

## ANALYSIS AND OPTIMAL CONTROL OF SOME SOLIDIFICATION PROCESSES

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**ABSTRACT.** In this paper we consider a mathematical model that describes the solidification of a binary alloy. We prove some existence and uniqueness results for a regularized problem, depending on a small parameter  $\varepsilon$ . We also analyze the behavior of the regularized solutions as  $\varepsilon \rightarrow 0$ . Then, we consider some associated optimal control problems. We prove existence and optimality results and we present and discuss some iterative methods.

**1. Introduction. The mathematical model.** The solidification of metals is one of the most difficult problems to model and analyze in engineering. The complex nature of the processes is an obstacle to obtain solutions in a simple way.

Indeed, to accomplish this task, we have to use sophisticated mathematical models based on systems of nonlinear partial differential equations. However, by using correctly the laws governing solidification processes and appropriate mathematical and numerical techniques, it is possible to gain insight in the phenomena, obtain products of good quality and, also, diminish the related costs.

This paper deals with the theoretical analysis and optimal control of a model of solidification for a binary alloy. The plan is the following. In the remainder of this Section we present the considered model and also a regularized version. Then, in Section 2 we study the existence and uniqueness of the weak solution to the regularized problem, as well as its behaviour as the regularizing parameter  $\varepsilon$  goes to zero. Section 3 deals with a first optimal control problem for the regularized solidification problem; here, the control variable is a heat source. We deduce the existence of optimal controls and we present the associated optimality system; some iterative algorithms are also introduced and discussed. Finally, in Section 4, we consider and solve a second optimal control problem where the solidification time plays a crucial role.

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2010 *Mathematics Subject Classification.* Primary: 93C20, 35Q93, 49K20, 35A01, 35A02; Secondary: 76D05.

*Key words and phrases.* Nonlinear PDEs, solidification models, regularization, weak solutions, optimal control.

The first author is partially supported by Universidad del Bío-Bío grant GI121909/C (Chile), FONDECYT grant 1140074 (Chile) and by MICINN grant MTM2012-32325 (Spain). The second and third authors were supported by MICINN grant MTM2010-15992 (Spain).

**1.1. The example of a cavity.** In order to present the basic ideas of solidification processes, we consider a situation where the mould is modelled as a rectangular cavity  $\Omega$  filled with an incompressible and diluted binary alloy, initially at liquid state, with uniform temperature and composition, under the influence of gravity. The components of the mould are the solute and the solvent; together, they form the melting. The variable that indicates the proportion of solute in the melting is called the concentration.

The alloy is deposited in the mould in such a way that, at time  $t = 0$ , the temperature of the left side of  $\Omega$  is instantaneously dropped and kept under the cooling point, while the other sides of  $\Omega$  are kept thermally isolated (see Figure 1.1). This is the origin of a temperature gradient in the alloy. The coupled action of gravity forces, convection, diffusion and reaction may introduce changes in the alloy density.

On the other hand, the region next to the left side of  $\Omega$  experiences a phase change, passing from the liquid to the solid state. The corresponding interface is called the solidification front. In general, it may have a highly irregular geometry and may exhibit dendritic forms for rapid solidification. The formation of dendrites is a consequence of the instability of growth of the solidification front.

**Remark 1.** Solidification is a multi-scale problem, varying from meters to micrometers (and even nanometers). Because of this, it is very difficult to present a model involving all the relevant variables and phenomena occurring at each scale. In this paper, we will consider a model that can capture the dynamics of the phenomena at the macroscopic (mould) scale. To describe appropriately the very rich and complex dynamics of dendritic growth, it is necessary to consider other models (see for instance [2], [15] and the references therein). On the other hand, in order to avoid some technical (and maybe nontrivial) difficulties, latent heat effects have been neglected.

After a while, the alloy is solidifies. If we analyze the composition of the resultant material, we will probably find variations of the solute. These variations are produced at two different scales: from the macroscopic viewpoint, the solidification front acts like a filter on the solute, that is rejected from the solid to the liquid state (this phenomenon is called macro-segregation); at another (microscopic) scale, the solute is partially trapped by the dendrites of the solidification front, generating highly concentrated solute grains (this is the micro-segregation phenomenon).

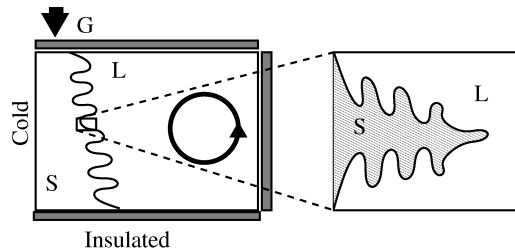


FIGURE 1. A schematic view of the cavity problem, with details of the solidification front.

**1.2. The solidification problem.** In the sequel,  $\Omega$  is a connected, open and bounded open set in  $\mathbb{R}^d$  ( $d = 2, 3$ ) with Lipschitz-continuous boundary  $\partial\Omega$ , such

that  $\partial\Omega = \Gamma_D \cup \Gamma_N$ ,  $\Gamma_D \cap \Gamma_N = \emptyset$  and  $\Gamma_N \neq \emptyset$ . Let us assume that  $T > 0$  and let us set  $Q := \Omega \times (0, T)$ .

Since it is very difficult to work with the highly irregular geometry of solidification front, it is convenient to perform an averaging process on the main variables of the problem in a such way that the front is replaced by a smooth phase change zone called the *mushy or moisture zone*, where we have coexistence of the liquid and solid states. Then, an acceptable mathematical model for the solidification problem is the following (see for example [3, 4, 5]):

$$c_t + \nabla \cdot (\mathbf{v}c_l(c, \theta) - D\nabla c) = 0, \quad (1)$$

$$\theta_t + \nabla \cdot (\mathbf{v}\theta - \chi\nabla\theta) = h_\theta, \quad (2)$$

$$\mathbf{v}_t + \nabla \cdot (\mathbf{v} \otimes \mathbf{v} - \nu\nabla\mathbf{v}) + F_i(c, \theta)\mathbf{v} + \nabla p = \mathbf{F}_e(c, \theta), \quad (3)$$

$$\nabla \cdot \mathbf{v} = 0. \quad (4)$$

In (1)–(4),  $h_\theta$  is a known function and, for any  $\mathbf{a}$  and  $\mathbf{b}$ ,  $\mathbf{a} \otimes \mathbf{b}$  stands for the tensor whose  $(i, j)$  component is  $a_i b_j$ ;  $c$  and  $c_l$  are respectively the concentration and the liquid concentration of solute of the binary alloy;  $\theta$  is the temperature of the moisture;  $\mathbf{v}$  is the velocity of the liquid and  $p$  is the pressure;  $D$ ,  $\chi$  and  $\nu$  are positive constants, respectively denoting the diffusion coefficient of the solute, the thermal conductivity and the kinematic viscosity;  $F_i$  and  $\mathbf{F}_e$  are functions associated to the internal and external forces acting on the system (1)–(4).

In general,  $F_i$  and  $\mathbf{F}_e$  are bounded functions depending on  $c$  and  $\theta$ . By introducing the solid fraction  $f_s$  (the function denoting the proportion of solid in the mould) and using the *Carman-Kozeny approximation* to model the effects in the mould as a porous media and the *Boussinesq approximation* to model the thermic and solutal stresses, we get the following expressions:

$$F_i = M_0 \frac{f_s(c, \theta)^2}{(1 - f_s(c, \theta))^3}, \quad (5)$$

$$\mathbf{F}_e = \mathbf{g}(1 + \beta_c c_l(c, \theta) + \beta_\theta \theta). \quad (6)$$

Here,  $M_0$  denotes a positive constant depending on the material,  $\mathbf{g}$  is the gravity force,  $\beta_\theta$  and  $\beta_c$  are constants representing the thermal and solute expansion coefficients and one has

$$c = c_s f_s + (1 - f_s)c_l,$$

where  $c_s$  is the solid concentration of solute, given by  $c_s = r c_l$  with  $0 < r < 1$ .

**1.3. The phase diagram.** Assume that  $t \geq 0$ . By using the solid fraction  $f_s$ , we can identify the following sets:

$$\Omega_s(t) = \{\mathbf{x} \in \Omega : f_s(\mathbf{x}, t) = 1\}, \quad \Omega_l(t) = \{\mathbf{x} \in \Omega : f_s(\mathbf{x}, t) = 0\},$$

$$\Omega_m(t) = \{\mathbf{x} \in \Omega : f_s(\mathbf{x}, t) \in (0, 1)\}.$$

This allows the *solid* and *non-solid* regions to be defined as

$$Q_s = \{(\mathbf{x}, t) : \mathbf{x} \in \Omega_s(t), \quad t \in (0, T)\}$$

and

$$Q_{ml} = \{(\mathbf{x}, t) : \mathbf{x} \in \Omega_m(t) \cup \Omega_l(t), \quad t \in (0, T)\},$$

respectively; here, “*ml*” stands for “moisture-liquid”.

The equations (1) and (2) must hold in the whole cylinder  $Q$ , with  $\mathbf{v} = 0$  in  $Q_s$ . The equations (3) and (4) must hold in  $Q_{ml}$ .

The sets  $Q_{ml}$  and  $Q_s$  can be computed from the phase diagram by using the values of  $c$  and  $\theta$  (see Figure 2). In this diagram,  $\theta_f$  and  $\theta_e$  denote the *fusion* and *eutectic* temperature, respectively. By simplicity, we assume that the solid and liquid curves  $\theta = \eta_s(c)$  and  $\theta = \eta_l(c)$  are straight lines; they respectively indicate the couples  $(c, \theta)$  where the solid alloy begins to melt and the couples where the liquid begins to solidify.

Specifically, we have:

$$\eta_l(c) = \theta_f - (\theta_f - \theta_e) \frac{c}{c_e} \quad \text{and} \quad \eta_s(c) = \theta_f - (\theta_f - \theta_e) \frac{c}{c_a},$$

where  $c_a$  and  $c_e$  are characteristic concentration values. Also, we can identify in the phase diagram the following sets:

$$L = \{ (c, \theta) : c > c_e \text{ or } \theta > \eta_l(c) \}, \tag{7}$$

$$M = \{ (c, \theta) : 0 \leq c \leq c_e, \max(\eta_s(c), \theta_e) \leq \theta \leq \eta_l(c) \}, \tag{8}$$

$$S = \{ (c, \theta) : 0 \leq c \leq c_e, \theta < \max(\eta_s(c), \theta_e) \}. \tag{9}$$

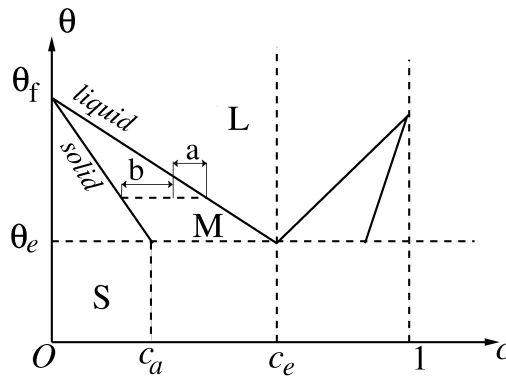


FIGURE 2. A typical phase diagram for a binary alloy

The temperature and the concentration can be used to determine the solid fraction  $f_s$  through the following equalities:

$$f_s(c, \theta) = \begin{cases} 0, & \text{if } c \geq c_e, \\ 0, & \text{if } 0 \leq c \leq c_e, \theta > \eta_l(c), \\ \frac{\eta_l(c) - \theta}{\eta_l(c) - \max(\eta_s(c), \theta_e)}, & \text{if } 0 \leq c \leq c_e, \text{ and} \\ & \max(\eta_s(c), \theta_e) \leq \theta \leq \eta_l(c), \\ 1, & \text{otherwise.} \end{cases} \tag{10}$$

Taking into account this definition of  $f_s$ , we can deduce that the liquid concentration is given by:

$$c_l(c, \theta) = \begin{cases} c_e, & \text{if } c \geq c_e, \\ c, & \text{if } 0 \leq c \leq c_e, \theta > \eta_l(c), \\ (1 - f_s)c, & \text{if } 0 \leq c \leq c_e, \max(\eta_s(c), \theta_e) \leq \theta \leq \eta_l(c), \\ 0, & \text{otherwise.} \end{cases} \tag{11}$$

In the sequel, we will always assume that  $h_\theta = h1_\omega$  for some (small) non-empty open set  $\omega \subset \Omega$  ( $1_\omega$  is the characteristic function of  $\omega$ ). In practice, this means

that we only act on the system through the right hand side of the transport-heat equation (2), by imposing a heat source localized in  $\omega \times (0, T)$ .

In fact, it would have been more realistic to assume that the action is performed through (a part of) the boundary, for instance by imposing a non-zero Dirichlet condition on  $\theta$ . However, this leads to a more complex analysis involving technical difficulties and we have preferred to consider the present situation and deal with distributed or internal controls.

**1.4. The regularized problem.** Notice that the interfaces that separate the solid and the non-solid region are not known a priori; this is a serious difficulty. Moreover, the Carman-Kozeny term is singular in  $Q_s$ , because the solid fraction  $f_s$  reaches 1 there. Accordingly, we will introduce a parameter  $\varepsilon \in (0, 1]$  and we will replace the function  $F_i(c, \theta)$  defined in (5) by the following:

$$F_i^\varepsilon = M_0 \frac{f_s(c, \theta)^2}{(1 - f_s(c, \theta) + \varepsilon)^3}. \quad (12)$$

This leads to the so called regularized problem:

$$c_t + \nabla \cdot (\mathbf{v}c_l(c, \theta) - D\nabla c) = 0, \quad (13)$$

$$\theta_t + \nabla \cdot (\mathbf{v}\theta - \chi\nabla\theta) = h1_\omega, \quad (14)$$

$$\mathbf{v}_t + \nabla \cdot (\mathbf{v} \otimes \mathbf{v} - \nu\nabla\mathbf{v}) + F_i^\varepsilon(c, \theta)\mathbf{v} + \nabla p = \mathbf{F}_e(c, \theta), \quad (15)$$

$$\nabla \cdot \mathbf{v} = 0. \quad (16)$$

Now, the four equations (13)–(16) must hold in the whole set  $Q$ . The system is completed with boundary conditions for  $c$ ,  $\theta$  and  $\mathbf{v}$  on  $\partial\Omega \times (0, T)$ :

$$(D\nabla c) \cdot \mathbf{n} = 0 \text{ on } \partial\Omega \times (0, T), \quad (17)$$

$$(\chi\nabla\theta) \cdot \mathbf{n} = 0 \text{ on } \Gamma_N \times (0, T), \quad (18)$$

$$\theta = 0 \text{ on } \Gamma_D \times (0, T), \quad (19)$$

$$\mathbf{v} = \mathbf{0} \text{ on } \partial\Omega \times (0, T). \quad (20)$$

Finally, we add initial conditions:

$$c(\mathbf{x}, 0) = c_0(\mathbf{x}); \quad \theta(\mathbf{x}, 0) = \theta_0(\mathbf{x}); \quad \mathbf{v}(\mathbf{x}, 0) = \mathbf{v}_0(\mathbf{x}) \text{ in } \Omega. \quad (21)$$

Let us now justify the introduction of (13)–(16). Assume that, as  $\varepsilon \rightarrow 0$ , the associated solutions to (13)–(16) remain bounded. For small  $\varepsilon$ , the term  $F_i^\varepsilon$  becomes very large in the solid part of the domain, where  $f_s \approx 1$ ; thus, in this set the velocity field is at least  $O(\varepsilon^3)$  and converges to zero. Contrarily, in any open set  $\mathcal{O} \subset\subset Q_{ml}$ ,  $F_i^\varepsilon$  remains bounded and converges in some sense to  $F_i$ . This gives the motion equation (3) in the limit.

This explanation clarifies the role of  $F_i^\varepsilon$  in the regularized problem:  $F_i^\varepsilon$  is a coefficient that blows up in the solidified part of the domain and remains bounded in the other part (there, it is related to dissipation). These properties of  $F_i^\varepsilon$  will be established rigorously when  $d = 2$  in Section 2.3.

**2. Existence and uniqueness results.** In this Section, we analyze the existence of weak solutions to the regularized solidification problem. The problem is given by equations (13)–(16) and the boundary and initial conditions are given by (17)–(21). We will also prove a uniqueness result when  $d = 2$ . Finally, we will show that, at least when  $d = 2$ , the solutions to the regularized problems converge (in an appropriate sense) towards a weak solution to the original problem.

The proofs of the results that follow are more or less standard. Maybe, the most interesting points are the following:

- The estimates  $0 \leq c \leq c_\varepsilon$ .
- The energy estimates of  $c^\varepsilon$ ,  $\theta^\varepsilon$  and  $\mathbf{v}^\varepsilon$ , that are independent of  $\varepsilon$ .
- The fact that  $c^\varepsilon$  and  $\theta^\varepsilon$  are actually strong solutions if  $c^0$  and  $\theta^0$  are regular enough and
- The estimates of  $c^\varepsilon$  and  $\theta^\varepsilon$  in a space of Hölder-continuous functions in  $\bar{Q}$  when  $d = 2$ .

Some previous works concerning this topic are [6, 10, 9].

