2(0,T;V_1) \cap L^\infty(0,T;H_1) \cap W^{1,2}(0,T;V_1^*),$$
$$\langle u_t^*, \eta\rangle_{V_1^*} = -\int_{\Omega_1} (k\nabla u + \sigma_M(u)\nabla\theta_1)\nabla\eta\, dx \quad \text{for all } \eta \in V_1 \text{ a.e. on } [0,T],$$
$$u(0,\cdot) = u_0 \quad \text{on } \Omega_1.$$

The first mathematical result is:

Theorem 2.1. *Let $T > 0$ and $M > 0$. If $u_0 \in H_1$ and $\nabla\theta_1 \in L^\infty(0,T;H_1^2)$, then there exists a weak solution u of $(P)_M$ on $[0,T]$.*

Next, in order to define a weak solution of $(\mathrm{P})_M(\varepsilon)$ we put

$$u^\varepsilon = \chi_1 u_1^\varepsilon + \chi_2 u_2^\varepsilon.$$

Definition 2.2. For $M > 0$ and $\varepsilon > 0$ a function $u^\varepsilon : [0,T] \to H$ is called a weak solution of $(\mathrm{P})_M(\varepsilon)$ on $[0,T]$, if

$$u^\varepsilon \in L^2(0,T;V) \cap L^\infty(0,T;H) \cap W^{1,2}(0,T;V^*),$$
$$\langle u_t^\varepsilon, \eta\rangle_{V^*} = -\int_{\Omega_1} (k\nabla u_1^\varepsilon + \sigma_M(u_1^\varepsilon)\nabla\theta_1)\nabla\eta\, dx - \varepsilon\int_{\Omega_2} \nabla u_2^\varepsilon \nabla\eta\, dx \text{ for } \eta \in V \text{ a.e. on } [0,T],$$
$$u_1^\varepsilon(0,\cdot) = u_0 \quad \text{on} \quad \Omega_1, u_2^\varepsilon(0,\cdot) = c \quad \text{on} \quad \Omega_2.$$

Theorem 2.2. *Let $T > 0$, $M > 0$ and $\varepsilon > 0$. If $u_0 \in H$ and $\nabla\theta_1 \in L^\infty(0,T;H_1^2)$, then there exists a weak solution u^ε of $(\mathrm{P})_M(\varepsilon)$ on $[0,T]$.*

Theorem 2.2 can be proved in a similar way as Theorem 2.1. Therefore, we omit a proof of Theorem 2.2.

3 Proof of existence for solutions

We have to go through several steps to prove Theorem 2.1. At first, since $\nabla\theta_1 = \left(\frac{\partial\theta_1}{\partial x}, \frac{\partial\theta_1}{\partial y}\right) \in L^2(0,T;H_1^2)$, we take $\{a_{1\epsilon}\}, \{a_{2\epsilon}\} \subset C^\infty(\overline{(0,T)\times\Omega_1})$ such that

$$a_{1\epsilon} \to \frac{\partial\theta_1}{\partial x}, a_{2\epsilon} \to \frac{\partial\theta_1}{\partial y} \quad \text{in } L^2(0,T;H_1) \text{ as } \epsilon \to 0. \tag{3.1}$$

Then it is easy to see that for each $\epsilon > 0$ there exists $K_\epsilon > 0$ such that

$$|a_\epsilon|_{L^\infty(\Omega_1)^2} \le K_\epsilon.$$

Here, we put $a_\epsilon = (a_{1\epsilon}, a_{2\epsilon})$ and denote by $(\mathrm{P})_\epsilon$ the following problem:

$$\begin{cases} u_t = \operatorname{div}(k\nabla u + \sigma_M(u)a_\epsilon) & \text{in } Q_1(T), \\ (k\nabla u + \sigma_M(u)a_\epsilon)\cdot\nu_1 = 0 & \text{on } S_1(T), \\ (k\nabla u + \sigma_M(u)a_\epsilon)\cdot\nu = 0 & \text{on } S(T), \\ u(0,\cdot) = u_0 & \text{on } \Omega_1. \end{cases}$$

Next, for $u_0 \in H_1$ we take $\{u_{0\ell}\} \subset C^\infty(\overline{\Omega_1})$ such that $u_{0\ell} \to u_0$ in H_1 as $\ell \to \infty$, and we denote by $(\mathrm{P})_{\epsilon,\ell}$ the following problem:

$$\begin{cases} u_t = \operatorname{div}(k\nabla u + \sigma_M(u)a_\epsilon) & \text{in } Q_1(T), \\ (k\nabla u + \sigma_M(u)a_\epsilon)\cdot\nu_1 = 0 & \text{on } S_1(T), \\ (k\nabla u + \sigma_M(u)a_\epsilon)\cdot\nu = 0 & \text{on } S(T), \\ u(0,\cdot) = u_{0\ell} & \text{on } \Omega_1. \end{cases}$$

Moreover, for $\tilde{u} \in L^2(0,T;H_1)$ we consider the auxiliary problem $(\mathrm{AP})_{\epsilon,\ell}(\tilde{u})$ to solve $(\mathrm{P})_{(\epsilon,\ell)}$ in the following way:

$$(\mathrm{AP})_{\epsilon,\ell}(\tilde{u}) \begin{cases} u_t = \mathrm{div}(k\nabla u + \sigma_M(\tilde{u})a_\epsilon) & \text{in } Q_1(T), \\ (k\nabla u + \sigma_M(\tilde{u})a_\epsilon)\cdot \nu_1 = 0 & \text{on } S_1(T), \\ (k\nabla u + \sigma_M(\tilde{u})a_\epsilon)\cdot \nu = 0 & \text{on } S(T), \\ u(0,\cdot) = u_{0\ell} & \text{on } \Omega_1. \end{cases}$$

Finally, we approximate $\tilde{u}$ by $\tilde{u}_m$ to prove existence of solutions of $(\mathrm{AP})_{\epsilon,\ell}(\tilde{u})$. For $\tilde{u} \in L^2(0,T;H_1)$, there exists $\{\tilde{u}_m\} \subset C^\infty(\overline{(0,T)\times\Omega_1})$ such that $\tilde{u}_m \to \tilde{u}$ in $L^2(0,T;H_1)$ as $m \to \infty$.

By the classical theory for parabolic equations, for instance [1], for $m = 1,2,\dots$ there exists one and only one $u_m \in W^{1,2}(0,T;H_1) \cap L^\infty(0,T;V_1) \cap L^2(0,T;W^{2,2}(\Omega_1))$ satisfying

$$\int_{\Omega_1} u_{mt}\eta \, dx = -\int_{\Omega_1} (k\nabla u_m + \sigma_M(\tilde{u}_m)a_\epsilon)\nabla\eta \, dx \text{ for all } \eta \in V_1 \text{ a.e. in } [0,T], \tag{3.2}$$
$$u_m(0,\cdot) = u_{0\ell} \quad \text{on } \Omega_1.$$

The first lemma is concerned with the existence of a weak solution to $(\mathrm{AP})_{\epsilon,\ell}(\tilde{u})$ for $\tilde{u} \in L^2(0,T;H_1)$.

Lemma 3.1. *Let $\epsilon > 0$ and $\ell = 1,2,\dots$ If $\tilde{u} \in L^2(0,T;H_1)$, there exists a weak solution u of $(AP)_{\epsilon,\ell}(\tilde{u})$ such that*

$$\begin{aligned} & u \in L^2(0,T;V_1) \cap L^\infty(0,T;H_1) \cap W^{1,2}(0,T;V_1^*)(\subset C([0,T];V_1^*)), \\ & \langle u_t^*, \eta\rangle_{V_1^*} = -\int_{\Omega_1} (k\nabla u + \sigma_M(\tilde{u})a_\epsilon)\nabla\eta \, dx \textit{ for } \eta \in V_1 \textit{ a.e. on } [0,T], \\ & u_m(0,\cdot) = u_{0\ell} \quad \textit{on } \Omega_1. \end{aligned}$$

Proof. For each m by putting $\eta = u_m$ in (3.2) we have

$$\int_{\Omega_1} u_{mt}u_m \, dx = -\int_{\Omega_1} (k\nabla u_m + \sigma_M(\tilde{u}_m)a_\epsilon)\nabla u_m \, dx \quad \text{a.e. on } [0,T].$$

Therefore we get

$$\begin{aligned} \frac{1}{2}\frac{d}{dt}\int_{\Omega_1} |u_m|^2 \, dx + \frac{k}{2}\int_{\Omega_1} |\nabla u_m|^2 \, dx & \le \frac{1}{2k}\int_{\Omega_1} |\sigma_M(\tilde{u}_m)|^2 |a_\epsilon|^2 \, dx \\ & \le \frac{|bM|^2}{2k}|a_\epsilon|_{H_1} \text{ a.e. on } [0,T]. \end{aligned}$$

By integrating it over $[0,t]$, we obtain

$$\begin{aligned} & \int_{\Omega_1} |u_m(t)|^2 \, dx + k\int_0^t \int_{\Omega_1} |\nabla u_m(t)|^2 \, dxdt \\ \le & \int_{\Omega_1} |u_m(0)|^2 \, dx + \frac{|bM|^2}{2k}\int_0^T |a_\epsilon(\tau)|_{H_1} d\tau \quad \text{for } t \in [0,T]. \end{aligned}$$

This yields that there exists a $C_1 > 0$ such that

$$|u_m|_{H_1}^2 \le C_1 \text{ on } [0,T] \text{ and } \int_0^T |\nabla u_m(t)|_{H_1}^2\, dt \le C_1 \quad \text{for } m = 1,2,\dots$$