**2.1. Preliminaries and weak formulation.** In the sequel, we consider the usual Sobolev spaces, given by

$$W^{m,p}(\Omega) = \{ f \in L^p(\Omega) : \partial^\alpha f \in L^p(\Omega) \quad \forall |\alpha| \leq m \}$$

for all  $m \geq 1$  and  $1 \leq p \leq +\infty$ . When  $p = 2$ , we write  $H^m(\Omega)$  instead of  $W^{m,2}(\Omega)$ ; we will denote by  $H_0^m(\Omega)$  the closure of  $C_0^\infty(\Omega)$  in  $H^m(\Omega)$ . Sometimes, we will also need to work with the Sobolev spaces  $W^{r,p}(\Omega)$ , where  $r \in \mathbb{R}_+$ ; for the definitions and main properties, see for instance [1]. If there is no confusion, we write  $L^p$  instead of  $L^p(\Omega)$ ,  $H^m$  instead of  $H^m(\Omega)$ , etc.

For any  $\tau \in [0, 1)$ , we will denote by  $C^{0,\tau,\tau/2}(\bar{Q})$  the space of functions  $\varphi \in C^0(\bar{Q})$  that are Hölder-continuous in the following sense:

$$\sup_{(\mathbf{x},t),(\mathbf{x}',t') \in \bar{Q}} \frac{|\varphi(\mathbf{x},t) - \varphi(\mathbf{x}',t')|}{|\mathbf{x} - \mathbf{x}'|^\tau + |t - t'|^{\tau/2}} < +\infty.$$

In general, we will denote by  $\|\cdot\|_X$  the norm of the normed space  $X$ . If  $X$  is a Banach space and  $1 \leq q \leq +\infty$ , we denote by  $L^q(0, T; X)$  the Banach space of the  $X$ -valued (classes of) functions defined on the interval  $[0, T]$  that are  $L^q$ -integrable in the sense of Bochner. On the other hand,  $C^0([0, T]; X)$  and  $C_w^0([0, T]; X)$  will respectively denote the spaces of continuous and weakly continuous functions  $f : [0, T] \mapsto X$ . Sometimes we write  $L^q(X)$  instead of  $L^q(0, T; X)$ , etc.

Spaces of  $\mathbb{R}^d$ -valued functions, as well as their elements, are usually denoted by bold faced letters.

We will consider the space

$$\mathcal{V}(\Omega) = \{ \mathbf{v} \in C_0^\infty(\Omega) : \nabla \cdot \mathbf{v} = 0 \text{ in } \Omega \}.$$

Let  $\mathbf{H}$  and  $\mathbf{V}$  respectively stand for the closures of  $\mathcal{V}(\Omega)$  in  $L^2(\Omega)$  and  $\mathbf{H}^1(\Omega)$ . It is then possible to show that

$$\begin{aligned} \mathbf{H} &= \{ \mathbf{v} \in L^2(\Omega) : \nabla \cdot \mathbf{v} = 0 \text{ in } \Omega, \mathbf{v} \cdot \mathbf{n} = 0 \text{ on } \partial\Omega \}, \\ \mathbf{V} &= \{ \mathbf{v} \in \mathbf{H}_0^1(\Omega) : \nabla \cdot \mathbf{v} = 0 \text{ in } \Omega \}, \end{aligned}$$

where  $\mathbf{n}$  is the outward unit normal vector to  $\partial\Omega$ , see for instance [19].

In the sequel, we denote by  $C$  a generic positive constant depending only on  $\Omega$  and the other data of the problem. As usual, it may have different values in different expressions. We will sometimes emphasize that the constants may have different values by putting  $C_1, C_2, \dots$ . We will emphasize that  $C$  depends on a specific data  $D$  (a set, a parameter,  $\dots$ ), by writing  $C(D)$ .

For the weak formulation of the regularized solidification problem described by (13)–(21), we will also need the following space:

$$\mathcal{H}_\theta(\Omega) = \{ \psi \in H^1(\Omega) : \psi = 0 \text{ on } \Gamma_D \}.$$

Notice that the function  $c_l$  in (11) satisfies

$$c_l \in W_{loc}^{1,\infty}(\mathbb{R}^2). \tag{22}$$

This is a consequence of the fact that  $f_s$  is Lipschitz-continuous. Moreover,  $c_l \equiv c_e$  for  $c \geq c_e$  and  $c_l \equiv 0$  for  $c \leq 0$ .

From now on, we will assume that

$$h \in L^2(\omega \times (0, T)), \tag{23}$$

$$c_0 \in L^\infty(\Omega), \quad 0 \leq c_0(\mathbf{x}) \leq c_e \quad \text{a.e. in } \Omega, \tag{24}$$

$$\theta_0 \in L^2(\Omega), \tag{25}$$

$$\mathbf{v}_0 \in \mathbf{H}, \tag{26}$$

$$\mathbf{g} \in L^\infty(\Omega). \tag{27}$$

**Definition 2.1.** We say that  $(c, \theta, \mathbf{v})$  is a *weak solution* of (13)–(21) if

$$c \in L^2(0, T; H^1(\Omega)) \cap L^\infty(0, T; L^2(\Omega)), \tag{28}$$

$$\theta \in L^2(0, T; \mathcal{H}_\theta(\Omega)) \cap L^\infty(0, T; L^2(\Omega)), \tag{29}$$

$$\mathbf{v} \in L^2(0, T; \mathbf{V}) \cap L^\infty(0, T; \mathbf{H}), \tag{30}$$

the following relations hold in  $(0, T)$

$$\langle c_t, \varphi \rangle + \int_\Omega \mathbf{v} \cdot \nabla c_l(c, \theta) \varphi + \int_\Omega D \nabla c \cdot \nabla \varphi = 0, \tag{31}$$

$$\langle \theta_t, \psi \rangle + \int_\Omega \mathbf{v} \cdot \nabla \theta \psi + \int_\Omega \chi \nabla \theta \cdot \nabla \psi = \int_\omega h \psi, \tag{32}$$

$$\langle \mathbf{v}_t, \mathbf{w} \rangle + \int_\Omega (\mathbf{v} \cdot \nabla) \mathbf{v} \cdot \mathbf{w} + \int_\Omega \nu \nabla \mathbf{v} \cdot \nabla \mathbf{w} + \int_\Omega F_i^\varepsilon(c, \theta) \mathbf{v} \cdot \mathbf{w} = \int_\Omega \mathbf{F}_e \cdot \mathbf{w}, \tag{33}$$

for all  $\varphi \in H^1(\Omega)$ ,  $\psi \in \mathcal{H}_\theta(\Omega)$  and  $\mathbf{w} \in \mathbf{V}$  and

$$c|_{t=0} = c_0, \quad \theta|_{t=0} = \theta_0, \quad \mathbf{v}|_{t=0} = \mathbf{v}_0. \tag{34}$$

Let us assume that (23)–(27) holds. It can be shown that any  $(c, \theta, \mathbf{v})$  satisfying (28)–(30) and (31)–(33) also satisfies  $c \in C^0([0, T]; L^2(\Omega))$  and, furthermore,  $\theta \in C^0([0, T]; L^2(\Omega))$  and  $\mathbf{v} \in C^0([0, T]; \mathbf{H})$  if  $d = 2$  and  $\theta \in C_w^0([0, T]; L^2(\Omega))$  and  $\mathbf{v} \in C_w^0([0, T]; \mathbf{H})$  if  $d = 3$ ; the argument is given below, in the proof of Theorem 2.2. In particular, the initial conditions (34) make sense.

Another property satisfied by  $c$  is the following. Let us introduce the quantity

$$c_g := \int_\Omega c_0(\mathbf{x}),$$

i.e. the initial total amount of solute in the moisture. By using (24), we see that  $0 \leq c_g \leq c_e |\Omega| < +\infty$ . Furthermore, if we take  $\varphi = 1$  in (31), a short computation shows that

$$\frac{d}{dt} \int_\Omega c(\mathbf{x}, t) = - \int_{\partial\Omega} (\mathbf{v} \cdot \mathbf{n}) c_l d\Gamma = 0 \quad \forall t \in (0, T).$$

Thus,  $\int_{\Omega} c(\mathbf{x}, t)$  is constant in time and

$$\int_{\Omega} c(\mathbf{x}, t) = c_g = \int_{\Omega} c_0(\mathbf{x}) \quad \forall t \in (0, T).$$

In other words, the amount of solute in the moisture does not depend on time.

**2.2. On the existence and uniqueness of solution of the regularized problem.** In the proof of existence of a weak solution to the regularized problem, we will use the following result:

**Proposition 1.** *Assume that  $(c, \theta, \mathbf{v})$  is a weak solution to (13)–(21). Then*

$$0 \leq c(\mathbf{x}, t) \leq c_e \quad \text{a.e. in } Q.$$

*Proof.* Let us denote by  $\varphi_+$  (resp.  $\varphi_-$ ) the positive (resp. negative) part of  $\varphi$ . For each  $t \in [0, T]$ , let us choose  $\varphi = c_-(\cdot, t)$  in (31). Since  $c = c_+ - c_-$ , taking into account the definition of  $c_l$ , we easily get:

$$-\frac{1}{2} \frac{d}{dt} \|c_-\|_{L^2}^2 - D \|\nabla c_-\|_{L^2}^2 = 0.$$

Integrating in time, we have

$$-\frac{1}{2} \|c_-(\cdot, t)\|_{L^2}^2 - D \int_0^t \|\nabla c_-\|_{L^2}^2 ds = -\frac{1}{2} \|(c_0)_-\|_{L^2}^2 = 0.$$

Therefore,  $\|c_-(\cdot, t)\|_{L^2} = 0$  for all  $t$ , that is,  $c \geq 0$ .

Now, for each  $t \in [0, T]$ , we choose  $\varphi = (c - c_e)_+(\cdot, t)$  in (31). By using an argument similar to the previous one, we obtain that

$$\frac{1}{2} \|(c(\cdot, t) - c_e)_+\|_{L^2}^2 + D \int_0^t \|\nabla (c - c_e)_+\|_{L^2}^2 ds = \frac{1}{2} \|(c_0 - c_e)_+\|_{L^2}^2 = 0$$

for all  $t \in [0, T]$ , whence  $c \leq c_e$ . □

Our first result concerns the existence of a solution to (13)–(21):

**Theorem 2.2.** *There exists at least one weak solution  $(c, \theta, \mathbf{v})$  to the regularized problem (13)–(21), with  $0 \leq c \leq c_e$ .*

*Proof.* We will introduce Galerkin approximations. To this end, we will consider three “special” bases

$$\mathcal{B}_c = \{\varphi_k(\mathbf{x}) : k \in \mathbb{N}\}, \quad \mathcal{B}_\theta = \{\psi_k(\mathbf{x}) : k \in \mathbb{N}\} \quad \text{and}$$

$$\mathcal{B}_\mathbf{v} = \{\mathbf{w}_k(\mathbf{x}) : k \in \mathbb{N}\},$$

respectively in  $H^1(\Omega)$ ,  $\mathcal{H}_\theta(\Omega)$  and  $\mathbf{V}$ .

It will be assumed that they are orthogonal for the scalar product in  $H^1$  and orthonormal for the scalar product in  $L^2$ . Obviously, this is the case if the  $\varphi_k$  are the eigenfunctions of the Neumann Laplacian in  $\Omega$ , that is,

$$\begin{cases} -\Delta \varphi_k = \lambda_k \varphi_k, & x \in \Omega, \\ \nabla \varphi_k \cdot \mathbf{n} = 0, & x \in \partial\Omega, \\ \|\varphi_k\|_{L^2} = 1, \end{cases}$$

and similar definitions hold for  $\psi_k$  and  $\mathbf{w}_k$ .

Let us fix  $m \in \mathbb{N}$ . We consider the  $m$ -dimensional spaces  $\mathcal{S}_c^m$ ,  $\mathcal{S}_\theta^m$  and  $\mathcal{S}_\mathbf{v}^m$ , respectively spanned by the first  $m$  functions of  $\mathcal{B}_c$ ,  $\mathcal{B}_\theta$  and  $\mathcal{B}_\mathbf{v}$ .



For any  $t$ , we define the approximations  $c^m$ ,  $\theta^m$  and  $\mathbf{v}^m$  as follows:

$$\begin{aligned} c^m(\mathbf{x}, t) &= \sum_{k=1}^m \lambda_{k,m}(t) \varphi_k(\mathbf{x}), \\ \theta^m(\mathbf{x}, t) &= \sum_{k=1}^m \xi_{k,m}(t) \psi_k(\mathbf{x}), \\ \mathbf{v}^m(\mathbf{x}, t) &= \sum_{k=1}^m \sigma_{k,m}(t) \mathbf{w}_k(\mathbf{x}). \end{aligned}$$

The coefficients  $\lambda_{k,m}(t)$ ,  $\xi_{k,m}(t)$  and  $\sigma_{k,m}(t)$  are computed in such way that

$$\langle c_t^m, \varphi_k \rangle + \int_{\Omega} \mathbf{v}^m \cdot \nabla c_l(c^m, \theta^m) \varphi_k + \int_{\Omega} D \nabla c^m \cdot \nabla \varphi_k = 0, \tag{35}$$

$$\langle \theta_t^m, \psi_k \rangle + \int_{\Omega} \mathbf{v}^m \cdot \nabla \theta^m \psi_k + \int_{\Omega} \chi \nabla \theta^m \cdot \nabla \psi_k = \int_{\omega} h \psi_k, \tag{36}$$

$$\begin{aligned} \langle \mathbf{v}_t^m, \mathbf{w}_k \rangle + \int_{\Omega} (\mathbf{v}^m \cdot \nabla) \mathbf{v}^m \cdot \mathbf{w}_k + \int_{\Omega} \nu \nabla \mathbf{v}^m \cdot \nabla \mathbf{w}_k \\ + \int_{\Omega} F_i^\varepsilon(c^m, \theta^m) \mathbf{v}^m \cdot \mathbf{w}_k = \int_{\Omega} \mathbf{F}_e(c^m, \theta^m) \cdot \mathbf{w}_k, \end{aligned} \tag{37}$$

for all  $k = 1, \dots, m$  and

$$c^m(\cdot, 0) = P_{c,m}(c_0), \quad \theta^m(\cdot, 0) = P_{\theta,m}(\theta_0), \quad \mathbf{v}^m(\cdot, 0) = \mathbf{P}_{\mathbf{v},m}(\mathbf{v}_0). \tag{38}$$

Here,  $P_{c,m} : H^1(\Omega) \mapsto \mathcal{S}_c^m$ ,  $P_{\theta,m} : \mathcal{H}_\theta(\Omega) \mapsto \mathcal{S}_\theta^m$  and  $\mathbf{P}_{\mathbf{v},m} : \mathbf{V} \mapsto \mathcal{S}_{\mathbf{v}}^m$  are the orthogonal projectors.

For each  $m$ , (35)–(37) is an ordinary differential system for the unknowns  $\lambda_{k,m}(t)$ ,  $\xi_{k,m}(t)$  and  $\sigma_{k,m}(t)$ . It is complemented with the initial conditions (38). This initial value problem has a local in time solution  $(c^m, \theta^m, \mathbf{v}^m)$  defined in some interval  $[0, t^m)$ . In order to prove that  $t^m = T$ , we need to show some a priori estimates.

If we multiply equations (35), (36) and (37) by  $\lambda_{k,m}(t)$ ,  $\xi_{k,m}(t)$  and  $\sigma_{k,m}(t)$ , respectively, and we sum over  $k$ , we obtain (using that  $\mathbf{v}^m \in \mathbf{V}$ ):

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \|c^m\|_{L^2}^2 + D \|\nabla c^m\|_{L^2}^2 &= - \int_{\Omega} \mathbf{v}^m \cdot \nabla c_l(c^m, \theta^m) c^m \\ \frac{1}{2} \frac{d}{dt} \|\theta^m\|_{L^2}^2 + \chi \|\nabla \theta^m\|_{L^2}^2 &= \int_{\omega} h \theta^m \\ \frac{1}{2} \frac{d}{dt} \|\mathbf{v}^m\|_{L^2}^2 + \nu \|\nabla \mathbf{v}^m\|_{L^2}^2 &= \int_{\Omega} \mathbf{F}_e(c^m, \theta^m) \cdot \mathbf{v}^m - \int_{\Omega} F_i^\varepsilon(c^m, \theta^m) |\mathbf{v}^m|^2 \end{aligned}$$

Now, we have to estimate the terms in the right-hand side of these inequalities. By using (22) and Hölder and Young inequalities, we can bound the first term as follows:

$$\begin{aligned} \left| \int_{\Omega} \mathbf{v}^m \cdot \nabla c_l(c^m, \theta^m) c^m \right| &= \left| - \int_{\Omega} c_l(c^m, \theta^m) \mathbf{v}^m \cdot \nabla c^m \right| \\ &\leq \frac{D}{2} \|\nabla c^m\|_{L^2}^2 + C_1 \|\mathbf{v}^m\|_{L^2}^2. \end{aligned} \tag{39}$$

By using Poincaré and Young inequalities, we find the following for the second term:

$$\int_{\omega} h\theta^m \leq C_2 \|h\|_{L^2(\omega)}^2 + \frac{\chi}{2} \|\nabla\theta^m\|_{L^2}^2. \tag{40}$$

Finally, for the third term we have

$$\begin{aligned} \left| \int_{\Omega} \mathbf{F}_e(c^m, \theta^m) \cdot \mathbf{v}^m \right| &\leq C_3 \|\theta^m\|_{L^2} \|\mathbf{v}^m\|_{L^2} + C_4 + \frac{1}{2} \|\mathbf{v}^m\|_{L^2}^2 \\ &\leq C_4 + C_3 \|\mathbf{v}^m\|_{L^2}^2 + C_5 \|\theta^m\|_{L^2}^2. \end{aligned} \tag{41}$$

Taking into account (39)–(41), we deduce that

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} (\|c^m\|_{L^2}^2 + \|\theta^m\|_{L^2}^2 + \|\mathbf{v}^m\|_{L^2}^2) \\ \leq C_6 (1 + \|h\|_{L^2(\omega)}^2) + C_7 (\|c^m\|_{L^2}^2 + \|\theta^m\|_{L^2}^2 + C_3 \|\mathbf{v}^m\|_{L^2}^2). \end{aligned} \tag{42}$$

Let us introduce  $f := \|c^m(t)\|_{L^2}^2 + \|\theta^m(t)\|_{L^2}^2 + \|\mathbf{v}^m(t)\|_{L^2}^2$ . Then, integrating (42) with respect to  $t$ , we obtain:

$$\begin{aligned} f(t) &\leq f(0) + C \int_0^t (1 + \|h\|_{L^2(\omega)}^2) ds + C \int_0^t f(s) ds \\ &\leq f(0) + C \int_0^T (1 + \|h\|_{L^2(\omega)}^2) ds + C \int_0^t f(s) ds \end{aligned}$$

From Gronwall’s lemma, we have for all  $t \in [0, T]$

$$f(t) \leq \left( f(0) + C \int_0^T (1 + \|h\|_{L^2(\omega)}^2) ds \right) e^{Ct}.$$

We conclude that  $t^m = T$  and, also, that the following estimates hold:

$$\begin{aligned} c^m \text{ and } \theta^m \text{ are bounded in } L^2(0, T; H^1) \cap L^\infty(0, T; L^2), \\ \mathbf{v}^m \text{ is bounded in } L^2(0, T; \mathbf{V}) \cap L^\infty(0, T; \mathbf{H}). \end{aligned} \tag{43}$$

Unfortunately, (43) does not suffice to pass to the limit in (35)–(38). We also need uniform estimates of  $c_t^m$ ,  $\theta_t^m$  and  $\mathbf{v}_t^m$ , for instance in  $L^\sigma(0, T; (H^1(\Omega))')$ ,  $L^\sigma(0, T; (\mathcal{H}_\theta(\Omega))')$  and  $L^\sigma(0, T; \mathbf{V}')$  for some  $\sigma > 1$ . We will now prove that this is indeed the case.

Thus, we first notice that

$$\langle c_t^m, \varphi_k \rangle = - \int_{\Omega} \mathbf{v}^m \cdot \nabla c_l(c^m, \theta^m) \varphi_k - \int_{\Omega} D\nabla c^m \cdot \nabla \varphi_k$$

for all  $k = 1, \dots, m$ . Consequently,  $c_t^m = \tilde{P}_{c,m} (-\mathbf{v}^m \cdot \nabla c_l(c^m, \theta^m) - D\Delta c^m)$ , where  $\tilde{P}_{c,m} : (H^1(\Omega))' \mapsto \mathcal{S}_c^m$  is the usual orthogonal projector. In view of the choice that we have made of  $\mathcal{B}_c$ , we have:

$$\begin{aligned} \|c_t^m\|_{(H^1)'} &= \left\| \tilde{P}_{c,m} (-\mathbf{v}^m \cdot \nabla c_l(c^m, \theta^m) - D\Delta c^m) \right\|_{(H^1)'} \\ &\leq C \|c_l(c^m, \theta^m) \mathbf{v}^m + D\nabla c^m\|_{L^2} \\ &\leq C (\|\mathbf{v}^m\|_{L^2} + \|\nabla c^m\|_{L^2}), \end{aligned}$$

which is uniformly bounded in  $L^2(0, T)$ , by (43). Consequently,

$$\|c_t^m\|_{L^2(0,T;(H^1)')} \leq C \quad \text{if } d = 2, 3.$$

A similar argument shows that

$$\|\theta_t^m\|_{(\mathcal{H}_\theta)'} \leq C (\|\theta^m \mathbf{v}^m\|_{L^2} + \|\nabla \theta^m\|_{L^2} + \|h\|_{L^2(\omega)}). \tag{44}$$

Notice that

$$\begin{aligned} \|\theta^m \mathbf{v}^m\|_{L^2} &\leq C \|\theta^m\|_{L^4} \|\mathbf{v}^m\|_{L^4} \\ &\leq C \|\theta^m\|_{L^2}^\alpha \|\nabla \theta^m\|_{L^2}^{1-\alpha} \|\mathbf{v}^m\|_{L^2}^\alpha \|\nabla \mathbf{v}^m\|_{L^2}^{1-\alpha} \\ &\leq C + C \|\nabla \theta^m\|_{L^2}^{2(1-\alpha)} + C \|\nabla \mathbf{v}^m\|_{L^2}^{2(1-\alpha)} \end{aligned} \tag{45}$$

where  $\alpha = 1/2$  for  $d = 2$  and  $\alpha = 1/4$  if  $d = 3$ . From (43), (44) and (45), it is immediate that

$$\|\theta_t^m\|_{L^\sigma(0,T;(\mathcal{H}_\theta)')} \leq C,$$

where  $\sigma = 2$  if  $d = 2$  and  $\sigma = 4/3$  if  $d = 3$ . In a very similar way, it can be shown that

$$\|\mathbf{v}_t^m\|_{L^\sigma(0,T;\mathbf{V}')} \leq C.$$

Therefore, the classical compactness method can be applied in order to deduce a strong convergence property and we can now pass to the limit in (35)–(38):

We can extract several subsequences of  $\{c^m(t)\}_m$ ,  $\{\theta^m(t)\}_m$  and  $\{\mathbf{v}^m(t)\}_m$ , all them being indexed again with  $m$ , with appropriate convergence properties:

$$\begin{aligned} c^m &\rightarrow c \text{ weakly in } L^2(H^1), \text{ weakly-* in } L^\infty(L^2) \text{ and strongly in } L^2(L^2), \\ \theta^m &\rightarrow \theta \text{ weakly in } L^2(\mathcal{H}_\theta), \text{ weakly-* in } L^\infty(L^2) \text{ and strongly in } L^2(L^2), \\ \mathbf{v}^m &\rightarrow \mathbf{v} \text{ weakly in } L^2(\mathbf{V}), \text{ weakly-* in } L^\infty(\mathbf{H}) \text{ and strongly in } L^2(\mathbf{H}). \end{aligned}$$

Here, the notation has been abridged. For instance,  $L^2(H^1)$  stands for  $L^2(0, T; H^1(\Omega))$ , etc.

These sequences can be chosen in such way that they converge a.e. in  $Q$ . It is now well known that we can take limits in (35)–(37) and obtain

$$\begin{aligned} \langle c_t, \varphi_k \rangle + \int_\Omega \mathbf{v} \cdot \nabla c_l(c, \theta) \varphi_k + \int_\Omega D \nabla c \cdot \nabla \varphi_k &= 0, \\ \langle \theta_t, \psi_k \rangle + \int_\Omega \mathbf{v} \cdot \nabla \theta \psi_k + \int_\Omega \chi \nabla \theta \cdot \nabla \psi_k &= \int_\omega h \psi_k, \\ \langle \mathbf{v}_t, \mathbf{w}_k \rangle + \int_\Omega (\mathbf{v} \cdot \nabla) \mathbf{v} \cdot \mathbf{w}_k + \int_\Omega \nu \nabla \mathbf{v} \cdot \nabla \mathbf{w}_k \\ &+ \int_\Omega F_i^\varepsilon(c, \theta) \mathbf{v} \cdot \mathbf{w}_k = \int_\Omega \mathbf{F}_e(c, \theta) \cdot \mathbf{w}_k, \end{aligned}$$

for all  $k \geq 1$ .

It is also clear that one can take limits as  $m \rightarrow +\infty$  in (38). Indeed, we have

$$c^m(\cdot, 0) \rightarrow c(\cdot, 0) \text{ weakly in } L^2$$

and

$$c^m(\cdot, 0) = P_{c,m}(c_0) \rightarrow c_0 \text{ strongly in } L^2,$$

whence  $c(\cdot, 0) = c_0$ . Similarly, we can prove that  $\theta(\cdot, 0) = \theta_0$  and  $\mathbf{v}(\cdot, 0) = \mathbf{v}_0$ .

Recall that the functions  $c_t^m$  are uniformly bounded in  $L^2(0, T; (H^1(\Omega))')$  and this implies  $c_t \in L^2(0, T; (H^1(\Omega))')$  and, consequently,  $c \in C^0([0, T]; L^2(\Omega))$ .

When  $d = 2$ , the functions  $\theta_t^m$  are uniformly bounded in  $L^2(0, T; (\mathcal{H}_\theta(\Omega))')$  whence, again,  $\theta \in C^0([0, T]; L^2(\Omega))$ . For a similar reason, we also have  $\mathbf{v} \in C^0([0, T]; \mathbf{H})$ . When  $d = 3$ ,  $\theta_t^m$  is only uniformly bounded in  $L^{4/3}(0, T; (\mathcal{H}_\theta(\Omega))')$  and all we can deduce is that  $\theta \in C_w^0([0, T]; L^2(\Omega))$ , see [19]. Analogously, we only get in this case  $\mathbf{v} \in C_w^0([0, T]; \mathbf{H})$ .

In view of proposition 1, we see that  $(c, \theta, \mathbf{v})$  is a weak solution of the regularized problem (13)–(21). □

We will now prove that, when  $d = 2$ , (13)–(21) possesses at most one weak solution:

**Theorem 2.3.** *Assume that  $d = 2$ . Then (13)–(21) possesses exactly one weak solution.*

*Proof.* Let us assume that  $(c^1, \theta^1, \mathbf{v}^1)$  and  $(c^2, \theta^2, \mathbf{v}^2)$  are weak solutions of the regularized problem and let us set  $(c, \theta, \mathbf{v}) = (c^1, \theta^1, \mathbf{v}^1) - (c^2, \theta^2, \mathbf{v}^2)$ . Then we have for some  $p$ :

$$c_t + \nabla \cdot (\mathbf{v}^1 c_l(c^1, \theta^1) - \mathbf{v}^2 c_l(c^2, \theta^2) - D\nabla c) = 0 \tag{46}$$

$$\theta_t + \nabla \cdot (\mathbf{v}^1 \theta^1 - \mathbf{v}^2 \theta^2 - \chi \nabla \theta) = 0 \tag{47}$$

$$\begin{aligned} \mathbf{v}_t + \nabla \cdot (\mathbf{v}^1 \otimes \mathbf{v}^1 - \mathbf{v}^2 \otimes \mathbf{v}^2 - \nu \nabla \mathbf{v}) + F_i^1 \mathbf{v}^1 - F_i^2 \mathbf{v}^2 + \nabla p \\ = \mathbf{F}_e(c^1, \theta^1) - \mathbf{F}_e(c^2, \theta^2) \end{aligned} \tag{48}$$

$$\nabla \cdot \mathbf{v} = 0 \tag{49}$$

where we have put  $F_i^k = F_i^\varepsilon(c^k, \theta^k)$  for  $k = 1, 2$ .

By summing and subtracting  $\nabla \cdot (\mathbf{v}^1 c_l(c^2, \theta^2))$  in (46),  $\mathbf{v}^1 \theta^2$  in (47) and  $\mathbf{v}^1 \otimes \mathbf{v}^2$  and  $F_i^1 \mathbf{v}^2$  in (48), we obtain:

$$c_t + \nabla \cdot (\mathbf{v}^1 [c_l^1 - c_l^2] + \mathbf{v} c_l^2 - D\nabla c) = 0, \tag{50}$$

$$\theta_t + \nabla \cdot (\mathbf{v}^1 \theta + \mathbf{v} \theta^2 - \chi \nabla \theta) = 0, \tag{51}$$

$$\begin{aligned} \mathbf{v}_t + \nabla \cdot (\mathbf{v}^1 \otimes \mathbf{v} - \mathbf{v} \otimes \mathbf{v}^2 - \nu \nabla \mathbf{v}) + F_i^1 \mathbf{v} + (F_i^1 - F_i^2) \mathbf{v}^2 + \nabla p \\ = (\beta_\theta \theta + \beta_c (c_l^1 - c_l^2)) \mathbf{g}, \end{aligned} \tag{52}$$

$$\nabla \cdot \mathbf{v} = 0. \tag{53}$$

Here, we have put  $c_l^k = c_l(c^k, \theta^k)$  for  $k = 1, 2$ .

Now, we multiply (50), (51) and (52) respectively by  $c$ ,  $\theta$  and  $\mathbf{v}$  and we integrate in space:

$$\frac{1}{2} \frac{d}{dt} \|c\|_{L^2}^2 + \frac{D}{2} \|\nabla c\|_{L^2}^2 = \int_{\Omega} c_l^2 \mathbf{v} \cdot \nabla c + \int_{\Omega} [c_l^1 - c_l^2] \mathbf{v}^1 \cdot \nabla c, \tag{54}$$

$$\frac{1}{2} \frac{d}{dt} \|\theta\|_{L^2}^2 + \frac{\chi}{2} \|\nabla \theta\|_{L^2}^2 = \int_{\Omega} \theta^2 \mathbf{v} \cdot \nabla \theta, \tag{55}$$

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \|\mathbf{v}\|_{L^2}^2 + \frac{\nu}{2} \|\nabla \mathbf{v}\|_{L^2}^2 + \int_{\Omega} F_i^1 |\mathbf{v}|^2 = - \int_{\Omega} \nabla \cdot (\mathbf{v} \otimes \mathbf{v}^2) \cdot \mathbf{v} \\ - \int_{\Omega} (F_i^1 - F_i^2) \mathbf{v}^2 \cdot \mathbf{v} + \int_{\Omega} (\beta_\theta \theta + \beta_c (c_l^1 - c_l^2)) \mathbf{g} \cdot \mathbf{v}. \end{aligned} \tag{56}$$

In view of (22), we have

$$\left| \int_{\Omega} c_l^2 \mathbf{v} \cdot \nabla c \right| \leq \delta \|\nabla c\|_{L^2}^2 + C_\delta \|\mathbf{v}\|_{L^2}^2 \quad \forall \delta > 0 \tag{57}$$

and, on the other hand,

$$\begin{aligned}
\left| \int_{\Omega} [c_l^1 - c_l^2] \mathbf{v}^1 \cdot \nabla c \right| &\leq C \int_{\Omega} (|c| + |\theta|) |\mathbf{v}^1| |\nabla c| \\
&\leq C (\|c\|_{L^4} + \|\theta\|_{L^4}) \|\mathbf{v}^1\|_{L^4} \|\nabla c\|_{L^2} \\
&\leq C \left( \|c\|_{L^2}^{1/2} \|\nabla c\|_{L^2}^{1/2} + \|\theta\|_{L^2}^{1/2} \|\nabla \theta\|_{L^2}^{1/2} \right) \|\mathbf{v}^1\|_{L^4} \|\nabla c\|_{L^2} \\
&\leq \delta \|\nabla c\|_{L^2}^2 + C_{\delta} \|\mathbf{v}^1\|_{L^4}^4 \|c\|_{L^2}^2 + \delta \|\nabla c\|_{L^2}^{4/3} \|\nabla \theta\|_{L^2}^{2/3} + C_{\delta} \|\mathbf{v}^1\|_{L^4}^4 \|\theta\|_{L^2}^2 \\
&\leq C\delta \|\nabla c\|_{L^2}^2 + C\delta \|\nabla \theta\|_{L^2}^2 + C_{\delta} \|\mathbf{v}^1\|_{L^4}^4 (\|\theta\|_{L^2}^2 + \|c\|_{L^2}^2).
\end{aligned} \tag{58}$$

(Notice that the last three inequalities only hold when  $d = 2$ ).

Let us introduce the function  $H_{\varepsilon} : [0, 1] \mapsto \mathbb{R}$ , with  $H_{\varepsilon}(f) = M_0 f^2 (1 - f + \varepsilon)^{-3}$  for all  $f \in [0, 1]$ . From (12), we can write:

$$\begin{aligned}
F_i^1 - F_i^2 &= F_i^{\varepsilon}(c^1, \theta^1) - F_i^{\varepsilon}(c^2, \theta^2) = H_{\varepsilon}(f_s(c^1, \theta^1)) - H_{\varepsilon}(f_s(c^2, \theta^2)) \\
&= H'_{\varepsilon}(\hat{f})(f_s(c^1, \theta^1) - f_s(c^2, \theta^2)) = H'_{\varepsilon}(\hat{f})(a_s^{1,2}c + b_s^{1,2}\theta)
\end{aligned}$$

for some  $\hat{f}, a_s^{1,2}, b_s^{1,2} \in L^{\infty}(\Omega)$ , with  $0 \leq \hat{f} \leq 1$ . Then

$$\begin{aligned}
\left| -\int_{\Omega} (F_i^1 - F_i^2) \mathbf{v}^2 \cdot \mathbf{v} \right| &= \left| -\int_{\Omega} H'_{\varepsilon}(\hat{f})(a_s^{1,2}c + b_s^{1,2}\theta) \mathbf{v}^2 \cdot \mathbf{v} \right| \\
&\leq C_1 \int_{\Omega} |c| |\mathbf{v}^2| |\mathbf{v}| + C_2 \int_{\Omega} |\theta| |\mathbf{v}^2| |\mathbf{v}|.
\end{aligned} \tag{59}$$

Arguing as before, we thus find that

$$\begin{aligned}
\left| -\int_{\Omega} (F_i^1 - F_i^2) \mathbf{v}^2 \cdot \mathbf{v} \right| &\leq C\delta (\|\nabla c\|_{L^2}^2 + \|\nabla \theta\|_{L^2}^2 + \|\nabla \mathbf{v}\|_{L^2}^2) \\
&\quad + C_{\delta} \|\mathbf{v}^2\|_{L^4}^4 (\|c\|_{L^2}^2 + \|\theta\|_{L^2}^2),
\end{aligned} \tag{60}$$

for all  $\delta > 0$ .