For all $v \in V_1$ (3.2) implies that

$$\begin{aligned} |\langle u_{mt}, v\rangle_{V_1^*}| &= \left|\int_{\Omega_1} u_{mt} v\, dx\right| \\ &\le \int_{\Omega_1} (k|\nabla u_m| + |\sigma_M(\tilde{u}_m) a_\epsilon||\nabla v|)\, dx \\ &\le (k|\nabla u_m|_{H_1} + |bM||a_\epsilon|_{H_1})|v|_{V_1} \quad \text{a.e. on } [0,T]. \end{aligned}$$

Thus, we get

$$|u_{mt}(t)|_{V_1^*} \le k|\nabla u_m(t)|_{H_1} + |bM||a_\epsilon(t)|_{H_1} \quad \text{for a.e. } t \in [0,T],$$

and there exists a $C_2 > 0$ such that

$$\int_0^T |u_{mt}(t)|_{V_1^*}^2\, dt \le C_2 \quad \text{for all } m.$$

Since $\{u_m\}$ is bounded in $L^\infty(0,T;H_1) \cap L^2(0,T;V_1) \cap W^{1,2}(0,T;V_1^*)$, by applying Aubin's compact theorem (cf. [4]) we can take a subsequence $\{m_j\}$ and $u \in L^\infty(0,T;H_1) \cap L^2(0,T;V_1) \cap W^{1,2}(0,T;V_1^*)$ such that $u_{m_j} \to u$ weakly in $L^2(0,T;V_1), W^{1,2}(0,T;V_1^*)$, weakly* in $L^\infty(0,T;H_1)$, and in $L^2(0,T;H_1)$ as $j \to \infty$. Moreover, since the dual space H_1^* of H_1 is compactly embedded into V_1^*, we may consider that

$$u_{m_j} \to u \text{ in } C([0,T];V_1^*) \text{ as } j \to \infty. \tag{3.3}$$

Let $\eta \in L^2(0,T;V_1)$. On account of Lipschitz continuity of σ_M we have

$$\begin{aligned} &\left|\int_0^T \int_{\Omega_1} \sigma_M(\tilde{u}_{m_j}) a_\epsilon \nabla\eta\, dxdt - \int_0^T \int_{\Omega_1} \sigma_M(\tilde{u}) a_\epsilon \nabla\eta\, dxdt\right| \\ \le\ & K_\epsilon \int_0^T \int_{\Omega_1} |\sigma_M(\tilde{u}_{m_j}) - \sigma_M(\tilde{u})||\nabla\eta|\, dxdt \to 0\ (j \to \infty). \end{aligned}$$

Now, it holds

$$\int_0^T \int_{\Omega_1} u_{mt}\eta\, dxdt + \int_0^T \int_{\Omega_1} (k\nabla u_m + \sigma_M(\tilde{u}_m) a_\epsilon)\nabla\eta\, dxdt = 0,$$

for all $\eta \in L^2(0,T;V_1)$ and $m = 1.2,\dots$ Therefore, the above convergences guarantee that Lemma 3.1 is true. □

Lemma 3.2. *Let $\epsilon > 0$ and $\ell = 1,2,\dots$ For $\tilde{u} \in L^2(0,T;H_1)$ the problem $(AP)_{\epsilon,\ell}(\tilde{u})$ has at most one weak solution.*

Proof. For $\tilde{u} \in L^2(0,T;H_1)$ let u_1 and u_2 be solutions of $(\mathrm{AP})_{\epsilon,\ell}(\tilde{u})$. Then, it holds that

$$\langle u_{it}, \eta \rangle_{V_1^*} = -\int_{\Omega_1} (k\nabla u_i + \sigma_M(\tilde{u})a_\epsilon)\nabla\eta \, dx \text{ a.e. on } [0,T] \text{ for } \eta \in V_1, i = 1,2. \tag{3.4}$$

Easily, we get

$$\langle u_{1t} - u_{2t}, \eta \rangle_{V_1^*} = -\int_{\Omega_1} k\nabla(u_1 - u_2)\nabla\eta \, dx \text{ a.e. on } [0,T] \text{ for } \eta \in V_1, i = 1,2. \tag{3.5}$$

Here, we substitute $\eta = F^{-1}(u_1 - u_2) \in V_1$ into (3.5). Then by (2.1) and (2.2) we have

$$\begin{aligned} &((u_1 - u_2)_t, u_1 - u_2)_{V_1^*} + (u_1 - u_2, F^{-1}(u_1 - u_2))_{V_1} \\ =& \left(\int_{\Omega_1} (u_1 - u_2) \, dx\right)\left(\int_{\Omega_1} F^{-1}(u_1 - u_2) \, dx\right) \quad \text{a.e. on } [0,T], \end{aligned}$$

and

$$\begin{aligned} &\frac{1}{2}\frac{d}{dt}|u_1 - u_2|^2_{V_1^*} + \langle u_1 - u_2, u_1 - u_2 \rangle_{V_1^*} \\ =& \left(\int_{\Omega_1} (u_1 - u_2) \, dx\right)\left(\int_{\Omega_1} F^{-1}(u_1 - u_2) \, dx\right) \quad \text{a.e. on } [0,T]. \end{aligned}$$

Here, we note that

$$\langle u_1 - u_2, u_1 - u_2 \rangle_{V_1^*} = \int_{\Omega_1} |u_1 - u_2|^2 \, dx \quad \text{a.e. on } [0,T].$$

Also, by taking $\eta = 1$ in (3.5) we see that $\langle u_{it}, 1 \rangle_{V_*} = 0$ a.e. on $[0,T]$ so that $\langle u_1 - u_2, 1 \rangle_{V_1^*} = 0$ on $[0,T]$. Hence, we observe that

$$\begin{aligned} &\left(\int_{\Omega_1} F^{-1}(u_1 - u_2) \, dx\right)\left(\int_{\Omega_1} 1 \, dx\right) \\ =& (F^{-1}(u_1 - u_2), 1)_{V_1} - k\int_{\Omega_1} \nabla F^{-1}(u_1 - u_2) \cdot \nabla 1 \, dx \\ =& \langle u_1 - u_2, 1 \rangle_{V_1^*} = 0 \quad \text{on } [0,T]. \end{aligned}$$

Thus, we obtain

$$\frac{1}{2}\frac{d}{dt}|u_1^* - u_2^*|^2_{V_1^*} + \int_{\Omega_1} |u_1 - u_2|^2 \, dx = 0.$$

Now, by integrating it over $[0,T]$ we conclude that $u_1 = u_2$ a.e. on $Q_1(T)$. □

Lemma 3.3. *Let* $\epsilon > 0$ *and* $\ell = 1,2,\ldots$ $(P)_{\epsilon,\ell}$ *has a unique weak solution on* $[0,T]$.

Proof. Lemmas 3.1 and 3.2 implies that for any $\tilde{u} \in L^2(0,T;H_1)$ there exists one and only one weak solution of $(\mathrm{AP})_{\epsilon,\ell}(\tilde{u})$. Then, we can define a function $\Lambda : L^2(0,T;H_1) \to L^2(0,T;H_1)$ by $\Lambda\tilde{u} = u$.

Let $\tilde{u}$ and $\tilde{u}' \in L^2(0,T;H_1)$, there exist $\{\tilde{u}_m\}$ and $\{\tilde{u}'_m\} \subset C^\infty(\overline{(0,T)\times\Omega_1})$ such that

$$\tilde{u}_m \to \tilde{u},\ \tilde{u}'_m \to \tilde{u}' \text{ in } L^2(0,T;H_1) \text{ as } m \to \infty. \tag{3.6}$$

By putting $\Lambda\tilde{u}_m = u_m$ and $\Lambda\tilde{u} = u$ we have

$$u_m(t) \to u(t) \text{ weakly in } H_1 \text{ as } m \to \infty \text{ for } t \in [0,T]. \tag{3.7}$$

In fact, on account of (3.3) and the uniqueness of a solution to $(\mathrm{AP})_{\epsilon,\ell}(\tilde{u})$ we see that

$$u_m \to u \text{ in } C([0,T];V_1^*) \text{ as } m \to \infty.$$

Let $t \in [0,T]$ and $\eta \in H_1$ and take $\{\eta_i\} \subset V_1$ such that $\eta_i \to \eta$ in H_1 as $i \to \infty$. Since $\{u_m\}$ is bounded in $L^\infty(0,T;H_1)$ as in the proof of Lemma 3.1, it is obvious that

$$\begin{aligned}
&\left|\int_{\Omega_1}(u_m(t)-u_{m'}(t))\eta\,dx\right| \\
\le\ &\left|\int_{\Omega_1}(u_m(t)-u_{m'}(t))\eta_i\,dx\right| + \left|\int_{\Omega_1}(u_m(t)-u_{m'}(t))(\eta_i^\eta)\,dx\right| \\
\le\ &|u_m(t)-u_{m'}(t)|_{V_1^*}|\eta_i|_{V_1} + (|u_m(t)|_{H_1}+|u_{m'}(t)|_{H_1})|\eta_i-\eta|_{H_1} \to 0 \text{ as } m,m' \to \infty.
\end{aligned}$$

Therefore, from $H_1^* \subset V_1^*$ it follows the convergence (3.7). Similarly, the same convergence for $\Lambda\tilde{u}'_m = u'_m$, $\Lambda\tilde{u}' = u'$ holds.