Finally, since  $\mathbf{g} \in \mathbf{L}^{\infty}(\Omega)$ , we also have

$$\begin{aligned}
\left| \int_{\Omega} (\beta_{\theta}\theta + \beta_c(c_l^1 - c_l^2)) \mathbf{g} \cdot \mathbf{v} \right| &\leq C_1 \int_{\Omega} |\theta| |\mathbf{v}| + C_2 \int_{\Omega} |c_l^1 - c_l^2| |\mathbf{v}| \\
&\leq C_3 \int_{\Omega} |c| |\mathbf{v}| + C_4 \int_{\Omega} |\theta| |\mathbf{v}| \\
&\leq C (\|c\|_{L^2}^2 + \|\theta\|_{L^2}^2 + \|\mathbf{v}\|_{L^2}^2).
\end{aligned} \tag{61}$$

Therefore, taking into account (54)–(61), we obtain that

$$\begin{aligned} & \frac{1}{2} \frac{d}{dt} \left( \|c\|_{L^2}^2 + \|\theta\|_{L^2}^2 + \|\mathbf{v}\|_{L^2}^2 \right) + C \left( \|\nabla c\|_{L^2}^2 + \|\nabla \theta\|_{L^2}^2 + \|\nabla \mathbf{v}\|_{L^2}^2 \right) \\ & \leq C \left( 1 + \|\mathbf{v}^1\|_{L^4}^4 + \|\mathbf{v}^2\|_{L^4}^4 \right) \left( \|c\|_{L^2}^2 + \|\theta\|_{L^2}^2 + \|\mathbf{v}\|_{L^2}^2 \right), \end{aligned}$$

and, from Gronwall’s lemma and the fact that  $\mathbf{v}^i \in \mathbf{L}^4(Q)$ , we see at once that  $c = \theta = 0$ ,  $\mathbf{v} = 0$  and  $(c^1, \theta^1, \mathbf{v}^1)$  and  $(c^2, \theta^2, \mathbf{v}^2)$  must coincide.

This ends the proof. □

**2.3. Generalized solutions for the true solidification problem.** In this Section, we will consider the original solidification system (1)–(4), completed with adequate boundary and initial conditions. First, we will specify what is a weak solution to this problem. Then, we will prove that, at least when  $d = 2$ , the control belongs to  $L^\infty$  and the initial data are regular enough, the solution to the regularized problems (13)–(21) converge in an appropriate sense to a weak solution of (1)–(4).

Our arguments are similar to those in [14, 7, 10]; see also [6, 9] for some results for related stationary problems. Notice that, for stationary problems, the passage to the limit as  $\varepsilon \rightarrow 0^+$  is much simpler, since it is relatively easy to check that  $c^\varepsilon$  and  $\theta^\varepsilon$  belongs to a compact set of  $C^0(\bar{\Omega})$  and  $\mathbf{v}^\varepsilon$  belongs to a compact set of  $\mathbf{H}$ .

As in the previous Section, it will be assumed that (22)–(27) hold. Additionally, we will suppose that

$$c_0, \theta_0 \in C^0(\bar{\Omega}).$$

**Definition 2.4.** We say that  $(c, \theta, \mathbf{v})$  is a weak solution to the solidification model (1)–(4), (17)–(21) if

$$\begin{aligned} c & \in L^2(0, T; H^1(\Omega)) \cap C^0(\bar{Q}), \\ \theta & \in L^2(0, T; \mathcal{H}_\theta(\Omega)) \cap C^0(\bar{Q}), \\ \mathbf{v} & \in L^2(0, T; \mathbf{V}) \cap C_w^0([0, T]; \mathbf{H}), \end{aligned}$$

the equalities (31) and (32) are satisfied for all  $\varphi \in H^1(\Omega)$  and  $\psi \in \mathcal{H}_\theta(\Omega)$  and  $t$  a.e. in  $(0, T)$ ,

$$\begin{aligned} & \mathbf{v} = 0 \quad \text{in} \quad \text{int } Q_s, \\ & \iint_Q (-\mathbf{v} \cdot \mathbf{w}_t + (\mathbf{v} \cdot \nabla) \mathbf{v} \cdot \mathbf{w} + \nu \nabla \mathbf{v} \cdot \nabla \mathbf{w} + F_i(c, \theta) \mathbf{v} \cdot \mathbf{w}) = \iint_Q F_\varepsilon(c, \theta) \cdot \mathbf{w} \end{aligned}$$

for all  $\mathbf{w} \in C_0^\infty(Q)$  with  $\text{Supp } \mathbf{w} \subset Q_{ml}$  and  $\nabla \cdot \mathbf{w} \equiv 0$ , the first two equalities of (34) hold and, finally,

$$\mathbf{v}(\mathbf{x}, 0) = \mathbf{v}_0(\mathbf{x}) \quad \text{in} \quad \Omega_{ml}(0).$$

The following result holds:

**Theorem 2.5.** *In addition to the previous assumptions, let us assume that  $d = 2$ ,  $h \in L^\infty(\omega \times (0, T))$ ,  $c_0 \in H^2(\Omega)$ ,  $\theta_0 \in H^2(\Omega)$  and  $\mathbf{v}_0 \in \mathbf{H}$ . Then, there exists at least one weak solution to the solidification model (1)–(4), (17)–(21).*

*Proof.* We will first prove that, under the present conditions, for each  $\varepsilon > 0$  the unique solution to the regularized problem solves this system in the strong sense and the  $c^\varepsilon$  and  $\theta^\varepsilon$  belong to a compact set in  $C^0(\bar{Q})$ . Then, it will be shown that an appropriate subsequence converges to a weak solution of (1)–(4), (17)–(21).

Let  $\varepsilon > 0$  be given and let  $(c^\varepsilon, \theta^\varepsilon, \mathbf{v}^\varepsilon)$  be the unique solution to (13)–(21). Then  $c^\varepsilon$ ,  $\theta^\varepsilon$  and  $\mathbf{v}^\varepsilon$  are uniformly bounded respectively in  $L^\infty(Q) \cap L^2(0, T; H^1(\Omega))$ ,  $L^\infty(0, T; L^2(\Omega)) \cap L^2(0, T; \mathcal{H}_\theta(\Omega))$  and  $L^\infty(0, T; \mathbf{H}) \cap L^2(0, T; \mathbf{V})$ .

Indeed, if we take  $\mathbf{w} = \mathbf{v}^\varepsilon(\cdot, t)$  in (33) (resp.  $\psi = \theta^\varepsilon(\cdot, t)$  in (32)) for  $t$  a.e. in  $(0, T)$ , we get

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \|\mathbf{v}^\varepsilon\|_{L^2}^2 + \nu \|\nabla \mathbf{v}^\varepsilon\|_{L^2}^2 + \int_{\Omega} F_i^\varepsilon(c^\varepsilon, \theta^\varepsilon) |\mathbf{v}^\varepsilon|^2 &\leq C \int_{\Omega} (1 + |c_l(c^\varepsilon, \theta^\varepsilon)| + |\theta^\varepsilon|) |\mathbf{v}^\varepsilon| \\ &\leq C \int_{\Omega} (1 + |\theta^\varepsilon|) |\mathbf{v}^\varepsilon| \end{aligned}$$

and

$$\frac{1}{2} \frac{d}{dt} \|\theta^\varepsilon\|_{L^2}^2 + \chi \|\nabla \theta^\varepsilon\|_{L^2}^2 = \int_{\omega} h \theta^\varepsilon \leq C \int_{\omega} |h| |\theta^\varepsilon|.$$

Taking into account that  $F_i^\varepsilon \geq 0$ , we easily deduce from these inequalities that

$$\|\theta^\varepsilon\|_{L^\infty(L^2)} + \|\theta^\varepsilon\|_{L^2(\mathcal{H}_\theta)} + \|\mathbf{v}^\varepsilon\|_{L^\infty(\mathbf{H})} + \|\mathbf{v}^\varepsilon\|_{L^2(\mathbf{V})} \leq C \tag{62}$$

and, in particular,  $\mathbf{v}^\varepsilon$  is uniformly bounded in  $L^\infty(0, T; \mathbf{H}) \cap L^2(0, T; \mathbf{V})$ . In a similar way, it can also be checked that

$$\|c^\varepsilon\|_{L^2(H^1)} \leq C.$$

Since  $d = 2$ , the previous estimates imply that  $\mathbf{v}^\varepsilon$  is uniformly bounded in  $L^4(Q)$ .

Let  $q$  be given, with  $2 \leq q < 4$ . Then  $\theta_0 \in H^2(\Omega) \cap \mathcal{H}_\theta(\Omega) \subset W^{2-\frac{2}{q}, q}(\Omega)$ . Hence, in view of theorem 9.1, Chap. IV in [13], the following holds:  $\theta^\varepsilon \in L^q(0, T; W^{2, q}(\Omega))$ ,  $\theta_t^\varepsilon \in L^q(Q)$ ,  $\theta^\varepsilon$  solves (14) in the strong sense and

$$\|\theta^\varepsilon\|_{L^q(W^{2, q})} + \|\theta_t^\varepsilon\|_{L^q(Q)} \leq C_q. \tag{63}$$

Also, similar arguments show that  $c^\varepsilon \in L^q(0, T; W^{2, q}(\Omega))$ ,  $c_t^\varepsilon \in L^q(Q)$ ,  $c^\varepsilon$  solves (13) in the strong sense and

$$\|c^\varepsilon\|_{L^q(W^{2, q})} + \|c_t^\varepsilon\|_{L^q(Q)} \leq C_q. \tag{64}$$

In view of (63) and (64), the sequences  $\{c^\varepsilon\}$  and  $\{\theta^\varepsilon\}$  are bounded in a space of Hölder-continuous functions. More precisely, one has

$$\|c^\varepsilon\|_{C^{0, \tau, \tau/2}(\overline{Q})} + \|\theta^\varepsilon\|_{C^{0, \tau, \tau/2}(\overline{Q})} \leq C_\tau \tag{65}$$

for all  $\tau \in (0, 1)$ ; see [13], p. 80. Consequently,  $c^\varepsilon$  and  $\theta^\varepsilon$  belong to a compact set in  $C^0(\overline{Q})$  and we have the following at least for a subsequence:

$$c^\varepsilon \rightarrow c \text{ and } \theta^\varepsilon \rightarrow \theta \text{ weakly in } L^2(H^2), \tag{66}$$

$$c_t^\varepsilon \rightarrow c_t \text{ and } \theta_t^\varepsilon \rightarrow \theta_t \text{ weakly in } L^2(Q), \tag{67}$$

$$c^\varepsilon \rightarrow c \text{ and } \theta^\varepsilon \rightarrow \theta \text{ strongly in } C^0(\overline{Q}). \tag{68}$$

On the other hand, it is not restrictive to assume that

$$\mathbf{v}^\varepsilon \rightarrow \mathbf{v} \text{ weakly-* in } L^\infty(\mathbf{H}) \text{ and weakly in } L^2(\mathbf{V}), \tag{69}$$

$$\mathbf{v}^\varepsilon \rightarrow \mathbf{v} \text{ weakly in } L^4(Q). \tag{70}$$

Let us introduce the open set

$$Q_{ml} = \{(\mathbf{x}, t) \in Q : f_s(c(\mathbf{x}, t), \theta(\mathbf{x}, t)) < 1\}.$$

We will now see that, at least for a subsequence, one has

$$\mathbf{v}^\varepsilon \rightarrow \mathbf{v} \text{ a.e. in } Q_{ml}. \tag{71}$$

To this end, we first notice that  $Q_{ml}$  can be written as a countable union of open sets of the form  $\mathcal{O} \times I$ , with

$$\mathcal{O} \subset \Omega, \quad I \subset (0, T) \text{ (an open interval)}, \quad \sup_{\mathcal{O} \times I} f_s(c, \theta) < 1. \tag{72}$$

Indeed, we first have

$$Q_{ml} = \bigcup_{n \geq 1} Q_{ml}^{(n)}, \quad \text{with } Q_{ml}^{(n)} = \{(\mathbf{x}, t) \in Q : f_s(c(\mathbf{x}, t), \theta(\mathbf{x}, t)) < 1 - \frac{1}{n}\};$$

then, any  $Q_{ml}^{(n)}$  can be written as a countable non-decreasing union of compact sets  $K_m^{(n)}$ ; finally, each  $K_m^{(n)}$  can be covered by a finite union of sets  $\mathcal{O} \times I$  satisfying (72).

Consequently, it will suffice to check that, for any such set  $\mathcal{O} \times I$ , we have

$$\mathbf{v}^\varepsilon \rightarrow \mathbf{v} \text{ a.e. in } \mathcal{O} \times I \tag{73}$$

at least for a subsequence.

Thus, let  $\mathcal{O}$  and  $I$  be given, satisfying (72). Let us introduce the space  $\mathbf{V}(\mathcal{O})$ , with

$$\mathbf{V}(\mathcal{O}) = \{ \mathbf{w} \in \mathbf{H}_0^1(\mathcal{O}) : \nabla \cdot \mathbf{w} = 0 \text{ in } \mathcal{O} \} \tag{74}$$

and let us denote by  $\mathbf{V}(\mathcal{O})'$  the dual of  $\mathbf{V}(\mathcal{O})$ . Let  $\mathbf{u}^\varepsilon$  denote the restriction to  $\mathcal{O} \times I$  of the field  $\mathbf{v}^\varepsilon$ . We obviously have

$$\| \mathbf{u}^\varepsilon \|_{L^2(I; \mathbf{H}^1(\mathcal{O}))} \leq C. \tag{75}$$

On the other hand, for any  $\mathbf{w} \in \mathbf{V}(\mathcal{O})$  and any  $t \in I$ , one has:

$$\begin{aligned} \langle \mathbf{u}_t^\varepsilon, \mathbf{w} \rangle &= \int_{\Omega} \mathbf{v}_t^\varepsilon \cdot \mathbf{w} = \int_{\Omega} ((\mathbf{v}^\varepsilon \cdot \nabla) \mathbf{w} \cdot \mathbf{v}^\varepsilon + \nu \nabla \mathbf{v}^\varepsilon \cdot \nabla \mathbf{w} - (\mathbf{F}_e^\varepsilon - F_i^\varepsilon \mathbf{v}^\varepsilon) \cdot \mathbf{w}) \\ &\leq C(\mathcal{O} \times I) (1 + \| \mathbf{v}^\varepsilon \|_{L^4}^2 + \| \nabla \mathbf{v}^\varepsilon \|_{L^2}) \| \mathbf{w} \|_{\mathbf{V}(\mathcal{O})}, \end{aligned}$$

where we have used (69), (70) and the fact that, for any sufficiently small  $\varepsilon$ ,  $F_i^\varepsilon$  is uniformly bounded in  $\mathcal{O} \times I$ . These estimates show that

$$\| \mathbf{u}_t^\varepsilon \|_{\mathbf{V}(\mathcal{O})'} \leq C(\mathcal{O} \times I) (1 + \| \mathbf{v}^\varepsilon \|_{L^4}^2 + \| \nabla \mathbf{v}^\varepsilon \|_{L^2})$$

and, consequently,

$$\| \mathbf{u}_t^\varepsilon \|_{L^2(I; \mathbf{V}(\mathcal{O})')} \leq C(\mathcal{O} \times I). \tag{76}$$

From (75) and (76), we deduce from well known compactness results that  $\mathbf{u}^\varepsilon$  belongs to a compact set in  $L^2(\mathcal{O} \times I)$ . Therefore, we get (73) at least for a subsequence, as desired. This proves (71).

From (70) and (71), we obtain:

$$\mathbf{v}^\varepsilon \rightarrow \mathbf{v} \text{ strongly in } L^p(Q_{ml}) \quad \forall p \in [1, 4).$$

On the other hand, (69) and (71) give

$$(\mathbf{v}^\varepsilon \cdot \nabla) \mathbf{v}^\varepsilon \rightarrow (\mathbf{v} \cdot \nabla) \mathbf{v} \text{ weakly in } L^{4/3}(Q_{ml}). \tag{77}$$

We can now take limits in the equations satisfied by  $c^\varepsilon$ ,  $\theta^\varepsilon$  and  $\mathbf{v}^\varepsilon$ . Thus, using (66)–(77), we find that  $c$  and  $\theta$  satisfy (31), (32) and the first two equalities of (34).



Also, using (69), (70) and (68), the following is found for every  $\mathbf{w} \in C_0^\infty(Q)$  with  $\text{Supp } \mathbf{w} \subset Q_{ml}$  and  $\nabla \cdot \mathbf{w} \equiv 0$ :

$$\begin{aligned} & \iint_Q (-\mathbf{v} \cdot \mathbf{w}_t + (\mathbf{v} \cdot \nabla) \mathbf{v} \cdot \mathbf{w} + \nu \nabla \mathbf{v} \cdot \nabla \mathbf{w} + (F_i(c, \theta) \mathbf{v} - \mathbf{F}_e(c, \theta)) \cdot \mathbf{w}) \\ &= \lim_{\varepsilon \rightarrow 0} \iint_Q (-\mathbf{v}^\varepsilon \cdot \mathbf{w}_t + (\mathbf{v}^\varepsilon \cdot \nabla) \mathbf{v}^\varepsilon \cdot \mathbf{w} + \nu \nabla \mathbf{v}^\varepsilon \cdot \nabla \mathbf{w} + (F_i^\varepsilon \mathbf{v}^\varepsilon - \mathbf{F}_e^\varepsilon) \cdot \mathbf{w}) = 0. \end{aligned}$$

In order to check that  $\mathbf{v}|_{t=0} = \mathbf{v}_0$  in  $\Omega_{ml}(0)$ , we argue as follows.

Let  $\mathcal{O} \subset \subset \Omega_{ml}(0)$  be a non-empty open set and let us denote again by  $\mathbf{V}(\mathcal{O})$  the space (74). Let  $\rho > 0$  be such that  $\mathcal{O} \times [0, \rho] \subset Q_{ml} \cup (\Omega \times \{0\})$ ; the definition of  $Q_{ml}$  and the fact that  $c$  and  $\theta$  are uniformly continuous prove that such a  $\rho$  exists. Let us denote by  $\mathbf{u}^\varepsilon$  (resp.  $\mathbf{u}$ ) the restriction of  $\mathbf{v}^\varepsilon$  (resp.  $\mathbf{v}$ ) to  $\mathcal{O} \times (0, \rho)$  and let  $\mathbf{u}_0$  be the restriction of  $\mathbf{v}_0$  to  $\mathcal{O}$ . Then

$$\|\mathbf{u}^\varepsilon\|_{L^2(0, \rho; \mathbf{H}^1(\mathcal{O}))} + \|\mathbf{u}^\varepsilon\|_{L^\infty(0, \rho; L^2(\mathcal{O}))} \leq C$$

and an argument similar to the proof of (76) shows that

$$\|\mathbf{u}_i^\varepsilon\|_{L^2(0, \rho; \mathbf{V}(\mathcal{O})')} \leq C(\mathcal{O} \times (0, \rho)).$$

Hence,  $\mathbf{u}^\varepsilon$  can be regarded as a continuous  $\mathbf{V}(\mathcal{O})'$ -valued function and, also, as a weakly continuous  $\mathbf{L}^2(\mathcal{O})$ -valued function. Furthermore,

$$\|\mathbf{u}^\varepsilon\|_{C^0([0, \rho]; \mathbf{V}(\mathcal{O})')} \leq C(\mathcal{O} \times (0, \rho))$$

and

$$\|(\mathbf{u}^\varepsilon, \varphi)_{\mathbf{L}^2(\mathcal{O})}\|_{C^0([0, \rho])} \leq C(\mathcal{O} \times (0, \rho), \varphi) \quad \forall \varphi \in \mathbf{L}^2(\mathcal{O}).$$

This shows that  $\mathbf{u}$  can also be regarded as a  $\mathbf{L}^2(\mathcal{O})$ -valued weakly continuous function and  $\mathbf{u}^\varepsilon|_{t=0}$  converges weakly in  $\mathbf{L}^2(\mathcal{O})$  to  $\mathbf{u}|_{t=0}$ . But we also have  $\mathbf{u}^\varepsilon|_{t=0} = \mathbf{u}_0$ . Therefore,  $\mathbf{u}|_{t=0} = \mathbf{u}_0$  in  $\mathcal{O}$  and, since  $\mathcal{O}$  is arbitrary, the desired initial condition is satisfied by  $\mathbf{v}$ .

Let us finally prove that  $\mathbf{v} = 0$  in  $\text{int } Q_s$ . To this purpose, we will view again  $(\mathbf{v}^\varepsilon, p^\varepsilon)$  as a weak solution to (15) satisfying (62).

From De Rham's lemma, we have  $\nabla p^\varepsilon \in W^{-1, \infty}(0, T; \mathbf{H}^{-1}(\Omega))$  and

$$\|\nabla p^\varepsilon\|_{W^{-1, \infty}(0, T; \mathbf{H}^{-1}(\Omega))} \leq C.$$

Indeed, we can write (15) in the form

$$\langle \mathbf{S}^\varepsilon, \varphi \rangle = 0 \quad \forall \varphi \in \mathcal{V}(\Omega),$$

where

$$\mathbf{S}^\varepsilon := \mathbf{v}_i^\varepsilon + \nabla \cdot (\mathbf{v}^\varepsilon \otimes \mathbf{v}^\varepsilon - \nu \nabla \mathbf{v}^\varepsilon) + F_i^\varepsilon(c^\varepsilon, \theta^\varepsilon) \mathbf{v}^\varepsilon - \mathbf{F}_e^\varepsilon(c^\varepsilon, \theta^\varepsilon)$$

is uniformly bounded in  $W^{-1, \infty}(0, T; \mathbf{L}^2(\Omega)) \cap L^2(0, T; \mathbf{H}^{-1}(\Omega))$ . Accordingly,  $\mathbf{S}$  can be viewed as a distribution in  $\mathbf{L}^2(\Omega; W^{-1, \infty}(0, T))$  that vanishes when it is applied to any  $\varphi$  in  $\mathcal{V}(\Omega)$ , see for instance [18]; therefore,  $\mathbf{S}^\varepsilon$  must be a gradient, that is,  $\mathbf{S}^\varepsilon = -\nabla p^\varepsilon$  for some  $\nabla p^\varepsilon$  uniformly bounded in  $\mathbf{H}^1(\Omega; W^{-1, \infty}(0, T)) \cong W^{-1, \infty}(0, T; \mathbf{H}^{-1}(\Omega))$ .

Thus, it can be assumed that

$$\nabla p^\varepsilon \rightarrow \nabla p \text{ weakly-* in } W^{-1, \infty}(0, T; \mathbf{H}^{-1}(\Omega)). \tag{78}$$

Let  $\varphi \in C_0^\infty(Q)$  be given, with  $K := \text{Supp } \varphi \subset \text{int } Q_s$ . Notice that

$$f_s(c^\varepsilon, \theta^\varepsilon) \rightarrow 1 \text{ and } \varepsilon^3 F_i^\varepsilon \rightarrow 1 \text{ uniformly in } K \text{ as } \varepsilon \rightarrow 0. \tag{79}$$

Also,

$$\begin{aligned} 0 &= \varepsilon^3 \iint_Q (\mathbf{v}_t^\varepsilon + (\mathbf{v}^\varepsilon \cdot \nabla) \mathbf{v}^\varepsilon - \nu \Delta \mathbf{v} + F_i^\varepsilon \mathbf{v}^\varepsilon + \nabla p^\varepsilon - \mathbf{F}_e^\varepsilon) \cdot \varphi \\ &= \varepsilon^3 \iint_Q (\mathbf{v}_t^\varepsilon + (\mathbf{v}^\varepsilon \cdot \nabla) \mathbf{v}^\varepsilon + \nabla p^\varepsilon - \mathbf{F}_e^\varepsilon) \cdot \varphi \\ &\quad + \nu \varepsilon^3 \iint_Q \nabla \mathbf{v}^\varepsilon \cdot \nabla \varphi + \varepsilon^3 \iint_Q F_i^\varepsilon \mathbf{v}^\varepsilon \cdot \varphi \end{aligned}$$

Taking limits as  $\varepsilon \rightarrow 0$  and using (65), (69), (78) and (79), we deduce that

$$\iint_Q \mathbf{v} \cdot \varphi = 0.$$

Since this must hold for all  $\varphi \in C_0^\infty(Q)$  with  $\text{Supp } \varphi \subset \text{int } Q_s$ , we find that  $\mathbf{v}$  vanishes in  $\text{int } Q_s$ .

This shows that  $(c, \theta, \mathbf{v})$  solves the solidification problem in the sense of definition 2.4 and ends the proof.  $\square$

**Remark 2.** The regularity assumptions on  $c_0$  and  $\theta_0$  have been needed to ensure the uniform Hölder-continuity of  $c^\varepsilon$  and  $\theta^\varepsilon$  and thus the compactness of these functions in  $C^0(\overline{Q})$ . On the other hand, the last passage to the limit in the previous proof relies, among other things, on the fact that

$$\iint_Q \mathbf{v}_t^\varepsilon \cdot \varphi = - \iint_Q \mathbf{v}^\varepsilon \cdot \varphi_t$$

and consequently converges as  $\varepsilon \rightarrow 0$ .

**Remark 3.** Observe that, if  $d = 3$  and  $(c^\varepsilon, \theta^\varepsilon, \mathbf{v}^\varepsilon)$  is a weak solution to the regularized problem for every  $\varepsilon$ , we can only prove that  $\mathbf{v}^\varepsilon$  is uniformly bounded in  $\mathbf{L}^{10/3}(Q)$ , see [8, 19]. But this is not enough to obtain (63) and (64) and we cannot deduce that  $c^\varepsilon$  and  $\theta^\varepsilon$  belong to a compact set of  $C^0(\overline{Q})$ ; we would need a uniform estimate in  $\mathbf{L}^{5/2}(Q)$ , see [13]. It is at this point that the argument begins to fail in the three-dimensional case. Consequently, the analog of theorem 2.5 in the three-dimensional case is open.

**3. Some first optimal control problems for the regularized solidification model.** Let us consider some first (standard) control problems for the regularized solidification system (13)–(21). The underlying goal is to govern the growth of a solidification front (and its geometrical shape) by imposing a heating mechanism that acts on the non-empty subset  $\omega \subset \Omega$ .

A mathematical formulation can be obtained under the form of an optimal control problem. More precisely, we will try to minimize an appropriate cost function subject to (13)–(21) and some additional constraints on the control  $h$ .

In this Section, we will propose several choices for the cost functional (see the definitions (81) and (82) below). In each case, our purpose will be to achieve three main tasks:

- To prove the existence of an optimal control.
- To characterize the optimal controls or, at least, to obtain necessary conditions for optimality.
- To provide iterative algorithms for the computation of optimal controls.

A very interesting question is what happens when  $\varepsilon \rightarrow 0$ , i.e. which is the behavior of the solutions to the optimal control problems when we take limits in (13)–(21) and we approach the original solidification model. This is a difficult question. It will not be analyzed in this paper, but will be the objective of a forthcoming work.

Let  $J = J(h, c, \theta, \mathbf{v})$  be a cost function. The considered optimal control problem will have the following general form:

$$\begin{cases} \text{Find } (h^*, c^*, \theta^*, \mathbf{v}^*) \in \mathcal{E} \text{ such that} \\ J(h^*, c^*, \theta^*, \mathbf{v}^*) = \min_{(h, c, \theta, \mathbf{v}) \in \mathcal{E}} J(h, c, \theta, \mathbf{v}), \end{cases} \tag{80}$$

where  $\mathcal{E}$  is a non-empty set that will be specified later.

In practice, any  $(h, c, \theta, \mathbf{v}) \in \mathcal{E}$  will be assumed to satisfy (13)–(21). Furthermore, it will be realistic to consider appropriate constraints on  $h$ , i.e. to impose that  $h$  belongs to a set of *admissible* controls  $\mathcal{U}_{ad} \subset L^2(\omega \times (0, T))$ .

Let  $\alpha, \beta, \gamma$  be nonnegative constants and let us assume that  $N > 0$ . We will consider the following two possible choices of  $J$ , that seem reasonable:

**First Choice:** Let  $c_d, \theta_d \in L^2(Q)$  and  $\mathbf{v}_d \in \mathbf{L}^2(Q)$  be given. We set

$$\begin{aligned} J(h, c, \theta, \mathbf{v}) &= \frac{\alpha}{2} \iint_Q |c - c_d|^2 + \frac{\beta}{2} \iint_Q |\theta - \theta_d|^2 + \frac{\gamma}{2} \iint_Q |\mathbf{v} - \mathbf{v}_d|^2 \\ &+ \frac{N}{2} \iint_{\omega \times (0, T)} |h|^2 \end{aligned} \tag{81}$$

**Second Choice:** Let  $c_e, \theta_e \in L^2(\Omega)$  and  $\mathbf{v}_e \in \mathbf{L}^2(\Omega)$  be given. We now set

$$\begin{aligned} J(h, c, \theta, \mathbf{v}) &= \frac{\alpha}{2} \int_{\Omega} |c(\mathbf{x}, T) - c_e(\mathbf{x})|^2 + \frac{\beta}{2} \int_{\Omega} |\theta(\mathbf{x}, T) - \theta_e(\mathbf{x})|^2 \\ &+ \frac{\gamma}{2} \int_{\Omega} |\mathbf{v}(\mathbf{x}, T) - \mathbf{v}_e(\mathbf{x})|^2 + \frac{N}{2} \iint_{\omega \times (0, T)} |h|^2 \end{aligned} \tag{82}$$

As usual, these objective functions correspond to the goal of having  $(c, \theta, \mathbf{v})$  close to a desired state in the cheapest feasible way.

**3.1. The existence of optimal controls.** Let us fix a non-empty set  $\mathcal{U}_{ad} \subset L^2(\omega \times (0, T))$ . Let us set

$$\mathcal{E} = \{ (h, c, \theta, \mathbf{v}) : h \in \mathcal{U}_{ad}, (c, \theta, \mathbf{v}) \text{ solves (13)–(21)} \}.$$

Notice that  $\mathcal{E}$  is a non-empty subset of  $L^2(\omega \times (0, T)) \times E$ , where  $E$  is the energy space for the weak solutions to (13)–(21), i.e. the space of triplets  $(c, \theta, \mathbf{v})$  satisfying (28)–(30). Of course,  $E$  is a Banach space for the norm

$$\|c\|_{L^2(H^1)} + \|c\|_{L^\infty(L^2)} + \|\theta\|_{L^2(\mathcal{H}_\theta)} + \|\theta\|_{L^\infty(L^2)} + \|\mathbf{v}\|_{L^2(\mathbf{V})} + \|\mathbf{v}\|_{L^\infty(\mathbf{H})}.$$

Let us consider the control problem (80). The following result holds:

**Theorem 3.1.** *Assume that  $\mathcal{U}_{ad}$  is weakly closed in  $L^2(\omega \times (0, T))$  and the following hypotheses are satisfied:*

1. *Either  $J$  is a coercive functional, that is,*

$$J(h^n, c^n, \theta^n, \mathbf{v}^n) \rightarrow +\infty \text{ if } (h^n, c^n, \theta^n, \mathbf{v}^n) \in \mathcal{E}, \quad \|h^n\|_{L^2(\omega \times (0, T))} \rightarrow +\infty,$$

*or  $\mathcal{U}_{ad}$  is a bounded set.*

2.  $J$  is sequentially weakly-\* lower semicontinuous, that is, if  $(h^n, c^n, \theta^n, \mathbf{v}^n) \rightarrow (h, c, \theta, \mathbf{v})$  weakly-\* in  $L^2(\omega \times (0, T)) \times E$ , then

$$\liminf_{n \rightarrow +\infty} J(h^n, c^n, \theta^n, \mathbf{v}^n) \geq J(h, c, \theta, \mathbf{v}).$$

Then, there exists at least one solution to (80), that is, an optimal control and its associated state.

*Proof.* The argument is standard and well known. However, for completeness, we will give a sketch.

Let  $\{(h^n, c^n, \theta^n, \mathbf{v}^n)\}$  be a minimizing sequence for (80). Then all the control-states  $(h^n, c^n, \theta^n, \mathbf{v}^n)$  belong to  $\mathcal{E}$  and the  $h^n$  are uniformly bounded in  $L^2(\omega \times (0, T))$ . Indeed, if this were not the case, it could be assumed that  $\|h^n\|_{L^2(\omega \times (0, T))} \rightarrow +\infty$ , whence we should have  $J(h^n, c^n, \theta^n, \mathbf{v}^n) \rightarrow +\infty$ , which is an absurd.

From the estimates in the proof of theorem 2.2, we easily get

$$0 \leq c^n \leq c_e, \quad \|(c^n, \theta^n, \mathbf{v}^n)\|_E \leq C,$$

and

$$\|c_t^n\|_{L^2(0, T; (H^1(\Omega))')} + \|\theta_t^n\|_{L^\sigma(0, T; (\mathcal{H}_\theta(\Omega))')} + \|\mathbf{v}_t^n\|_{L^\sigma(0, T; \mathbf{V}')} \leq C,$$

where  $\sigma = 2$  if  $d = 2$  and  $\sigma = 4/3$  if  $d = 3$ .

Consequently, at least for a new minimizing (sub)sequence, we have the weak and/or weak-\* convergence of  $h^n, c^n, \theta^n, \mathbf{v}^n, c_t^n, \theta_t^n$  and  $\mathbf{v}_t^n$  in appropriate spaces and the strong convergence of  $c^n, \theta^n$  and the components of  $\mathbf{v}^n$  in  $L^2(Q)$ . Thus, as in the proof of theorem 2.2, we deduce that the limit  $(h^*, c^*, \theta^*, \mathbf{v}^*)$  belongs to  $\mathcal{E}$ , i.e.  $h^* \in \mathcal{U}_{ad}$  (here we use that  $\mathcal{U}_{ad}$  is weakly closed) and  $(c^*, \theta^*, \mathbf{v}^*)$  solves (13)–(21) for  $h = h^*$ .