Now, we show that for some $l \in \mathbb{N}$, Λ^l is a contraction mapping. Indeed, for $m = 1,2,\dots$ we have

$$\begin{aligned}
&\int_{\Omega_1}(u_{mt}-u'_{mt})(u_m-u'_m)\,dx + \int_{\Omega_1}k\nabla(u_m-u'_m)\nabla(u_m-u'_m)\,dx \\
=\ &-\int_{\omega_1}(\sigma_M(\tilde{u}_m-\tilde{u}'_m))a_\epsilon\nabla(u_m-u'_m)\,dx \quad \text{a.e. on } [0,T],
\end{aligned}$$

and

$$\begin{aligned}
&\frac{1}{2}\frac{d}{dt}|u_m(t)-u'_m(t)|_{H_1}^2 + k\int_{\Omega_1}|\nabla(u_m-u'_m)|^2\,dx \\
\le\ &\int_{\Omega_1}M|\tilde{u}_m-\tilde{u}'_m||a_\epsilon||\nabla(u_m-u'_m)|\,dx \\
\le\ &\int_{\Omega_1}\left(\frac{k}{2}|\nabla(u_m-u'_m)|^2+\frac{M^2}{2k}|\tilde{u}_m-\tilde{u}'_m|^2|a_\epsilon|^2\right)dx \\
\le\ &\frac{k}{2}\int_{\Omega_1}|\nabla(u_m-u'_m)|^2\,dx + \frac{M^2}{2k}K_\epsilon^2\int_{\Omega_1}|\tilde{u}_m-\tilde{u}'_m|^2\,dx \quad \text{for a.e. } t \in [0,T].
\end{aligned}$$

Thus, we get

$$\frac{1}{2}|u_m(t)-u'_m(t)|_{H_1}^2 + \frac{k}{2}\int_0^t\int_{\Omega_1}|\nabla(u_m-u'_m)|^2\,dxd\tau$$

$$\leq \frac{M^2}{2k} K_\epsilon^2 \int_0^t |\tilde{u}_m - \tilde{u}'_m|_{H_1}^2 \; d\tau \quad \text{ for } t \in [0,T].$$

Therefore, there exists a $C_3 > 0$ such that

$$|u_m(t) - u'_m(t)|_{H_1}^2 \leq C_3 \int_0^t |\tilde{u}_m - \tilde{u}'_m|_{H_1}^2 \; d\tau \quad \text{ for } t \in [0,T] \text{ and } m.$$

Easily, we obtain

$$\liminf_{m\to\infty} |u_m(t) - u'_m(t)|_{H_1}^2 \leq C_3 \liminf_{m\to\infty} \int_0^t |\tilde{u}_m - \tilde{u}'_m|_{H_1}^2 \; d\tau.$$

By (3.6) and (3.7) we infer that

$$|u(t) - u'(t)|_{H_1}^2 \leq C_3 \int_0^t |\tilde{u} - \tilde{u}'|_{H_1}^2 d\tau \text{ for } t \in [0,T],$$

that is,

$$|\Lambda(\tilde{u})(t) - \Lambda(\tilde{u}')(t)|_{H_1}^2 \leq C_3 \int_0^t |\tilde{u} - \tilde{u}'|_{H_1}^2 d\tau \text{ for } t \in [0,T].$$

By applying this inequality, we have

$$\begin{aligned} |\Lambda^2(\tilde{u})(t) - \Lambda^2(\tilde{u}')(t)| &= |\Lambda(\Lambda(\tilde{u})(t)) - \Lambda(\Lambda(\tilde{u}')(t))|_{H_1}^2 \\ &\leq C_3 \int_0^t |\Lambda(\tilde{u})(\tau) - \Lambda(\tilde{u}')(\tau)|_{H_1}^2 \; d\tau \\ &\leq C_3^2 \int_0^t \int_0^t |\tilde{u}(t) - \tilde{u}'(t)|_{H_1}^2 \; d\tau dt \\ &\leq C_3^2 \cdot t \int_0^t |\tilde{u}(\tau) - \tilde{u}'(\tau)|_{H_1}^2 \; d\tau. \end{aligned}$$

Recursively, for $l = 1, 2, \ldots$, we have

$$|\Lambda^l(\tilde{u})(t) - \Lambda^l(\tilde{u}')(t)| \leq \frac{C_3^l \cdot t^{l-1}}{(l-1)!} \int_0^t |\tilde{u} - \tilde{u}'|_{H_1}^2 \; d\tau \text{ for } t \in [0,T].$$

Here, we can choose $l \in \mathbb{N}$ such that

$$\frac{C_3^l}{(l-1)!} \cdot T^{l-1} < 1.$$

This yields that Λ^l is a contraction mapping. By applying the Banach fixed point theorem, there exists a $u \in L^2(0,T;H_1)$ such that $\Lambda^l u = u$. Clearly, $\Lambda u = u$ and u is a weak solution of $(\mathrm{P})_\epsilon$ on $[0,T]$.

Next, we prove the uniqueness. Let u_1, u_2 be weak solutions of $(\mathrm{P})_{\epsilon,\ell}$. Similarly to the proof of Lemma 3.2, we have

$$\frac{1}{2}\frac{d}{dt}|u_1 - u_2|_{V_1^*}^2 + \int_{\Omega_1} |u_1 - u_2|^2 \; dx$$

$$= \quad -\int_{\Omega_1} (\sigma_M(u_1) - \sigma_M(u_2)) a_\epsilon \nabla F^{-1}(u_1 - u_2)\, dx \qquad \text{a.e. on } [0,T]. \tag{3.8}$$

We note that

$$|F^{-1}(u_1 - u_2)|_{V_1}^2 = k|\nabla F^{-1}(u_1 - u_2)|_{H_1}^2 + \left| \int_{\Omega_1} F^{-1}(u_1 - u_2)\, dx \right|^2,$$
$$|u_1 - u_2|_{V_1^*}^2 = |F^{-1}(u_1^* - u_2^*)|_{V_1}^2 \geq k|\nabla F^{-1}(u_1 - u_2)|_{H_1}^2.$$

Accordingly, we have

$$\begin{aligned} (\text{Right hand side of (3.8)}) \quad &\leq \quad K_\epsilon |b| |u_1 - u_2|_{H_1} |\nabla F^{-1}(u_1 - u_2)|_{H_1} \\ &\leq \quad \frac{|u_1 - u_2|_{H_1}^2}{2} + \frac{K_\epsilon^2 |b|^2 |u_1 - u_2|_{V_1^*}^2}{2k}. \end{aligned}$$

Now, by setting $K_1 = K_\epsilon^2 |b|^2 / k$ we get

$$\frac{d}{dt}|u_1 - u_2|_{V_1^*}^2 + |u_1 - u_2|_{H_1}^2 \leq K_1 |u_1 - u_2|_{V_1^*}^2 \qquad \text{a.e. on } [0,T].$$

Finally, Grönwall's inequality implies that

$$|u_1(t) - u_2(t)|_{V_1^*}^2 + \exp(Mt) \int_0^t |u_1 - u_2|_{H_1}^2 d\tau \leq \exp(Mt) |u_1(0) - u_2(0)|_{V_1^*}^2 = 0 \qquad \text{for } t \in [0,T].$$

Thus, $u_1 = u_2$ hold a.e. on $Q_1(T)$. □

Lemma 3.4. *For each* $\epsilon > 0$ $(P)_\epsilon$ *has a unique solution on* $[0,T]$.

Proof. For $\epsilon > 0$ and $\ell = 1, 2, \ldots$ by Lemma 3.3 we have one and only one weak solution u_ℓ of $(\mathrm{P})_{\epsilon,\ell}$ on $[0,T]$ such that

$$\begin{aligned} &u_\ell \in L^2(0,T;V_1) \cap L^\infty(0,T;H_1) \cap W^{1,2}(0,T;V_1^*), \\ &\langle u_{\ell t}, \eta \rangle_{V_1^*} = -\int_{\Omega_1} (k\nabla u_\ell + \sigma_M(u_\ell) a_\epsilon) \nabla \eta\, dx \text{ for } \eta \in V_1 \text{ a.e. on } [0,T], \\ &u_\ell(0,\cdot) = u_{0_\ell} \quad \text{on } \Omega_1. \end{aligned} \tag{3.9}$$

In the same way to that of the proof of Lemma 3.1 by taking $\eta = u_\ell$ in (3.9), there exists $C_4 > 0$ such that

$$|u_\ell(t)|_{H_1}^2 \leq C_4 \left(\int_0^T \int_{\Omega_1} |a_\epsilon|^2\, dxdt + 1 \right) \quad \text{for } 0 \leq t \leq T, \tag{3.10}$$

$$\int_0^T |\nabla u_\ell|_{H_1}^2 dt \leq C_4 \left(\int_0^T \int_{\Omega_1} |a_\epsilon|^2\, dxdt + 1 \right), \tag{3.11}$$

$$\int_0^T |u_{\ell t}(t)|_{V_1^*}^2 dt \leq C_4 \text{ for each } \ell. \tag{3.12}$$

From these estimates by applying Aubin's compact theorem, again, we can choose a subsequence $\{\ell_j\}$ and $u \in L^2(0,T;V_1) \cap L^\infty(0,T;H_1) \cap W^{1,2}(0,T;V_1^*)$ such that $u_{\ell_j} \to u$

weakly in $L^2(0,T;V_1)$ and $W^{1,2}(0,T;V_1^*)$, weakly* in $L^\infty(0,T;H_1)$ and in $L^2(0,T;H_1)$ as $j\to\infty$. Now, we know that for each j

$$\begin{cases} \int_0^T \langle u_{\ell_j t}, \eta\rangle_{V_1^*} dt = -\int_0^T \int_{\Omega_1} (k\nabla u_{\ell_j} + \sigma_M(u_{\ell_j})a_\epsilon)\nabla\eta\, dxdt \text{ for } \eta\in L^2(0,T;V_1),\\ u_{k_j}(0,\cdot) = u_{0_{k_j}} \quad \text{on } \Omega_1. \end{cases}$$

Therefore, the above convergences imply that u is a weak solution of $(\mathrm{P})_\epsilon$ on $[0,T]$.

The uniqueness is similarly proved in a way to that of Lemma 3.3. Thus, we have proved Lemma 3.4. □

Proof of Theorem 2.1. For $\epsilon>0$ Lemma 3.4 guarantees existence of a unique weak solution u_ϵ of $(\mathrm{P})_\epsilon$ on $[0,T]$. Then by estimates (3.10)–(3.12) we can take a subsequence $\{\epsilon_j\}$ and $u\in L^2(0,T;V_1)\cap L^\infty(0,T;H_1)\cap W^{1,2}(0,T;V_1^*)$ such that the following convergences as in the proof of Lemma 3.4 hold:

$u_{\epsilon_j}\to u$ weakly in $L^2(0,T;V_1)$ and $W^{1,2}(0,T;V_1^*)$, weakly* in $L^\infty(0,T;H_1)$ and in $L^2(0,T;H_1)$ as $j\to\infty$.

Moreover, we may suppose that $u_{\epsilon_j}\to u$ a.e. on $Q_1(T)$ as $j\to\infty$. Here, thanks to Lebesgue's dominated convergence theorem and (3.1) we infer that

$$\lim_{j\to\infty}\int_0^T\int_{\Omega_1}\sigma_M(u_{\ell_j})a_\epsilon\nabla\eta\, dxdt = \int_0^T\int_{\Omega_1}\sigma_M(u)\nabla\theta_1\nabla\eta\, dxdt \text{ for } \eta\in L^2(0,T;V_1).$$

Consequently, we can prove Theorem 2.1. □

4 Numerical results

4.1 Problem formulation for numerical simulation

For numerical simulation we approximate the system (1.1)–(1.9) as follows. Again, let χ_i be the characteristic function of Ω_i for $i=1,2$, let $\theta=\theta_1\chi_1+\theta_2\chi_2$, $C=C_1\chi_1+C_2\chi_2$, $\kappa=\kappa_1\chi_1+\kappa_2\chi_2$ and $s=s_1\chi_1+s_2\chi_2$. Then, the function θ is a weak solution of the following problem:

$$C\theta_t = \operatorname{div}(\kappa\nabla\theta + d\theta\chi_1\nabla u) + s \quad \text{in } Q(T), \tag{4.1}$$
$$(\kappa\nabla\theta + d\theta\chi_1\nabla u)\cdot\nu = 0 \quad \text{on } S(T). \tag{4.2}$$
$$\theta(0) = \chi\theta_{01} + \chi_2\theta_{02} =: \theta_0 \quad \text{on } \Omega, \tag{4.3}$$

where $Q(T)=(0,T)\times\Omega$. In order to get approximation problems we consider the following problem as an extension of u to Ω_2:

$$u_t = 0 \quad \text{in } Q_2(T), \tag{4.4}$$
$$u(0) = u_0 \quad \text{in } \Omega_2, \tag{4.5}$$

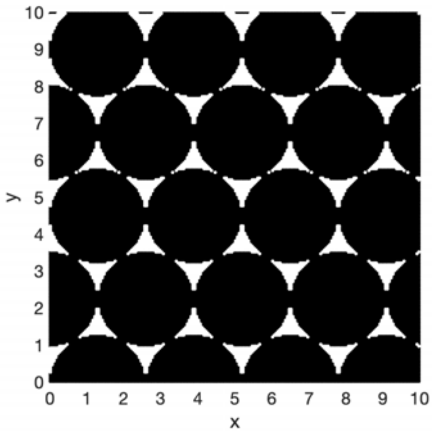

Figure 4.1: Problem domain $\Omega = \Omega_1 \cup \Omega_2$. The liquid part Ω_1 is black, the silver part Ω_2 is white.

where we extend u_0 to Ω_2, continuously.

As a next step, we approximate the system (1.4), (1.6), and (4.4) by: For small $\varepsilon > 0$,

$$
\begin{aligned}
&u_t = \operatorname{div}(k\nabla u + bu\nabla\theta_1) && \text{in } Q_1(T), && (4.6)\\
&u_t = \operatorname{div}(\varepsilon\nabla u) && \text{in } Q_2(T), && (4.7)\\
&(k\nabla u + bu\nabla\theta_1)\cdot\nu = 0 && \text{on } S(T), && (4.8)\\
&(k\nabla u + bu\nabla\theta_1)\cdot\nu = \varepsilon\nabla u\cdot\nu && \text{on } S_2(T). && (4.9)
\end{aligned}
$$

Finally, we take $\kappa_\varepsilon, \chi_\varepsilon, k_\varepsilon \in C^\infty(\overline{\Omega})$ for $\varepsilon > 0$ with

$$
\kappa_\varepsilon \to \kappa, \quad \chi_\varepsilon \to \chi_1, \quad k_\varepsilon \to k\chi_1 \quad \text{on } \Omega \quad \text{as } \varepsilon \downarrow 0, \tag{4.10}
$$

and $k_\varepsilon \geq \varepsilon$ on Ω_2. Thus we obtain the approximation system (4.11)–(4.15). for (4.1) and (4.3): For $\varepsilon > 0$ the problem is to find a pair $(\theta_\varepsilon, u_\varepsilon)$ satisfying

$$
\begin{aligned}
&C\theta_{\varepsilon t} = \operatorname{div}(\kappa_\varepsilon\nabla\theta_\varepsilon + d\theta_\varepsilon\chi_\varepsilon\nabla u_\varepsilon) + s && \text{in } Q(T), && (4.11)\\
&u_{\varepsilon t} = \operatorname{div}(k_\varepsilon\nabla u_\varepsilon + bu_\varepsilon\chi_\varepsilon\nabla\theta_\varepsilon) && \text{in } Q(T), && (4.12)\\
&(\kappa_\varepsilon\nabla\theta_\varepsilon + d\theta_\varepsilon\chi_\varepsilon\nabla u_\varepsilon)\cdot\nu = 0 && \text{on } S(T), && (4.13)\\
&(k_\varepsilon\nabla u_\varepsilon + bu_\varepsilon\chi_\varepsilon\nabla\theta_\varepsilon)\cdot\nu = 0 && \text{on } S(T), && (4.14)\\
&\theta(0) = \theta_0, \quad u(0) = u_0 && \text{on } \Omega. && (4.15)
\end{aligned}
$$

Because we are interested in modeling and simulating the Soret effect in this paper, we do not use a full Maxwell equations based description of the plasmonic heating. Instead we present a simplified heat source that has the same characteristics. Consider the problem domain in Figure 4.1, inspired by [6].

First, we approximate the silver region as seen in Figure 4.1 by triangles. The region between three touching circles is assumed to be triangular. Let K be such a triangle. For every point $P = (x, y) \in \Omega$, we compute the distance from P to the edge of the triangle.

Let us denote this distance with $d(P, K)$. Then the heat source q_K due to plasmonic heating by triangle K is modeled as

$$q_K(x, y) := \begin{cases} \exp(-\alpha_1 d^2(P, K)), & \text{if } P \text{ is inside triangle } K, \\ \exp(-\alpha_2 d^2(P, K)), & \text{if } P \text{ is outside triangle } K. \end{cases} \tag{4.16}$$

The total heat source q is the sum over all triangles K of the local heat source for each triangle. See Figure 4.2 for a two-triangle example. Note that the heat source is largest between the two triangles. This effect is what we aimed to achieve as it is also observed for plasmonic heating.

Figure 4.3 shows the heat source for the domain in Figure 4.1. Note the six spots around each circle where the heat source q has its maximum value.

Figure 4.2: Heat source for two triangles. From left to right: The two triangles, the heat source q_1 of the left triangle only, the heat source q_2 of the right triangle only, the sum of q_1 and q_2.

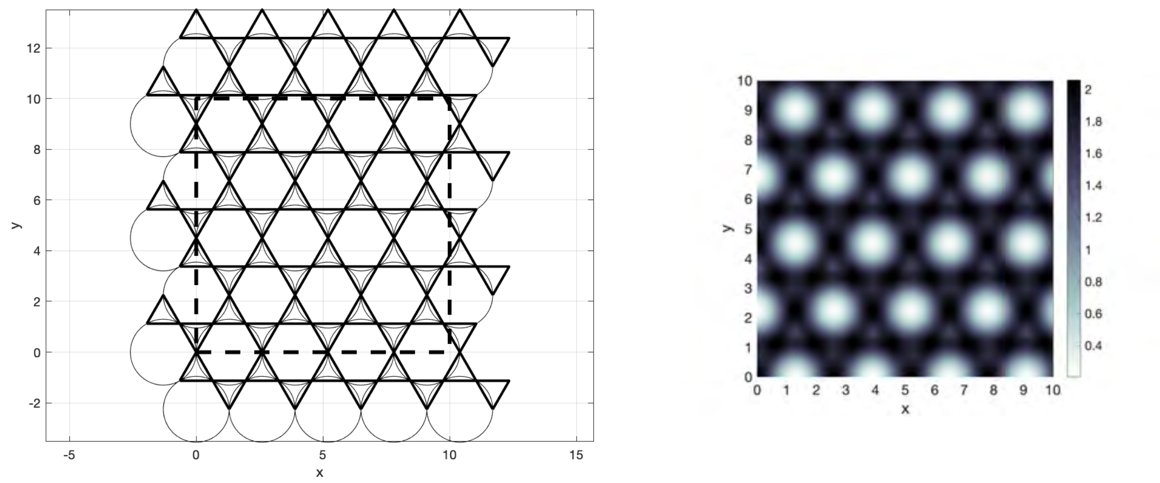

Figure 4.3: Circles, triangles and problem domain (dashed) on the left. Resulting heat source q on the right.