We also have

$$\liminf_{n \rightarrow +\infty} J(h^n, c^n, \theta^n, \mathbf{v}^n) \geq J(h^*, c^*, \theta^*, \mathbf{v}^*).$$

Hence,  $(h^*, c^*, \theta^*, \mathbf{v}^*)$  solves (80) and the proof is achieved. □

**Remark 4.** The hypotheses in this result are satisfied when  $J$  is given by (81) or (82) and  $\mathcal{U}_{ad} \subset L^2(\omega \times (0, T))$  is non-empty, closed and convex. Typical examples are the following:

$$\begin{aligned} \mathcal{U}_{ad} &= L^2(\omega \times (0, T)) \\ \mathcal{U}_{ad} &= \{h \in L^2(\omega \times (0, T)) : |h| \leq R \text{ a.e.}\} \\ \mathcal{U}_{ad} &= \{h \in L^2(\omega \times (0, T)) : h = \sum_{j=1}^m h_j(\mathbf{x})1_{I_j}(t), \quad h_j \in L^2(\omega)\} \end{aligned}$$

where  $R > 0$  and the  $I_j \subset (0, T)$  are disjoint intervals. Consequently, in these cases, there exists at least one solution to (80).

**3.2. The optimality system.** Next, we will deduce the optimality system associated to the previous control problems. We will need a regularity assumption on the optimal control-state  $(h^*, c^*, \theta^*, \mathbf{v}^*)$ :

$$\text{The set of points } (\mathbf{x}, t) \text{ where } \theta^* = \eta_l(c^*) \text{ or } \max(\eta_s(c^*), \theta_e) \text{ is negligible.} \quad (83)$$

In the case of the cost functional (81), the following holds:

**Theorem 3.2.** *Assume that  $\mathcal{U}_{ad} \subset L^2(\omega \times (0, T))$  is non-empty, closed and convex and  $J$  is given by (81). Let  $(h^*, c^*, \theta^*, \mathbf{v}^*)$  be an optimal solution to (80) satisfying (83) and assume that  $(c^*, \theta^*, \mathbf{v}^*)$  is the unique state associated to  $h^*$ . Then, there exists  $(\phi, \psi, \mathbf{w}) \in E$  such that one has:*

$$\left\{ \begin{array}{l} c_t^* + \mathbf{v}^* \cdot \nabla c_l^* - D\Delta c^* = 0, \\ \theta_t^* + \mathbf{v}^* \cdot \nabla \theta^* - \chi \Delta \theta^* = h^* 1_\omega, \\ \mathbf{v}_t^* + (\mathbf{v}^* \cdot \nabla) \mathbf{v}^* - \nu \Delta \mathbf{v}^* + (F_i^\varepsilon)^* \mathbf{v}^\varepsilon + \nabla p^\varepsilon = \mathbf{F}_e^*, \\ \nabla \cdot \mathbf{v}^* = 0, \\ (D\nabla c^*) \cdot \mathbf{n} = 0, \quad \mathbf{v}^* = 0 \quad \text{on } \partial\Omega \times (0, T), \\ (\chi \nabla \theta^*) \cdot \mathbf{n} = 0 \quad \text{on } \Gamma_N \times (0, T), \quad \theta^* = 0 \quad \text{on } \Gamma_D \times (0, T), \\ c^*(\mathbf{x}, 0) = c^0(\mathbf{x}); \quad \theta^*(\mathbf{x}, 0) = \theta^0(\mathbf{x}); \quad \mathbf{v}^*(\mathbf{x}, 0) = \mathbf{v}^0(\mathbf{x}) \quad \text{in } \Omega. \end{array} \right. \quad (84)$$

$$\left\{ \begin{array}{l} -\phi_t - (D_c c_l)^* \mathbf{v}^* \cdot \nabla \phi - D\Delta \phi = ((D_c \mathbf{F}_e)^* - (D_c F_i^\varepsilon)^* \mathbf{v}^*) \cdot \mathbf{w} \\ \quad + \alpha(c^* - c_d), \\ -\psi_t - \mathbf{v}^* \cdot \nabla \psi - \chi \Delta \psi = ((D_\theta \mathbf{F}_e)^* - (D_\theta F_i^\varepsilon)^* \mathbf{v}^*) \cdot \mathbf{w} \\ \quad + (D_\theta c_l)^* \mathbf{v}^* \cdot \nabla \phi + \beta(\theta^* - \theta_d), \\ -\mathbf{w}_t - \nu \Delta \mathbf{w} - (\mathbf{v}^* \cdot \nabla) \mathbf{w} + (\nabla \mathbf{v}^*)^t \mathbf{w} + (F_i^\varepsilon)^* \mathbf{w} + \nabla \pi \\ \quad = -\phi \nabla c_l^* - \psi \nabla \theta^* + \gamma(\mathbf{v}^* - \mathbf{v}_d), \\ \nabla \cdot \mathbf{w} = 0, \\ (D\nabla \phi) \cdot \mathbf{n} = 0, \quad \mathbf{w} = 0 \quad \text{on } \partial\Omega \times (0, T), \\ (\chi \nabla \psi) \cdot \mathbf{n} = 0 \quad \text{on } \Gamma_N \times (0, T), \quad \psi = 0 \quad \text{on } \Gamma_D \times (0, T), \\ \phi(\mathbf{x}, T) = 0; \quad \psi(\mathbf{x}, T) = 0; \quad \mathbf{w}(\mathbf{x}, T) = 0 \quad \text{in } \Omega. \end{array} \right. \quad (85)$$

$$\iint_{\omega \times (0, T)} (\psi + Nh^*)(h - h^*) \geq 0 \quad \forall h \in \mathcal{U}_{ad}, \quad h^* \in \mathcal{U}_{ad}. \quad (86)$$

Notice that the same conclusion is obtained if  $(h^*, c^*, \theta^*, \mathbf{v}^*)$  is only a local minimizer of  $J$ .

*Proof.* Let us take  $h = h^* + am$  with  $a \in \mathbb{R}_+$  (small),  $m \in L^2(\omega \times (0, T))$  and  $h^* + am \in \mathcal{U}_{ad}$ . Let  $(c, \theta, \mathbf{v})$  be a state associated to  $h$ . We can then write

$$(c, \theta, \mathbf{v}) = (c^*, \theta^*, \mathbf{v}^*) + a(z, y, \mathbf{u}) + a(z'_a, y'_a, \mathbf{u}'_a),$$

with

$$\left\{ \begin{array}{l} z_t + \mathbf{v}^* \cdot \nabla((D_c c_l)^* z + (D_\theta c_l)^* y) + \mathbf{u} \cdot \nabla c_l^* - D\Delta z = 0, \\ y_t + \mathbf{v}^* \cdot \nabla y + \mathbf{u} \cdot \nabla \theta^* - \chi \Delta y = m 1_\omega, \\ \mathbf{u}_t + (\mathbf{v}^* \cdot \nabla) \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{v}^* - \nu \Delta \mathbf{u} + (F_i^\varepsilon)^* \mathbf{u} \\ \quad + ((D_c F_i^\varepsilon)^* z + (D_\theta F_i^\varepsilon)^* y) \mathbf{v}^* + \nabla q = (D_c \mathbf{F}_e)^* z + (D_\theta \mathbf{F}_e)^* y, \\ \nabla \cdot \mathbf{u} = 0, \end{array} \right. \quad (87)$$

and

$$\left\{ \begin{array}{l} z'_{a,t} + \mathbf{v}^* \cdot \nabla((D_c c_l)^* z'_a + (D_\theta c_l)^* y'_a) + \mathbf{u}'_a \cdot \nabla c_l^* - D\Delta z'_a = -Z_a, \\ y'_{a,t} + \mathbf{v}^* \cdot \nabla y'_a + \mathbf{u}'_a \cdot \nabla \theta^* - \chi \Delta y'_a = -Y_a + ((D_c F_i^\varepsilon)^* z'_a, \\ \mathbf{u}'_{a,t} + (\mathbf{v}^* \cdot \nabla) \mathbf{u}'_a + (\mathbf{u}'_a \cdot \nabla) \mathbf{v}^* - \nu \Delta \mathbf{u}'_a + (F_i^\varepsilon)^* \mathbf{u}'_a \\ \quad + (D_\theta F_i^\varepsilon)^* y'_a) \mathbf{v}^* + \nabla q = (D_c \mathbf{F}_e)^* z'_a + (D_\theta \mathbf{F}_e)^* y'_a - U_a, \\ \nabla \cdot \mathbf{u}'_a = 0. \end{array} \right. \quad (88)$$

Here, we have used the following notation:

$$c_l^* = c_l(c^*, \theta^*), \quad (D_c c_l)^* = D_c c_l(c, \theta)|_{c=c^*, \theta=\theta^*}, \quad (F_i^\varepsilon)^* = F_i^\varepsilon(c^*, \theta^*), \dots$$

The functions  $(z, y, \mathbf{u})$  and  $(z'_a, y'_a, \mathbf{u}'_a)$  must satisfy the same boundary conditions than  $(c^*, \theta^*, \mathbf{v}^*)$  and homogeneous initial conditions at  $t = 0$ .

We have

$$Z_a = \nabla \cdot ((c_l(c, \theta) - c_l^*)(\mathbf{u} + \mathbf{u}'_a) + Z'_a),$$

where

$$\begin{aligned} Z'_a &= \left[ \frac{1}{a}(c_l(c, \theta) - c_l^*) - ((D_c c_l)^*(z + z'_a) + (D_\theta c_l)^*(y + y'_a)) \right] \mathbf{v}^* \\ &:= [D_{1,a}(z + z'_a) + D_{2,a}(y + y'_a)] \mathbf{v}^* \end{aligned}$$

Similar expressions hold for  $Y_a$  and  $U_a$ :

$$Y_a = a \nabla \cdot ((y + y'_a)(\mathbf{u} + \mathbf{u}'_a))$$

and

$$U_a = a \nabla \cdot ((\mathbf{u} + \mathbf{u}'_a) \otimes (\mathbf{u} + \mathbf{u}'_a)) + (F_i^\varepsilon(c, \theta) - (F_i^\varepsilon)^*)(\mathbf{u} + \mathbf{u}'_a) + U'_a,$$

where

$$\begin{aligned} U'_a &= \beta_c \left[ \frac{1}{a}(c_l(c, \theta) - c_l^*) - ((D_c c_l)^*(z + z'_a) + (D_\theta c_l)^*(y + y'_a)) \right] \mathbf{g} \\ &\quad + \left[ \frac{1}{a}(F_i^\varepsilon(c, \theta) - (F_i^\varepsilon)^*) - ((D_c F_i^\varepsilon)^*(z + z'_a) + (D_\theta F_i^\varepsilon)^*(y + y'_a)) \right] \mathbf{v}^* \\ &:= [D_{1,a}(z + z'_a) + D_{2,a}(y + y'_a)] \mathbf{g} + [D_{3,a}(z + z'_a) + D_{4,a}(y + y'_a)] \mathbf{v}^*. \end{aligned}$$

Here,  $D_{1,a}$  and  $D_{2,a}$  (resp.  $D_{3,a}$  and  $D_{4,a}$ ) denote appropriate combinations of the partial derivatives of  $c_l$  (resp.  $F_i^\varepsilon$ ). For instance,

$$D_{1,a} = \int_0^1 D_c c_l(c^* + sa(z + z'_a), \theta^* + sa(y + y'_a)) ds - (D_c c_l)^*. \tag{89}$$

Let us see that  $(z, y, \mathbf{u}), (z'_a, y'_a, \mathbf{u}'_a) \in E$ , with

$$\|(z, y, \mathbf{u})\|_E \leq C \|m\|_{L^2(\omega \times (0, T))}, \quad \|(z'_a, y'_a, \mathbf{u}'_a)\|_E \rightarrow 0 \text{ as } a \rightarrow 0^+. \tag{90}$$

Taking into account that  $(h^*, c^*, \theta^*, \mathbf{v}^*) \in \mathcal{E}$ ,  $0 \leq c \leq c_e$  and  $c_l \in W^{1, \infty}(\mathbb{R}^2)$ , from the usual energy estimates for linear parabolic systems, we easily deduce the first part of (90): by multiplying the first, second and third equations in (87) respectively by  $z, y$  and  $\mathbf{u}$ , integrating in space and setting  $e := (z, y, \mathbf{u})$  and  $\mu := \min(D, \chi, \nu)$ , we find that

$$\frac{d}{dt} \|e\|_{L^2}^2 + \mu \|\nabla e\|_{L^2}^2 \leq (1 + \|\nabla \theta^*\|_{L^2}^2 + \|\nabla \mathbf{v}^*\|_{L^2}^2) \|e\|_{L^2}^2 + \|m 1_\omega\|_{L^2}^2$$

for all  $t \in (0, T)$ . This leads to the desired estimate.

Also,  $\|(z'_a, y'_a, \mathbf{u}'_a)\|_E$  is bounded, independently of  $a$ . More precisely, using the expressions of  $Z_a, Z'_a, Y_a, U_a$  and  $U'_a$  and introducing  $e'_a := (z'_a, y'_a, \mathbf{u}'_a)$ , we now have

$$\begin{aligned} \frac{d}{dt} \|e'_a\|_{L^2}^2 + \mu \|\nabla e'_a\|_{L^2}^2 \\ \leq (1 + \|\nabla \theta^*\|_{L^2}^2 + \|\nabla \mathbf{v}^*\|_{L^2}^2 + \|\nabla y\|_{L^2}^2 + \|\nabla \mathbf{u}\|_{L^2}^2) \|e'_a\|_{L^2}^2 + M_a \end{aligned}$$

for all  $t \in (0, T)$ , where  $M_a = P_a + Q_a + R_a + S_a$ ,

$$P_a := C \int_\Omega |c_l(c, \theta) - c_l^*|^2 |\mathbf{u}|^2, \quad Q_a := C \int_\Omega |F_i^\varepsilon(c, \theta) - (F_i^\varepsilon)^*|^2 |\mathbf{u}|^2, \tag{91}$$

$$R_a := C \int_\Omega [|D_{1,a}|^2 |z|^2 + |D_{2,a}|^2 |y|^2] \tag{92}$$

and

$$S_a := C \int_{\Omega} [|D_{3,a}|^2(|\nabla z|^2 + |\nabla \mathbf{v}^*|^2) + |D_{4,a}|^2(|\nabla y|^2 + |\nabla \mathbf{v}^*|^2)]. \tag{93}$$

First, since  $M_a \leq C(1 + \|\nabla z\|_{L^2}^2 + \|\nabla y\|_{L^2}^2 + \|\nabla \mathbf{v}\|_{L^2}^2)$  for all  $a$  and  $t$ , we deduce that  $\|(z'_a, y'_a, \mathbf{u}'_a)\|_E$  is bounded by a constant depending on  $\|m\|_{L^2(\omega \times (0,T))}$ .

Secondly, observe that this yields uniform bounds for  $z'_{a,t}$  and  $y'_{a,t}$  respectively in  $L^\sigma(0, T; (H^1(\Omega))')$  and  $L^\sigma(0, T; (\mathcal{H}_\theta(\Omega))')$ . Indeed, it suffices to consider the first two equations in (88) and notice that  $Z_a$  and  $Y_a$  are uniformly bounded in these spaces. As a consequence, at least for a subsequence, we have that  $z'_a$  and  $y'_a$  converge strongly in  $L^2(Q)$ .

In view of (91) and Lebesgue’s theorem, we find that

$$\int_0^T P_a(t) dt \rightarrow 0 \quad \text{and} \quad \int_0^T Q_a(t) dt \rightarrow 0. \tag{94}$$

On the other hand, we also have

$$\int_0^T R_a(t) dt \rightarrow 0 \quad \text{and} \quad \int_0^T S_a(t) dt \rightarrow 0. \tag{95}$$

Indeed, the uniqueness of  $(c^*, \theta^*, \mathbf{v}^*)$  and the regularity assumption (83) imply that, for instance,  $D_{1,a} \rightarrow 0$  a.e. in  $Q$ , since  $c_i$  is  $C^1$  in a neighborhood of any  $(c, \theta)$  with  $\theta \neq \eta_i(c)$  and  $\theta \neq \max(\eta_s(c), \theta_e)$ . The same is true for  $D_{2,a}$ ,  $D_{3,a}$  and  $D_{4,a}$ . Consequently, Lebesgue’s theorem also leads to (95).

From (94) and (95), we find that

$$\int_0^T M_a(t) dt \rightarrow 0.$$

Since

$$\|e'_a\|_{L^2}^2(t) + \mu \int_0^t \|\nabla e'_a\|_{L^2}^2(s) ds \leq C \int_0^t M_a(s) ds \quad \forall t \in [0, T],$$

we deduce that, at least for a subsequence, the second part of (90) is fulfilled. Since this argument can be applied to any subsequence of  $\{(z'_a, y'_a, \mathbf{u}'_a)\}$ , the convergence must hold for the whole sequence. This proves (90).