4.2 Finite volume discretization

Both conservation laws (4.11) and (4.12) can be written as

$$C_\varphi \varphi_t = \operatorname{div}(\mathbf{f}_\varphi) + s_\varphi, \tag{4.17}$$

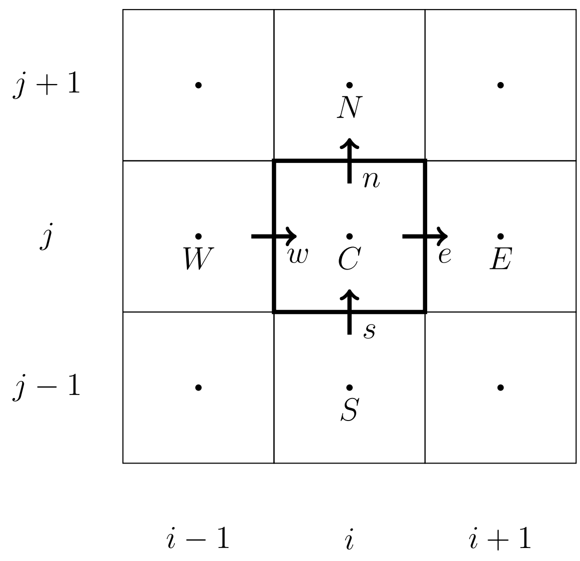

Figure 4.4: Control volume $\Omega_{i,j}$ (thick) with its surrounding cells. The arrows denote the normal components of the flux.

with $C_\varphi = C$ for $\varphi = \theta_\varepsilon$ and $C_\varphi = 1$ for $\varphi = u_\varepsilon$. The flux $\mathbf{f}_\varphi$ is defined by

$$\mathbf{f}_\varphi := D\nabla\varphi + \mathbf{u}\varphi, \tag{4.18}$$

where $D = \kappa_\varepsilon$, $\mathbf{u} = d\chi_\varepsilon \nabla u$, for $\varphi = \theta_\varepsilon$, and $D = k_\varepsilon$, $\mathbf{u} = b\nabla\theta_\varepsilon$, for $\varphi = u_\varepsilon$. Finally, $s_\varphi = -a(\theta_\varepsilon - \theta_{\mathrm{sub}}) + q$, for $\varphi = \theta_\varepsilon$, and $s = 0$, for $\varphi = u_\varepsilon$.

Integrating (4.17) over a fixed domain A and applying Gauss's theorem we obtain the integral form of the conservation law, i.e.,

$$\int_A C_\varphi \varphi_t \, dA = \oint_{\partial A} (\mathbf{f}_\varphi, \mathbf{n}) \, dr + \int_A s_\varphi \, dA, \tag{4.19}$$

where $\mathbf{n}$ is the outward unit normal on the boundary ∂A. In the finite volume method, we cover the domain with a finite number of disjunct control volumes or cells and impose the integral form (4.19) for each of these cells.

In two-dimensional Cartesian coordinates, we first choose the grid points $\mathbf{x}_{i,j} = (x_i, y_j)$ where the unknown φ has to be approximated. Next, we choose control volumes $\Omega_{i,j} := (x_{i-1/2}, x_{i+1/2}) \times (y_{j-1/2}, y_{j+1/2})$. Here $x_{i\pm1/2} := \frac{1}{2}(x_i + x_{i\pm1})$ and $y_{j\pm1/2} := \frac{1}{2}(y_j + y_{j\pm1})$ The boundary of control volume $\Omega_{i,j}$ is the union of four edges $\Gamma_{i\pm1/2,j}$ and $\Gamma_{i,j\pm1/2}$. See Figure 4.4.

Taking $A = \Omega_{i,j}$ in conservation law (4.19) and approximating all integrals with the midpoint rule, we find

$$C_\varphi \varphi_{t,i,j} \, \Delta x \, \Delta y \doteq \left(f_{x,i+1/2,j} - f_{x,i-1/2,j}\right) \Delta y + \left(f_{y,i,j+1/2} - f_{y,i,j-1/2}\right) \Delta x + s_{i,j} \, \Delta x \, \Delta y, \tag{4.20}$$

where we have used that the flux equals $\mathbf{f}_\varphi = f_x \, \mathbf{e}_x + f_y \, \mathbf{e}_y$. We discretize in time using a time step $\Delta t > 0$ and introduce time levels $t_n = n \cdot \Delta t$, $n = 0, 1, 2, \ldots$ If we use the implicit Euler method for time discretization, (4.20) becomes

$$\varphi_{i,j}^{(n+1)} = \varphi_{i,j}^{(n)} + \frac{1}{C_\varphi}\left(\frac{\Delta t}{\Delta x}\left(f_{x,i+1/2,j}^{(n+1)} - f_{x,i-1/2,j}^{(n+1)}\right) + \frac{\Delta t}{\Delta y}\left(f_{y,i,j+1/2}^{(n+1)} - f_{y,i,j-1/2}^{(n+1)}\right) + s_{i,j}^{(n+1)}\,\Delta t\right). \tag{4.21}$$

Here, $\varphi_{i,j}^{(n+1)}$ is the numerical approximation of $\varphi(t_{n+1}, x_i, y_j)$ and the superscripts and subscripts are similar for the other terms in the equation. The FVM has to be completed with numerical approximations F_x and F_y for the fluxes f_x and f_y in (4.21).

Let us suppress the time dependence in the notation for now and let us consider $\varphi = \theta_\varepsilon$. Then

$$f_x = \kappa_\varepsilon \frac{\partial \theta_\varepsilon}{\partial x} + d\chi_\varepsilon \frac{\partial u_\varepsilon}{\partial x}\theta_\varepsilon, \qquad f_y = \kappa_\varepsilon \frac{\partial \theta_\varepsilon}{\partial y} + d\chi_\varepsilon \frac{\partial u_\varepsilon}{\partial y}\theta_\varepsilon, \tag{4.22}$$

and we use the central difference approximations

$$F_{x,e} := \kappa_\varepsilon \frac{\theta_E - \theta_C}{\Delta x} + d\chi_\varepsilon \frac{u_E - u_C}{\Delta x}\frac{\theta_C + \theta_E}{2}, \quad F_{y,n} := \kappa_\varepsilon \frac{\theta_N - \theta_C}{\Delta y} + d\chi_\varepsilon \frac{u_N - u_C}{\Delta y}\frac{\theta_C + \theta_N}{2}. \tag{4.23}$$

Here we have used compass notation (cf. Figure 4.4): $F_{x,e} = F_{x,i+1/2,j}$, $\theta_C = \theta_{\varepsilon,i,j}$, etc.

Let us focus on the horizontal flux $F_{x,e}$. We have

$$F_{x,e} = \alpha_{x,e}\theta_C - \beta_{x,e}\theta_E, \quad \alpha_{x,e} := -\frac{\kappa_\varepsilon}{\Delta x} + \tfrac{1}{2}\chi_\varepsilon d\frac{u_E - u_C}{\Delta x}, \quad \beta_{x,e} := -\frac{\kappa_\varepsilon}{\Delta x} - \tfrac{1}{2}\chi_\varepsilon d\frac{u_E - u_C}{\Delta x}. \tag{4.24}$$

In (4.24), we choose $\kappa_\varepsilon = \kappa_1$ if both $\mathbf{x}_C = \mathbf{x}_{i,j} \in \Omega_1$ and $\mathbf{x}_E \in \Omega_1$. We choose $\kappa_\varepsilon = \kappa_2$ if $\mathbf{x}_C \in \Omega_2$ and $\mathbf{x}_E \in \Omega_2$. Finally, we choose κ_ε equal to the harmonic mean, that is $\kappa_\varepsilon = 2\kappa_1\kappa_2/(\kappa_1 + \kappa_2)$, in the other situations. This means that the flux is located at an interface between the liquid and silver regions. For χ_ε, we choose $\chi_\varepsilon = 1$ if both $\mathbf{x}_C \in \Omega_1$ and $\mathbf{x}_E \in \Omega_1$. We set $\chi_\varepsilon = 0$ in all other situations.

Similarly we can define $\alpha_{x,w}$, $\alpha_{y,n}$, $\alpha_{y,s}$ etc. Substitution of (4.24) and the equivalent in vertical direction into (4.21) yields

$$\begin{aligned}\theta_C^{(n+1)} = \theta_C^{(n)} &+ \frac{1}{C}\frac{\Delta t}{\Delta x}\left(-\beta_{x,e}\theta_E^{(n+1)} + (\alpha_{x,e} + \beta_{x,w})\theta_C^{(n+1)} - \alpha_{x,w}\theta_W^{(n+1)}\right) \\ &+ \frac{1}{C}\frac{\Delta t}{\Delta y}\left(-\beta_{y,n}\theta_N^{(n+1)} + (\alpha_{y,n} + \beta_{y,s})\theta_C^{(n+1)} - \alpha_{y,s}\theta_S^{(n+1)}\right) \\ &+ \frac{1}{C}\left(-a\left(\theta_C^{(n+1)} - \theta_{\text{sub}}\right) + q\right)\Delta t.\end{aligned} \tag{4.25}$$

Summarizing we have now discretized (4.11) and found the final form of the difference equation for θ_ε:

$$\begin{aligned}&\left(1 + \frac{a\Delta t}{C} - a_{x,e} - b_{x,w} - a_{y,n} - b_{y,s}\right)\theta_C^{(n+1)} \\ &\qquad + b_{x,e}\theta_E^{(n+1)} + a_{x,w}\theta_W^{(n+1)} \\ &\qquad + b_{y,n}\theta_N^{(n+1)} + a_{y,s}\theta_S^{(n+1)} = \theta_C^{(n)} + \frac{\Delta t}{C}(a\theta_{\text{sub}} + q),\end{aligned} \tag{4.26}$$

with

$$a_{x,e} := \frac{\Delta t}{C\Delta x^2}\left(-\kappa_\varepsilon + \tfrac{1}{2}d\chi_\varepsilon(u_E^{(n+1)} - u_C^{(n+1)})\right), \quad b_{x,e} := \frac{\Delta t}{C\Delta x^2}\left(-\kappa_\varepsilon - \tfrac{1}{2}d\chi_\varepsilon(u_E^{(n+1)} - u_C^{(n+1)})\right), \tag{4.27}$$

$$a_{x,w} := \frac{\Delta t}{C\Delta x^2}\left(-\kappa_\varepsilon + \tfrac{1}{2}d\chi_\varepsilon(u_C^{(n+1)} - u_W^{(n+1)})\right), \quad b_{x,w} := \frac{\Delta t}{C\Delta x^2}\left(-\kappa_\varepsilon - \tfrac{1}{2}d\chi_\varepsilon(u_C^{(n+1)} - u_W^{(n+1)})\right), \tag{4.28}$$

$$a_{y,n} := \frac{\Delta t}{C\Delta y^2}\left(-\kappa_\varepsilon + \tfrac{1}{2}d\chi_\varepsilon(u_N^{(n+1)} - u_C^{(n+1)})\right), \quad b_{y,n} := \frac{\Delta t}{C\Delta y^2}\left(-\kappa_\varepsilon - \tfrac{1}{2}d\chi_\varepsilon(u_N^{(n+1)} - u_C^{(n+1)})\right), \tag{4.29}$$

$$a_{y,s} := \frac{\Delta t}{C\Delta y^2}\left(-\kappa_\varepsilon + \tfrac{1}{2}d\chi_\varepsilon(u_C^{(n+1)} - u_S^{(n+1)})\right), \quad b_{y,s} := \frac{\Delta t}{C\Delta y^2}\left(-\kappa_\varepsilon - \tfrac{1}{2}d\chi_\varepsilon(u_C^{(n+1)} - u_S^{(n+1)})\right). \tag{4.30}$$

For $\varphi = u_\varepsilon$, the flux equals

$$f_x = k_\varepsilon \frac{\partial u_\varepsilon}{\partial x} + b\chi_\varepsilon \frac{\partial \theta_\varepsilon}{\partial x} u_\varepsilon, \qquad f_y = k_\varepsilon \frac{\partial u_\varepsilon}{\partial y} + b\chi_\varepsilon \frac{\partial \theta_\varepsilon}{\partial y} u_\varepsilon, \tag{4.31}$$

which we approximate by

$$F_{x,e} := k_\varepsilon \frac{u_E - u_C}{\Delta x} + b\chi_\varepsilon \frac{\theta_E - \theta_C}{\Delta x}\frac{u_C + u_E}{2}, \qquad F_{y,n} := k_\varepsilon \frac{u_N - u_C}{\Delta y} + b\chi_\varepsilon \frac{\theta_N - \theta_C}{\Delta y}\frac{u_C + u_N}{2}. \tag{4.32}$$

In (4.32), we choose k_ε as follows:

$$k = \begin{cases} k & \text{if both } \mathbf{x}_C = \mathbf{x}_{i,j} \in \Omega_1 \text{ and } \mathbf{x}_E \in \Omega_1, \\ \varepsilon & \text{if both } \mathbf{x}_C \in \Omega_2 \text{ and } \mathbf{x}_E \in \Omega_2, \\ \dfrac{2k\varepsilon}{k+\varepsilon} & \text{otherwise.} \end{cases}$$

Finally, we choose k_ε equal to the harmonic mean in the other situations. This means that the flux is located at an interface between the liquid and silver regions. For χ_ε, we choose $\chi_\varepsilon = 1$ if both $\mathbf{x}_C \in \Omega_1$ and $\mathbf{x}_E \in \Omega_1$. We set $\chi_\varepsilon = 0$ in all other situations.

If we follow the same steps as before, we find the following discretization of (4.12):

$$\begin{aligned}(1 - a_{x,e} - b_{x,w} - a_{y,n} - b_{y,s})\, u_C^{(n+1)} + b_{x,e}u_E^{(n+1)} + a_{x,w}u_W^{(n+1)} \\ + b_{y,n}u_N^{(n+1)} + a_{y,s}u_S^{(n+1)} = u_C^{(n)},\end{aligned} \tag{4.33}$$

with

$$a_{x,e} := \frac{\Delta t}{\Delta x^2}\left(-k_\varepsilon + \tfrac{1}{2}b\chi_\varepsilon(\theta_E^{(n+1)} - \theta_C^{(n+1)})\right), \quad b_{x,e} := \frac{\Delta t}{\Delta x^2}\left(-k_\varepsilon - \tfrac{1}{2}b\chi_\varepsilon(\theta_E^{(n+1)} - \theta_C^{(n+1)})\right), \tag{4.34}$$

$$a_{x,w} := \frac{\Delta t}{\Delta x^2}\left(-k_\varepsilon + \tfrac{1}{2}b\chi_\varepsilon(\theta_C^{(n+1)} - \theta_W^{(n+1)})\right), \quad b_{x,w} := \frac{\Delta t}{\Delta x^2}\left(-k_\varepsilon - \tfrac{1}{2}b\chi_\varepsilon(\theta_C^{(n+1)} - \theta_W^{(n+1)})\right), \tag{4.35}$$

$$a_{y,n} := \frac{\Delta t}{\Delta y^2}\left(-k_\varepsilon + \tfrac{1}{2}b\chi_\varepsilon(\theta_N^{(n+1)} - \theta_C^{(n+1)})\right), \quad b_{y,n} := \frac{\Delta t}{\Delta y^2}\left(-k_\varepsilon - \tfrac{1}{2}b\chi_\varepsilon(\theta_N^{(n+1)} - \theta_C^{(n+1)})\right), \tag{4.36}$$

$$a_{y,s} := \frac{\Delta t}{\Delta y^2}\left(-k_\varepsilon + \tfrac{1}{2}b\chi_\varepsilon(\theta_C^{(n+1)} - \theta_S^{(n+1)})\right), \quad b_{y,s} := \frac{\Delta t}{\Delta y^2}\left(-k_\varepsilon - \tfrac{1}{2}b\chi_\varepsilon(\theta_C^{(n+1)} - \theta_S^{(n+1)})\right). \tag{4.37}$$

The finite volume method formulation makes the treatment of the boundary conditions (4.13) and (4.14) straightforward. We choose the computational grid such that $\partial\Omega$ coincides with cell edges. All fluxes located at boundaries are set to zero, so if e.g. the horizontal flux F_e in (4.24) is on $\partial\Omega$, we set $\alpha_{x,e} = 0$ and $\beta_{x,e} = 0$.

4.3 Numerical results

We present numerical results for the following parameter values: $C_1 = C_2 = 1, \kappa_1 = 0.2, \kappa_2 = 1.3, k = 1, d = 0.05, b = -0.1, \theta_{\text{sub}} = 20, a = 0.7, \varepsilon = 10^{-6}, u_0 = 1, \theta_0 = \theta_{\text{sub}}$. The domain is as in Figure 4.1, so $\Omega = (0, 10) \times (0, 10)$. The circles in Figure 4.1 each have radius $r = 1.3$. In Ω, we choose a uniform grid of $N_x \times N_y$ control volumes with $N_x = N_y = 200$.

We solve the system of nonlinear equations in each time step using Newton iteration. The Newton iteration is stopped as soon as the 2-norm of the update of the solution is less than 10^{-5}. This typically takes two or three iteration steps.

To study the time behavior of the solutions, we take time steps with $\Delta t = 0.1$ and we plot both temperature and concentration along the central axes indicated in Figure 4.5. The results are shown in Figures 4.6 and 4.7.

To find the stationary solution we take twenty time steps with $\Delta t = 1$. Figure 4.8 shows the integral of the temperature over the domain. It proves that we have indeed reached the stationary situation. Figures 4.9, 4.10 and 4.11 show the stationary solutions.

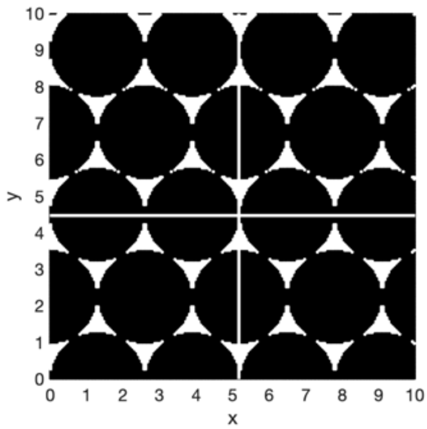

Figure 4.5: Central axes (in white) in the problem domain.

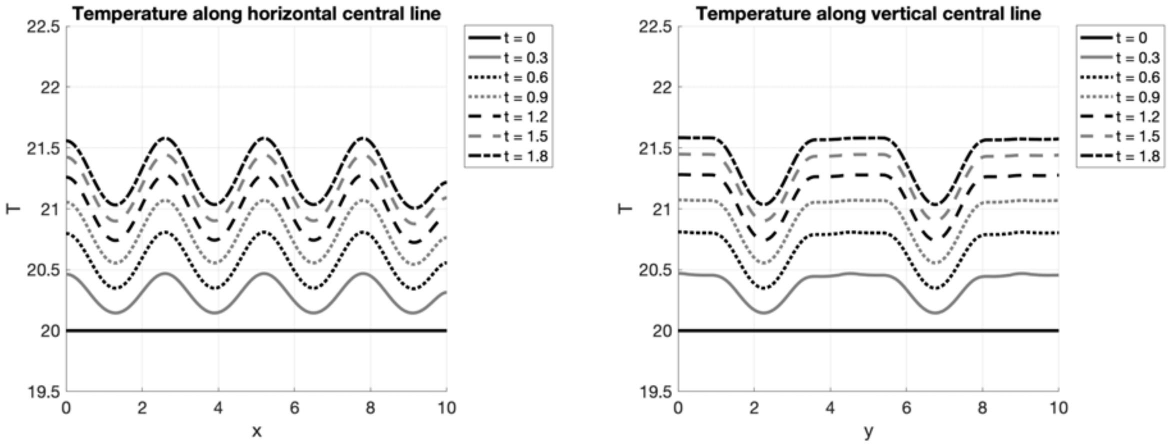

Figure 4.6: Development of temperature in time along horizontal central axis (left) and vertical (right).