By hypothesis,  $J(h, c, \theta, \mathbf{v}) - J(h^*, c^*, \theta^*, \mathbf{v}^*) \geq 0$ . Dividing by  $a$  and taking limits as  $a \rightarrow 0^+$ , we see that

$$\iint_Q (\alpha(c^* - c_d)z + \beta(\theta^* - \theta_d)y + \gamma(\mathbf{v}^* - \mathbf{v}_d) \cdot \mathbf{u}) + N \iint_{\omega \times (0,T)} h^* m \geq 0. \tag{96}$$

Let us introduce the linear (adjoint) system (85). From classical arguments, it is clear that (85) possesses at least one weak solution  $(\phi, \psi, \mathbf{w}) \in E$ . Furthermore, a straightforward integration by parts yields the following identity:

$$\iint_Q (\alpha(c^* - c_d)z + \beta(\theta^* - \theta_d)y + \gamma(\mathbf{v}^* - \mathbf{v}_d) \cdot \mathbf{u}) = \iint_{\omega \times (0,T)} \psi m.$$

This, together with (96), gives the inequality

$$\iint_{\omega \times (0,T)} (\psi + Nh^*) m \geq 0.$$

Since this must hold for any  $m$  of the form  $m = h - h^*$  with  $h \in \mathcal{U}_{ad}$ , we find (86). This ends the proof.  $\square$

For the second choice of the cost functional, given by (82), a very similar result can be obtained:

**Theorem 3.3.** *Assume that  $\mathcal{U}_{ad} \subset L^2(\omega \times (0, T))$  is non-empty, closed and convex and  $J$  is given by (82). Let  $(h^*, c^*, \theta^*, \mathbf{v}^*)$  be an optimal solution to (80) satisfying (83) and assume that  $(c^*, \theta^*, \mathbf{v}^*)$  is the unique state associated to  $h^*$ . Then, there exists  $(\phi, \psi, \mathbf{w}) \in E$  such that one has (84),*

$$\left\{ \begin{array}{l} -\phi_t - (D_c c_l)^* \mathbf{v}^* \cdot \nabla \phi - D \Delta \phi = ((D_c \mathbf{F}_e)^* - (D_c F_i^\varepsilon)^* \mathbf{v}^*) \cdot \mathbf{w}, \\ -\psi_t - \mathbf{v}^* \cdot \nabla \psi - \chi \Delta \psi = ((D_\theta \mathbf{F}_e)^* - (D_\theta F_i^\varepsilon)^* \mathbf{v}^*) \cdot \mathbf{w} \\ \quad + (D_\theta c_l)^* \mathbf{v}^* \cdot \nabla \phi, \\ -\mathbf{w}_t - \nu \Delta \mathbf{w} - (\mathbf{v}^* \cdot \nabla) \mathbf{w} + (\nabla \mathbf{v}^*)^t \mathbf{w} + (F_i^\varepsilon)^* \mathbf{w} + \nabla \pi \\ \quad = -\phi \nabla c_i^* - \psi \nabla \theta^*, \\ \nabla \cdot \mathbf{w} = 0, \\ (D \nabla \phi) \cdot \mathbf{n} = 0, \quad \mathbf{w} = 0 \quad \text{on } \partial \Omega \times (0, T), \\ (\chi \nabla \psi) \cdot \mathbf{n} = 0 \quad \text{on } \Gamma_N \times (0, T), \quad \psi = 0 \quad \text{on } \Gamma_D \times (0, T), \\ \phi(\mathbf{x}, T) = \alpha(c^*(\mathbf{x}, T) - c_e(\mathbf{x})); \quad \psi(\mathbf{x}, T) = \beta(\theta^*(\mathbf{x}, T) - \theta_e(\mathbf{x})) \quad \text{in } \Omega, \\ \mathbf{w}(\mathbf{x}, T) = \gamma(\mathbf{v}^*(\mathbf{x}, T) - \mathbf{v}_e(\mathbf{x})) \quad \text{in } \Omega. \end{array} \right. \tag{97}$$

and (86).

Again, notice that the same holds if  $(h^*, c^*, \theta^*, \mathbf{v}^*)$  is a local minimizer.

**Remark 5.** Observe that theorems 3.2 and 3.3 do not assert that  $h \mapsto J(h, c, \theta, \mathbf{v})$  is differentiable at  $h^*$ . In fact, nothing indicates that this function is well defined, since in general a control  $h$  close to  $h^*$  can have several associated states. Nevertheless, we have been able to express the variation of  $J$  at  $(h^*, c^*, \theta^*, \mathbf{v}^*)$  in the direction determined by  $m$  in the form

$$\iint_{\omega \times (0, T)} (\psi + N h^*) m,$$

where  $\psi$  solves, together with  $\phi$  and  $\mathbf{w}$ , the adjoint system (85) or (97). For this reason, we can interpret  $(\psi + N h^*)|_{\omega \times (0, T)}$  as the “gradient” of  $h \mapsto J(h, c, \theta, \mathbf{v})$  at  $h^*$ .

**Remark 6.** In the most simple case,  $\mathcal{U}_{ad} = L^2(\omega \times (0, T))$ , and (86) means that

$$h = -\frac{1}{N} \psi \quad \text{in } \omega \times (0, T). \tag{98}$$

More generally, since  $\mathcal{U}_{ad}$  is a closed convex set of  $L^2(\omega \times (0, T))$ , (86) is equivalent to

$$h = P_{ad} \left( -\frac{1}{N} \psi|_{\omega \times (0, T)} \right), \tag{99}$$

where  $P_{ad} : L^2(\omega \times (0, T)) \mapsto \mathcal{U}_{ad}$  is the orthogonal projector.

**3.3. Some iterative algorithms.** We will now propose some iterates to compute the solution to the previous optimal control problems.

For simplicity, we will only refer to the case where  $J$  is given by (81) and, consequently, the optimality system is (84)–(86). The adaptation to the case (82) is straightforward and will not be given.

The following algorithms rely on the ideas in the proof of theorem 3.2. Specifically, we notice that, if  $(h, c, \theta, \mathbf{v}) \in \mathcal{E}$  and the couple  $(c, \theta)$  is “regular” in the sense



of (83), then for any  $m \in L^2(\omega \times (0, T))$ , any small  $a > 0$  and any state  $(c', \theta', \mathbf{v}')$  associated to  $h' = h + am$ , one has

$$J(h', c', \theta', \mathbf{v}') = J(h, c, \theta, \mathbf{v}) + a \iint_{\omega \times (0, T)} (\psi + Nh^*) m + a O(a),$$

where  $\psi$  is, together with  $\phi$  and  $\mathbf{w}$ , the unique solution to

$$\begin{cases} -\phi_t - (D_c c_l) \mathbf{v} \cdot \nabla \phi - D \Delta \phi = ((D_c \mathbf{F}_e) - (D_c F_i^\varepsilon) \mathbf{v}) \cdot \mathbf{w} \\ \quad + \alpha(c - c_d) \\ -\psi_t - \mathbf{v} \cdot \nabla \psi - \chi \Delta \psi = ((D_\theta \mathbf{F}_e) - (D_\theta F_i^\varepsilon) \mathbf{v}) \cdot \mathbf{w} \\ \quad + (D_\theta c_l) \mathbf{v} \cdot \nabla \phi + \beta(\theta - \theta_d) \\ -\mathbf{w}_t - \nu \Delta \mathbf{w} - (\mathbf{v} \cdot \nabla) \mathbf{w} + (\nabla \mathbf{v})^t \mathbf{w} + (F_i^\varepsilon) \mathbf{w} + \nabla \pi \\ \quad = -\phi \nabla c_l - \psi \nabla \theta + \gamma(\mathbf{v} - \mathbf{v}_d) \\ \nabla \cdot \mathbf{w} = 0 \\ (D \nabla \phi) \cdot \mathbf{n} = 0, \quad \mathbf{w} = 0 \quad \text{on } \partial \Omega \times (0, T) \\ (\chi \nabla \psi) \cdot \mathbf{n} = 0 \quad \text{on } \Gamma_N \times (0, T), \quad \psi = 0 \quad \text{on } \Gamma_D \times (0, T) \\ \phi(\mathbf{x}, T) = 0; \quad \psi(\mathbf{x}, T) = 0; \quad \mathbf{w}(\mathbf{x}, T) = 0 \quad \text{in } \Omega \end{cases} \tag{100}$$

and  $O(a) \rightarrow 0$  as  $a \rightarrow 0^+$ .

The first proposed algorithm is the following:

**ALGORITHM 1**

- a.** Choose  $h^0 \in \mathcal{U}_{ad}$ ;
- b.** Then, for given  $n \geq 0$  and  $h^n \in \mathcal{U}_{ad}$ , do until convergence:
  - 1.** Solve (84) with  $h = h^n$ , to obtain  $(c^n, \theta^n, \mathbf{v}^n)$ ;
  - 2.** Solve (100) with  $(c, \theta, \mathbf{v}) = (c^n, \theta^n, \mathbf{v}^n)$ , to obtain  $(\phi^n, \psi^n, \mathbf{w}^n)$ ;
  - 3.** Set  $d^n = (\psi^n + Nh^n)|_{\omega \times (0, T)}$  and find  $\rho^n$  such that
 
$$j^n(\rho^n) = \inf_{\rho > 0} j^n(\rho).$$
 Here,  $j^n(\rho)$  is the value of  $J$  at any  $(h^n - \rho d^n, c^n(\rho), \theta^n(\rho) \mathbf{v}^n(\rho))$ , where  $(c^n(\rho), \theta^n(\rho), \mathbf{v}^n(\rho))$  is a state associated to  $h^n - \rho d^n$ ;
  - 4.** Set  $h^{n+1} = P_{ad}(h^n - \rho^n d^n)$ .

TABLE 1. The optimal step gradient method with projection.

Let us assume that (84) possesses exactly one weak solution  $(c, \theta, \mathbf{v})$  for each  $h \in \mathcal{U}_{ad}$  (this is the case if  $d = 2$ ) and that all the  $(h, c, \theta, \mathbf{v}) \in \mathcal{E}$  satisfy (83). Then algorithm 1 must be viewed as a classical optimal step gradient method.

Since (84) is nonlinear and we have to solve this system by using an iterative scheme, it is reasonable to introduce a variant where we perform mixed loops. This is described in Table 2.

**Remark 7.** A natural choice of the convergence criteria can be

$$\|k^{n+1} - k^n\|_{L^2(\omega \times (0, T))} < \kappa \|k^{n+1}\|_{L^2(\omega \times (0, T))},$$

for  $\kappa$  small enough. Notice however that this can be not completely significative for linear and not superlinear convergence. Consequently, this should be followed by an additional test where we check whether the necessary optimality conditions are satisfied. On the other hand, since the numerical computation of  $\rho^n$  can be

## ALGORITHM 2

- a. Choose  $h^0 \in \mathcal{U}_{ad}$  and  $(c^{-1}, \theta^{-1}, \mathbf{v}^{-1}) \in E$ ;
- b. Then, for given  $n \geq 0$  and  $h^n \in \mathcal{U}_{ad}$ , do until convergence:
  1. Solve (84) with  $h = h^n$ ,  $c_l$ ,  $F_i^\varepsilon$  and  $\mathbf{F}_e$  computed at  $(c^{n-1}, \theta^{n-1})$  and  $\mathbf{v} \cdot \nabla$  replaced by  $\mathbf{v}^{n-1} \cdot \nabla$ , to obtain  $(c^n, \theta^n, \mathbf{v}^n)$ ;
  2. Solve (100) with  $(c, \theta, \mathbf{v}) = (c^n, \theta^n, \mathbf{v}^n)$ , to obtain  $(\phi^n, \psi^n, \mathbf{w}^n)$ ;
  3. Do as in step 3 of algorithm 1;
  4. Do as in step 4 of algorithm 1.

TABLE 2. A “mixed-loop” alternative to algorithm 1.

expensive, it may be convenient to simplify algorithms 1 and 2 by replacing step 3 by the following:

- 3’.** Set  $d^n = (\psi^n + Nh^n)|_{\omega \times (0, T)}$  and  $\rho^n = \rho$  (a prescribed positive constant).

Of course, we can also consider a variant by performing step 3 only a few times (for instance for  $n = 10, 20, 30, \dots$ ) and keeping in between the same fixed  $\rho$  (equal to the last computed  $\rho^n$ ).

A second and more efficient and accurate strategy is to consider conjugate gradient methods. This leads to algorithms similar to those above, where the main difference is that the descent direction  $d^n$  is close but not identical to the “gradient”  $(\psi^n + Nh^n)|_{\omega \times (0, T)}$ .

Let us set

$$G_1(f, g) = \frac{\iint_{\omega \times (0, T)} |f|^2}{\iint_{\omega \times (0, T)} |g|^2} \quad \text{and} \quad G_2(f, g) = \frac{\iint_{\omega \times (0, T)} f(f - g)}{\iint_{\omega \times (0, T)} |g|^2}$$

for all  $f, g \in L^2(\omega \times (0, T))$  with  $g \neq 0$ . The proposed conjugate gradient algorithm (with projection) is given in Table 3.

There,  $G$  stands for one of the functions  $G_1$  or  $G_2$ ; the choice  $G = G_1$  (resp.  $G = G_2$ ) corresponds to the Fletcher-Reeves (resp. Polak-Ribière) version; see [12] for more details.

**Remark 8.** Of course, we can modify algorithm 3 as we did in remark 7 in order to avoid large computational costs concerning  $\rho^n$ . We can also linearize the state systems by simply computing  $c_l$ ,  $F_i^\varepsilon$  and  $\mathbf{F}_e$  at the previous  $(c^{n-1}, \theta^{n-1})$  and replacing  $\mathbf{v}^n$  by  $\mathbf{v}^{n-1}$  in the transport terms. This leads to the analog of algorithm 2. We omit the details.

**4. Minimizing the time needed to approach a desired state.** In this Section, we will consider another optimal control problem for (13)–(21), where the time needed to approach a desired state plays an essential role. We will prove an existence result and, then, we will deduce the optimality system.

**4.1. An existence result.** Let us fix  $T_0 > 0$  and let us introduce a closed convex set  $\mathcal{U}_{ad} \subset L^2(\omega \times (0, T_0))$  and the set

$$\mathcal{E}_0 = \{ (h, c, \theta, \mathbf{v}) : h \in \mathcal{U}_{ad}, (c, \theta, \mathbf{v}) \text{ solves (13)–(21) in } \Omega \times (0, T_0) \}.$$

<p><b>ALGORITHM 3</b></p> <ol style="list-style-type: none"> <li>a. Choose <math>h^0 \in \mathcal{U}_{ad}</math>;</li> <li>b. Perform one gradient step, i.e.             <ol style="list-style-type: none"> <li>1. Solve (84) with <math>h = h^0</math>, to obtain <math>(c^0, \theta^0, \mathbf{v}^0)</math>;</li> <li>2. Solve (100) with <math>(c, \theta, \mathbf{v}) = (c^0, \theta^0, \mathbf{v}^0)</math>, to obtain <math>(\phi^0, \psi^0, \mathbf{w}^0)</math>;</li> <li>3. Set <math>d^n = (\psi^n + Nh^n) _{\omega \times (0, T)}</math>, etc.</li> </ol> </li> <li>c. Then, for given <math>n \geq 1</math> and <math>h^n \in \mathcal{U}_{ad}</math>, do until convergence:             <ol style="list-style-type: none"> <li>1. Solve (84) with <math>h = h^n</math>, to obtain <math>(c^n, \theta^n, \mathbf{v}^n)</math>;</li> <li>2. Solve (100) with <math>(c, \theta, \mathbf{v}) = (c^n, \theta^n, \mathbf{v}^n)</math>, to obtain <math>(\phi^n, \psi^n, \mathbf{w}^n)</math>;</li> <li>3. Set <math>f^n = (\psi^n + Nh^n) _{\omega \times (0, T)}</math>, <math>\zeta^n = G(f^n, f^{n-1})</math>, <math>d^n = f^n + \zeta^n d^{n-1}</math> and compute <math>\rho^n</math> as in step 3 of algorithm 1 with this new <math>d^n</math>;</li> <li>4. Do as in step 4 of algorithm 1.</li> </ol> </li> </ol>
---

TABLE 3. The optimal step conjugate gradient method with projection.

Again,  $\mathcal{E}_0 \subset L^2(\omega \times (0, T_0)) \times E_0$ , where  $E_0$  is the energy space for the solutions to (13)–(21) in  $\Omega \times (0, T_0)$ .

Let  $\delta > 0$  be given and let us set

$$I(h, c, \theta, \mathbf{v}) = \frac{1}{2} T^*(\theta; \theta_e, \delta)^2 + \frac{N}{2} \iint_{\omega \times (0, T_0)} |h|^2 \tag{101}$$

where  $\theta_e \in L^2(\Omega)$  and, by definition,

$$T^*(\theta; \theta_e, \delta) = \inf \{ T \in [0, T_0] : \|\theta(\cdot, T) - \theta_e\|_{L^2} \leq \delta \}$$

(eventually, we can have  $T^*(\theta; \theta_e, \delta) = +\infty$ ).