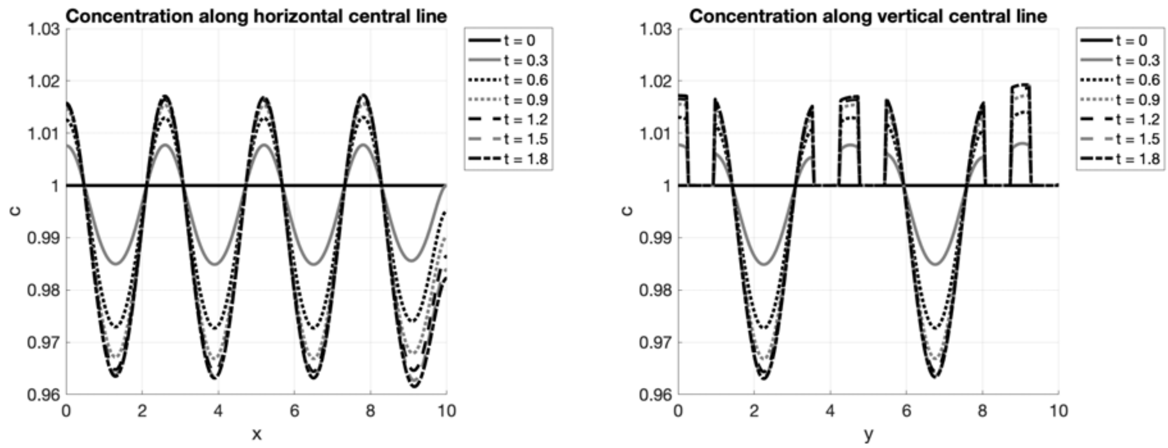

Figure 4.7: Development of concentration in time along horizontal central axis (left) and vertical (right).

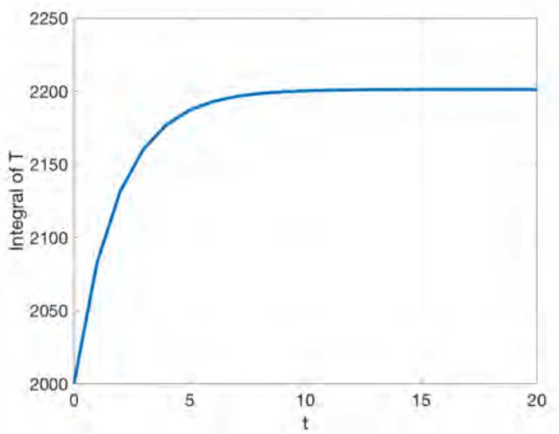

Figure 4.8: Temperature integrated over the domain as a function of time.

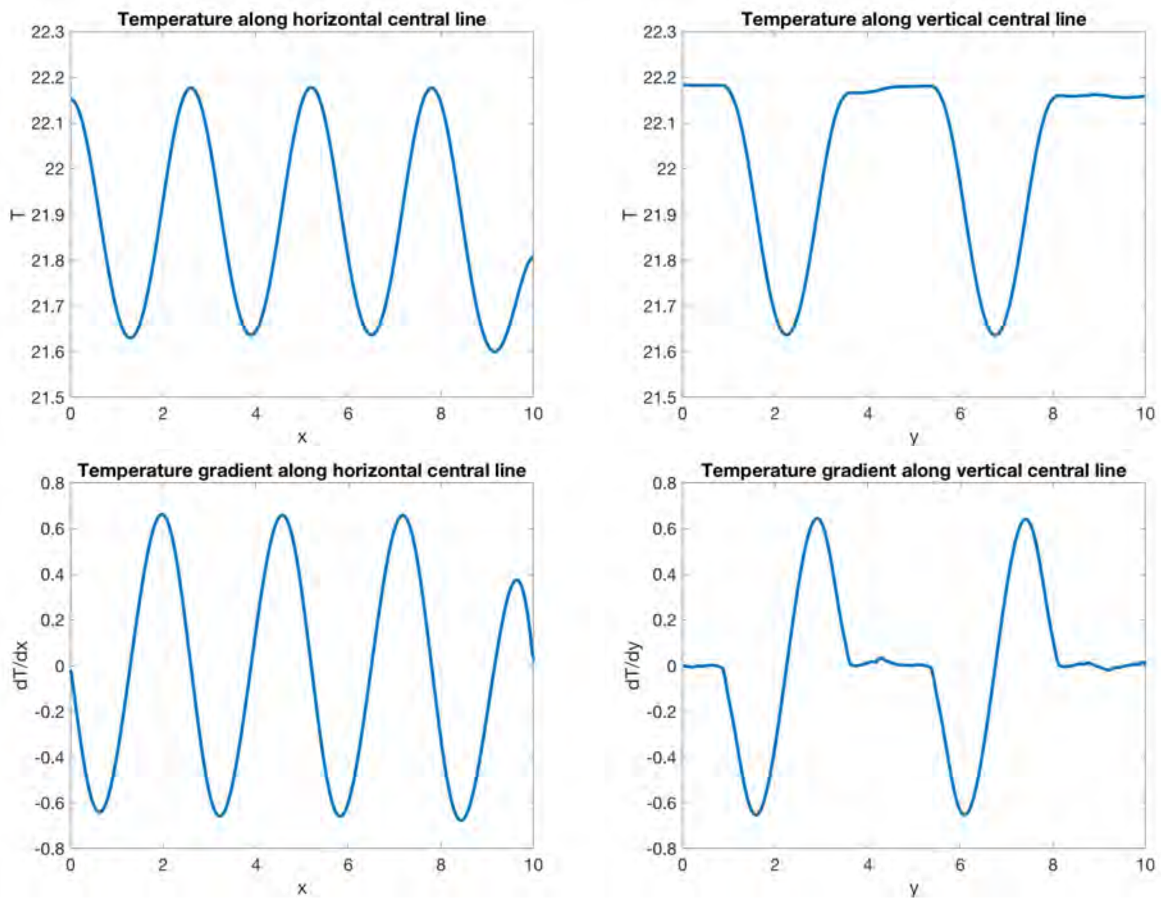

Figure 4.9: Stationary temperature and temperature gradient profiles along horizontal axis (left) and vertical (right).

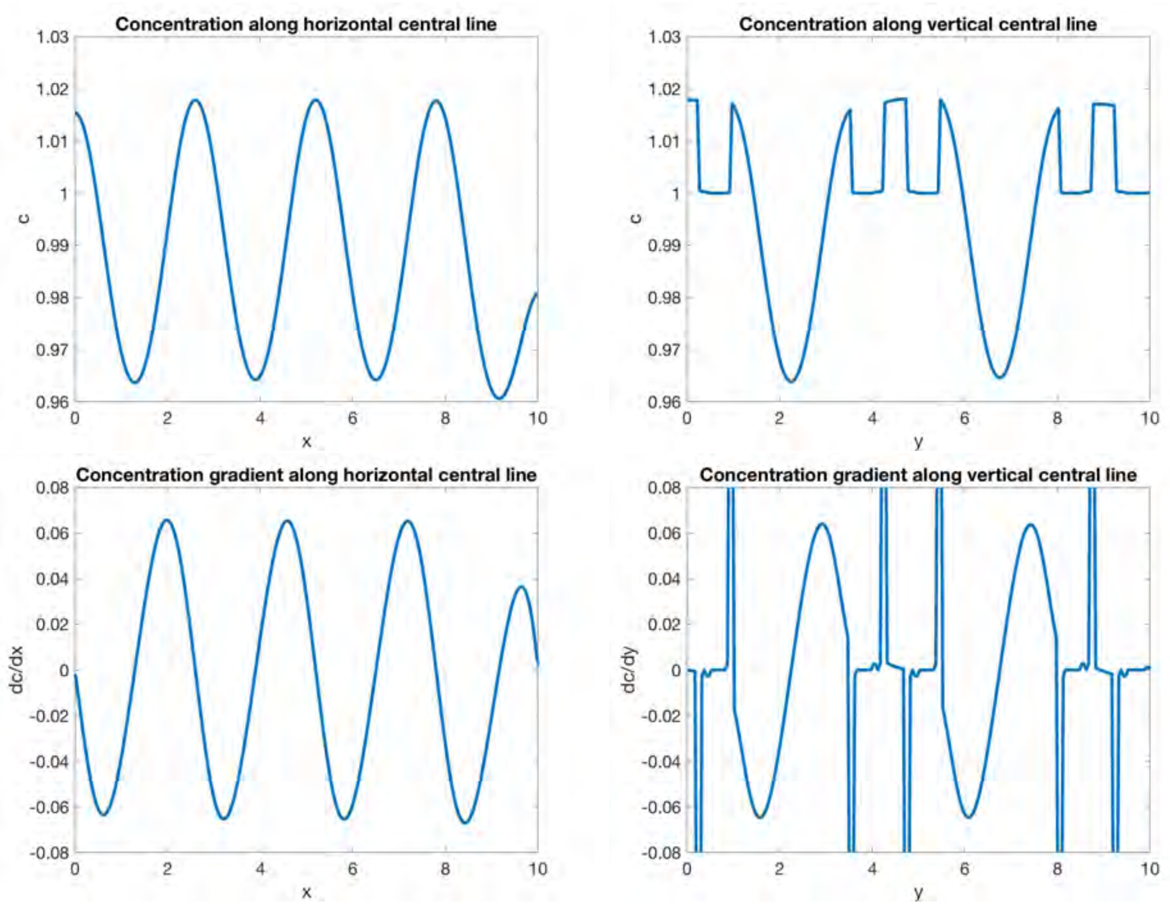

Figure 4.10: Stationary concentration and concentration gradient profiles along horizontal axis (left) and vertical (right).

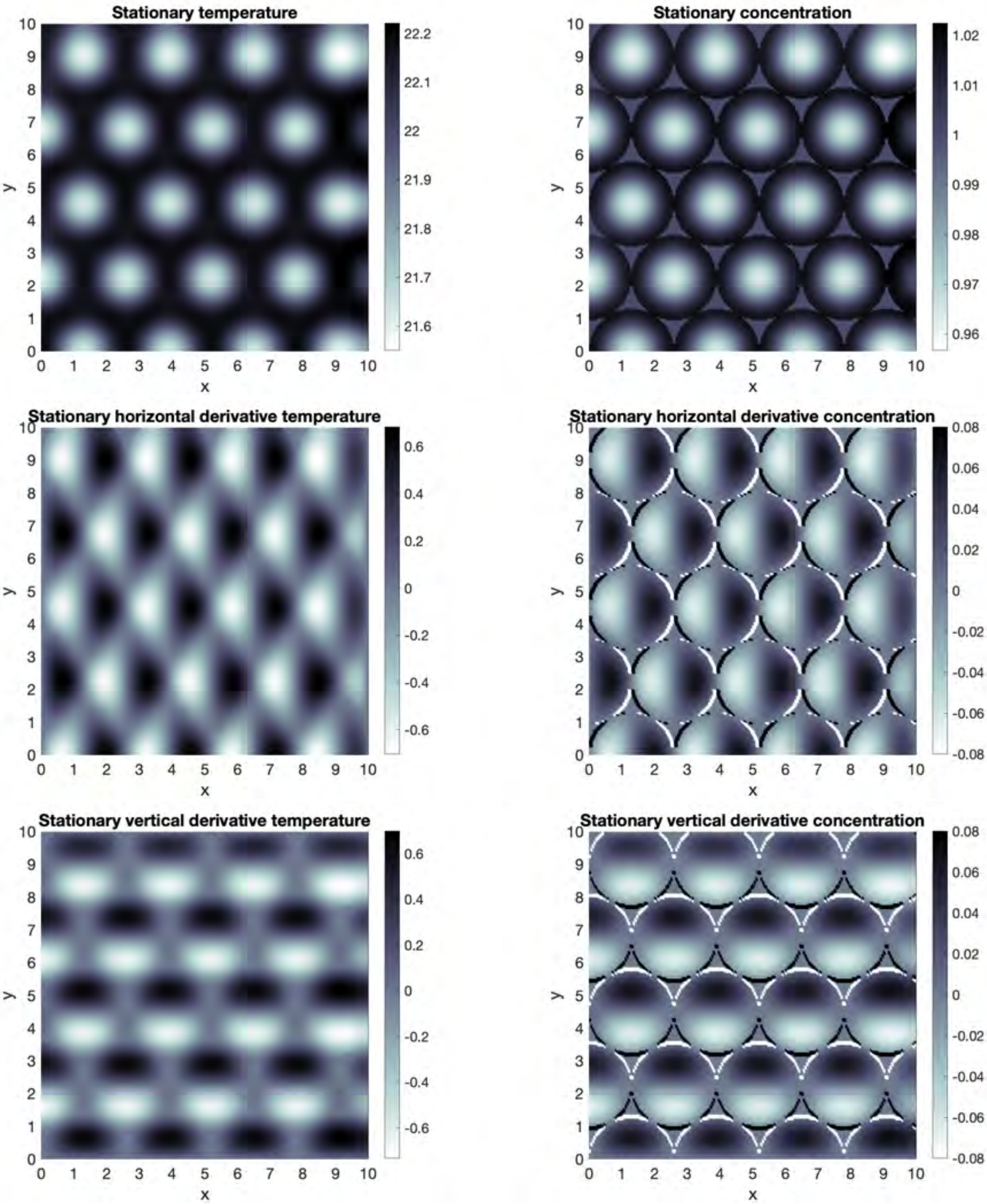

Figure 4.11: Stationary two-dimensional profiles.

4.4 Influence of the initial artificial concentration

The concentration u has been extended to Ω_2. Here we study the influence of the initial value for the concentration in Ω_2.

In Figure 4.10, we chose $u_0 = 1$ in Ω_2. We have also set $u_0 = 0$ in Ω_2 and $u_0 = 2$ in Ω_2. The results are shown in Figure 4.13. It is obvious that the value of u_0 in Ω_2 has little influence on the solution in Ω_1. We do observe in Figure 4.13 however that the maximum and minimum values of the concentration vary slightly.

We add two more cases. The first, $\varepsilon = 10^{-3}$, is shown in Figure 4.12. This value is obviously too large as the solution changes throughout the domain. The parameter ε was set to 10^{-6} for the simulations in Figure 4.13. If we redo the computations with $\varepsilon = 10^{-12}$, we see identical results for all three initial values of u_0 in Ω_2, see Figure 4.14.

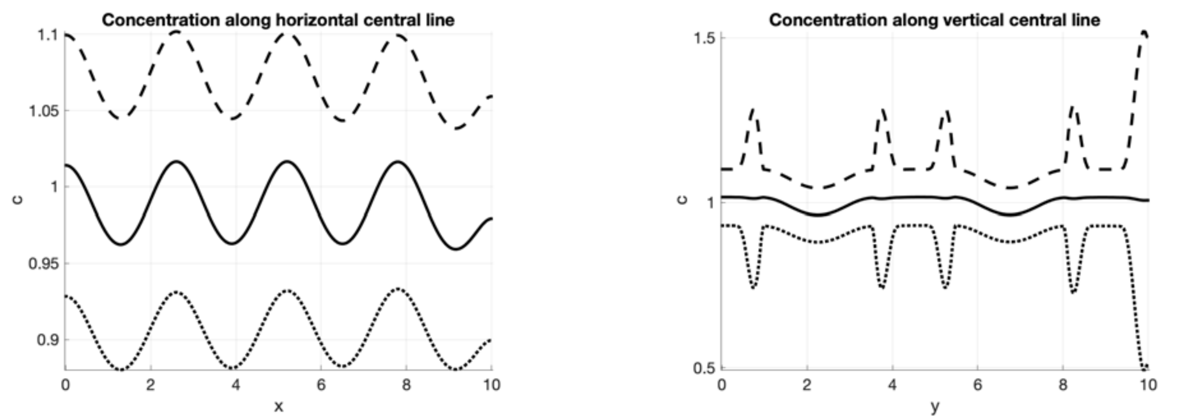

Figure 4.12: Influence of the initial artificial concentration for $\varepsilon = 10^{-3}$. The following values have been chosen: $u_0 = 1$ in Ω_2 (solid line), $u_0 = 0$ in Ω_2 (dotted) and $u_0 = 2$ in Ω_2 (dashed).

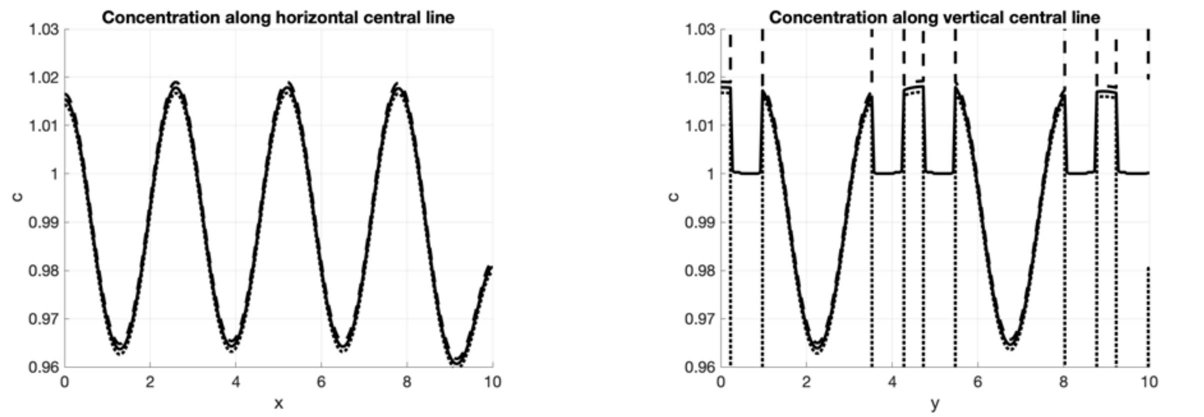

Figure 4.13: Influence of the initial artificial concentration for $\varepsilon = 10^{-6}$. The following values have been chosen: $u_0 = 1$ in Ω_2 (solid line), $u_0 = 0$ in Ω_2 (dotted) and $u_0 = 2$ in Ω_2 (dashed).

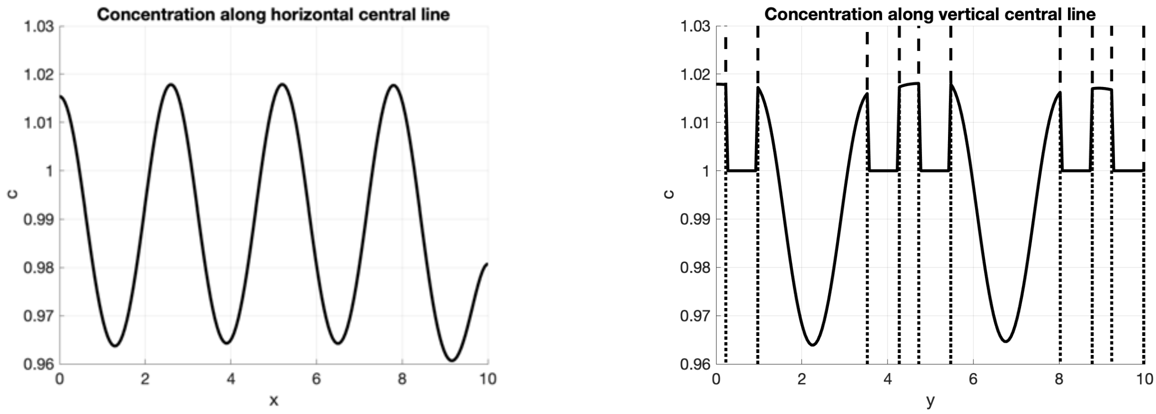

Figure 4.14: Influence of the initial artificial concentration for $\varepsilon = 10^{-12}$. The following values have been chosen: $u_0 = 1$ in Ω_2 (solid line), $u_0 = 0$ in Ω_2 (dotted) and $u_0 = 2$ in Ω_2 (dashed).

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