We will consider the following optimal control problem:

$$\left\{ \begin{array}{l} \text{Find } (\hat{h}, \hat{c}, \hat{\theta}, \hat{\mathbf{v}}) \in \mathcal{E}_0 \text{ such that} \\ I(\hat{h}, \hat{c}, \hat{\theta}, \hat{\mathbf{v}}) = \min_{(h, c, \theta, \mathbf{v}) \in \mathcal{E}_0} I(h, c, \theta, \mathbf{v}) \end{array} \right. \tag{102}$$

**Theorem 4.1.** *Assume that the set of  $(h, c, \theta, \mathbf{v}) \in \mathcal{E}_0$  such that  $I(h, c, \theta, \mathbf{v}) < +\infty$  is non-empty. Then, there exists at least one solution to (102).*

*Proof.* The set  $\mathcal{U}_{ad}$  is weakly closed in  $L^2(\omega \times (0, T_0))$  and  $I$  is coercive. Accordingly, we only have to check that this functional is sequentially weakly-\* lower semicontinuous for the norm of  $E_0$ .

Let  $\{(h^n, c^n, \theta^n, \mathbf{v}^n)\}$  be a sequence in  $\mathcal{E}_0$  such that  $h^n \rightarrow \hat{h}$  weakly in  $L^2(\omega \times (0, T_0))$  and  $(c^n, \theta^n, \mathbf{v}^n) \rightarrow (\hat{c}, \hat{\theta}, \hat{\mathbf{v}})$  weakly-\* in  $E_0$ . Then, arguing as in the proof of theorem 3.1, we see that  $(\hat{c}, \hat{\theta}, \hat{\mathbf{v}})$  must solve (13)–(21) in  $\Omega \times (0, T_0)$  for  $h = \hat{h}$ . We have

$$\liminf_{n \rightarrow +\infty} \iint_{\omega \times (0, T_0)} |h^n|^2 \geq \iint_{\omega \times (0, T_0)} |\hat{h}|^2.$$

On the other hand, if we set  $T_n^* := T^*(\theta^n; \theta_e, \delta)$  and  $T^* := T^*(\hat{\theta}; \theta_e, \delta)$ , we also have

$$\liminf_{n \rightarrow +\infty} T_n^* \geq T^*. \tag{103}$$

Indeed, if this assertion is false, it can be assumed that the  $T_n^*$  converge to a time  $\tilde{T}$  that satisfies

$$\tilde{T} = \lim_{n \rightarrow +\infty} T_n^* < T^*. \tag{104}$$

We will use the following result, whose proof is postponed to the end of this paragraph:

**Lemma 4.2.** *Under the assumption (104), we necessarily have:*

$$(\hat{\theta}(\cdot, \tilde{T}) - \theta_e, \psi)_{L^2} \leq \delta \|\psi\|_{L^2} \quad \forall \psi \in \mathcal{H}_\theta(\Omega). \tag{105}$$

In particular, if (104) holds, one has  $\|\hat{\theta}(\cdot, \tilde{T}) - \theta_e\|_{L^2} \leq \delta$ . On the other hand, in view of the definition of  $T^*$  and the fact that  $\tilde{T} < T^*$ , we must also have  $\|\hat{\theta}(\cdot, \tilde{T}) - \theta_e\|_{L^2} > \delta$ , which is the opposite inequality. Thus, we get an absurd and, necessarily,

$$\liminf_{n \rightarrow +\infty} T_n^* \geq T^*.$$

This completes the proof of theorem 4.1. □

*Proof of lemma 4.2.* Let  $\theta^n, T_n^*$  and  $\tilde{T}$  be as in the proof of theorem 4.1 and let us assume that (104) holds. We can write the following:

$$\begin{aligned} |(\hat{\theta}(\cdot, \tilde{T}) - \theta_e, \psi)_{L^2}| &\leq |(\hat{\theta}(\cdot, \tilde{T}) - \hat{\theta}(\cdot, T_n^*), \psi)_{L^2}| \\ &+ |(\hat{\theta}(\cdot, T_n^*) - \theta^n(\cdot, T_n^*), \psi)_{L^2}| + |(\theta^n(\cdot, T_n^*) - \theta_e, \psi)_{L^2}| \end{aligned} \tag{106}$$

Let us estimate the three terms in the right hand side of (106). To this end, we will use the following well known result by J. Simon (see [17]):

**Lemma 4.3.** *Let us consider three Banach spaces  $X \subset B \subset Y$  with compact embedding  $X \hookrightarrow B$  and continuous embedding  $B \hookrightarrow Y$ . Let  $F$  be bounded in  $L^\infty(0, T; X)$  and let  $\partial F / \partial t := \{ \partial f / \partial t : f \in F \}$  be bounded in  $L^r(0, T; Y)$ , where  $r > 1$ . Then,  $F$  is relatively compact in  $C^0([0, T]; B)$ .*

Since  $h^n$  is uniformly bounded in  $L^2(\omega \times (0, T_0))$  and the states  $(c^n, \theta^n, \mathbf{v}^n)$  are uniformly bounded in  $E_0$ , we also have

$$\|\theta_t^n\|_{L^\sigma(0, T_0; (\mathcal{H}_\theta(\Omega))')} \leq C$$

(recall that  $\sigma = 2$  if  $d = 2$  and  $\sigma = 4/3$  if  $d = 3$ ). This is a consequence of the identities

$$\theta_t^n = h^n 1_\omega + \chi \Delta \theta^n - \nabla \cdot (\theta^n \mathbf{v}^n)$$

and was already deduced in similar contexts in the proofs of theorems 2.2, 3.1 and 3.2.

In view of lemma 4.3,  $\theta^n$  belongs to a compact set in  $C^0([0, T_0]; B)$  for any Banach space  $B$  with  $L^2(\Omega) \subset B \subset (\mathcal{H}_\theta(\Omega))'$ , the first embedding being compact. In particular,  $\theta^n \rightarrow \hat{\theta}$  strongly in  $C^0([0, T_0]; (\mathcal{H}_\theta(\Omega))')$  and

$$|(\hat{\theta}(\cdot, T_n^*) - \theta^n(\cdot, T_n^*), \psi)_{L^2}| \leq C \|\hat{\theta}(\cdot, T_n^*) - \theta^n(\cdot, T_n^*)\|_{(\mathcal{H}_\theta)'} \|\psi\|_{\mathcal{H}_\theta} \rightarrow 0 \tag{107}$$

for all  $\psi \in \mathcal{H}_\theta(\Omega)$ . Also, since  $T_n^* \rightarrow \tilde{T}$  and  $\hat{\theta} \in C_w^0([0, T_0]; L^2(\Omega))$ , we have  $\hat{\theta}(\cdot, T_n^*) \rightarrow \hat{\theta}(\cdot, \tilde{T})$  weakly in  $L^2(\Omega)$ , whence

$$|(\hat{\theta}(\cdot, \tilde{T}) - \hat{\theta}(\cdot, T_n^*), \psi)_{L^2}| \rightarrow 0. \tag{108}$$

Finally,

$$|(\theta^n(\cdot, T_n^*) - \theta_e, \psi)_{L^2}| \leq \|\theta^n(\cdot, T_n^*) - \theta_e\|_{L^2} \|\psi\|_{L^2} \leq \delta \|\psi\|_{L^2} \tag{109}$$

by the definition of  $T_n^*$ . From (106) and (107)–(109), we deduce at once (105). □

4.2. **The optimality conditions.** Our second goal will be to characterize the solutions to (102) in terms of appropriate optimality conditions, i.e. to deduce a system of equations that the optimal solution, together with some appropriate multipliers, must satisfy.

Let us introduce the function  $\Phi$ , with

$$\Phi(T, h) = \frac{T^2}{2} + \frac{N}{2} \iint_{\omega \times (0, T_0)} |h|^2 \quad \forall (T, h) \in [0, T_0] \times L^2(\omega \times (0, T_0)). \quad (110)$$

Then, (102) can also be written in the form

$$\left\{ \begin{array}{l} \text{Minimize } \Phi(T, h) \\ \text{Subject to } \quad T \in [0, T_0] \\ \quad \quad \quad (h, c, \theta, \mathbf{v}) \in \mathcal{E}_0 \\ \quad \quad \quad \|\theta(\cdot, T) - \theta_e\|_{L^2} \leq \delta \end{array} \right. \quad (111)$$

For obvious reasons, it can also be written in the slightly different way

$$\left\{ \begin{array}{l} \text{Minimize } \Phi(T, h) \\ \text{Subject to } \quad T \in [0, T_0] \\ \quad \quad \quad (h, c, \theta, \mathbf{v}) \in \mathcal{E}_0 \\ \quad \quad \quad \|\theta(\cdot, T) - \theta_e\|_{L^2} = \delta \end{array} \right. \quad (112)$$

where the condition for  $\theta$  at  $T$  has been reformulated as an equality constraint.

The following result holds:

**Theorem 4.4.** *Let the assumptions of theorem 4.1 be satisfied and let  $(\hat{T}, \hat{h})$  be a solution to (112), with associated state  $(\hat{c}, \hat{\theta}, \hat{\mathbf{v}})$ . Let us assume that  $\hat{T} \in (0, T_0)$ ,  $(\hat{c}, \hat{\theta}, \hat{\mathbf{v}})$  is the unique state associated to  $(\hat{T}, \hat{h})$ , the set of points  $(\mathbf{x}, t)$  where  $\hat{\theta} = \eta(\hat{c})$  or  $\max(\eta_s(\hat{c}), \theta_e)$  is negligible,*

$$\exists \kappa > 0 \text{ such that } t \in [\hat{T} - \kappa, \hat{T}] \mapsto \hat{\theta}(\cdot, t) \in L^2(\Omega) \text{ is } C^1 \quad (113)$$

and

$$(\hat{\theta}(\cdot, \hat{T}) - \theta_e, \hat{\theta}_t(\cdot, \hat{T}))_{L^2} < 0 \quad (114)$$

and let us denote by  $\hat{E}$  the energy space associated to  $\hat{T}$ . Then, there exist  $\lambda \in \mathbb{R}$  and  $(\phi, \psi, \mathbf{w}) \in \hat{E}$  such that one has:

$$\left\{ \begin{array}{l} \hat{c}_t + \hat{\mathbf{v}} \cdot \nabla \hat{c}_t - D\Delta \hat{c} = 0 \\ \hat{\theta}_t + \hat{\mathbf{v}} \cdot \nabla \hat{\theta} - \chi \Delta \hat{\theta} = \hat{h} 1_\omega \\ \hat{\mathbf{v}}_t + (\hat{\mathbf{v}} \cdot \nabla) \hat{\mathbf{v}} - \nu \Delta \hat{\mathbf{v}} + (\hat{F}_i^\varepsilon) \mathbf{v}^\varepsilon + \nabla p^\varepsilon = \hat{\mathbf{F}}_e \\ \nabla \cdot \hat{\mathbf{v}} = 0 \\ (D\nabla \hat{c}) \cdot \mathbf{n} = 0, \quad \hat{\mathbf{v}} = 0 \text{ on } \partial\Omega \times (0, \hat{T}) \\ (\chi \nabla \hat{\theta}) \cdot \mathbf{n} = 0 \text{ on } \Gamma_N \times (0, \hat{T}), \quad \hat{\theta} = 0 \text{ on } \Gamma_D \times (0, \hat{T}) \\ \hat{c}(\mathbf{x}, 0) = c^0(\mathbf{x}); \quad \hat{\theta}(\mathbf{x}, 0) = \theta^0(\mathbf{x}); \quad \hat{\mathbf{v}}(\mathbf{x}, 0) = \mathbf{v}^0(\mathbf{x}) \text{ in } \Omega \end{array} \right. \quad (115)$$

$$\left\{ \begin{array}{l} -\phi_t - (D_c \hat{c}_l) \hat{\mathbf{v}} \cdot \nabla \phi - D \Delta \phi = \left( (D_c \hat{F}_e) - (D_c \hat{F}_i^\varepsilon) \hat{\mathbf{v}} \right) \cdot \mathbf{w} \\ -\psi_t - \hat{\mathbf{v}} \cdot \nabla \psi - \chi \Delta \psi = \left( (D_\theta \hat{F}_e) - (D_\theta \hat{F}_i^\varepsilon) \hat{\mathbf{v}} \right) \cdot \mathbf{w} \\ \quad + (D_\theta \hat{c}_l) \hat{\mathbf{v}} \cdot \nabla \phi \\ -\mathbf{w}_t - \nu \Delta \mathbf{w} - (\hat{\mathbf{v}} \cdot \nabla) \mathbf{w} + (\nabla \hat{\mathbf{v}})^t \mathbf{w} + (\hat{F}_i^\varepsilon) \mathbf{w} + \nabla \pi \\ \quad = -\phi \nabla \hat{c}_l - \psi \nabla \hat{\theta} \\ \nabla \cdot \mathbf{w} = 0 \\ (D \nabla \phi) \cdot \mathbf{n} = 0, \quad \mathbf{w} = 0 \quad \text{on } \partial \Omega \times (0, \hat{T}) \\ (\chi \nabla \psi) \cdot \mathbf{n} = 0 \quad \text{on } \Gamma_N \times (0, \hat{T}), \quad \psi = 0 \quad \text{on } \Gamma_D \times (0, \hat{T}) \\ \phi(\mathbf{x}, \hat{T}) = 0; \quad \psi(\mathbf{x}, \hat{T}) = \lambda(\hat{\theta}(\mathbf{x}, \hat{T}) - \theta_e(\mathbf{x})); \quad \mathbf{w}(\mathbf{x}, \hat{T}) = 0 \quad \text{in } \Omega \end{array} \right. \quad (116)$$

$$\iint_{\omega \times (0, \hat{T})} (\psi + N \hat{h})(h - \hat{h}) \geq 0 \quad \forall h \in \mathcal{U}_{ad}, \quad \hat{h} \in \mathcal{U}_{ad}, \quad (117)$$

$$\hat{T} = P_{[0, T_0]} \left( -\lambda(\hat{\theta}(\cdot, \hat{T}) - \theta_e, \hat{\theta}_t(\cdot, \hat{T})) \right), \quad (118)$$

$$\|\hat{\theta}(\cdot, \hat{T}) - \theta_e\|_{L^2} = \delta. \quad (119)$$

In (118),  $P_{[0, T_0]}$  stands for the usual orthogonal projector on  $[0, T_0]$ .

**Remark 9.** The assumption we have made on  $\hat{T}$  serves to discard trivial cases. The first two assumptions on  $(\hat{c}, \hat{\theta})$  are regularity hypotheses. The assumption (113) plays the role of a qualification hypothesis; this is explained in remark 10. On the other hand, it is a reasonable assumption, at least when  $\mathcal{U}_{ad} = L^2(\omega \times (0, T))$ ; this will be clarified below, see remark 11.

**Remark 10.** In order to understand the situation and to interpret theorem 4.4, it is convenient to argue as follows. Let us provisionally replace (13)–(21) by the much simpler system

$$\left\{ \begin{array}{l} \theta_t - \Delta \theta = h 1_\omega \quad \text{in } \Omega \times (0, T_0) \\ \theta = 0 \quad \text{on } \partial \Omega \times (0, T_0) \\ \theta(\mathbf{x}, 0) = \theta^0(\mathbf{x}) \quad \text{in } \Omega \end{array} \right. \quad (120)$$

Let  $(\hat{T}, \hat{h})$  be a solution to the problem

$$\left\{ \begin{array}{l} \text{Minimize } \Phi(T, h) \\ \text{Subject to } \quad T \in [0, T_0] \\ \quad (h, \theta) \text{ satisfies (120)} \\ \quad \|\theta(\cdot, T) - \theta_e\|_{L^2} = \delta \end{array} \right. \quad (121)$$

and assume that  $\hat{T} \in (0, T_0)$ ,  $\hat{h} \in \text{int } \mathcal{U}_{ad}$ . Let  $\hat{\theta}$  be the state associated to  $\hat{h}$  and assume that (113) holds. We can view  $(\hat{T}, \hat{h})$  as a minimizer of  $\Phi$  subject to the equality constraints

$$\begin{aligned} E(h, \theta) &:= (\theta_t - \Delta \theta - h 1_\omega, \theta(\cdot, 0) - \theta_0) = (0, 0) \\ V(T, \theta) &:= \frac{1}{2} \|\theta(\cdot, T) - \theta_e\|_{L^2}^2 - \frac{\delta^2}{2} \end{aligned}$$

Moreover,  $R(E'(\hat{h}, \hat{\theta}))$  is closed. Therefore, thanks to the classical Lagrange’s theorem, there exist multipliers  $\lambda_0, \lambda$  and  $(\psi, \eta)$  (not simultaneously zero) with

$$\lambda_0, \lambda \in \mathbb{R}, \quad \psi = \psi(\mathbf{x}, t), \quad \eta = \eta(\mathbf{x})$$

and

$$\begin{aligned} 0 &= \lambda_0 \langle \Phi'(\hat{T}, \hat{h}), (S, m) \rangle + \lambda \langle V'(\hat{T}, \hat{\theta}), (S, y) \rangle - \langle (\psi, \eta), E'(\hat{h}, \hat{\theta})(m, y) \rangle \\ &= \lambda_0 \left( \hat{T}S + N \iint_{\omega \times (0, T)} \hat{h} m \right) \\ &\quad + \lambda \left( (\hat{\theta}(\cdot, \hat{T}) - \theta_e, \hat{\theta}_t(\cdot, \hat{T}))_{L^2} + (\hat{\theta}(\cdot, \hat{T}) - \theta_e, y(\cdot, \hat{T}))_{L^2} \right) \\ &\quad - \iint_Q \psi(y_t - \Delta y - m1_\omega) - (\eta, y(\cdot, 0))_{L^2} \end{aligned}$$

for all  $S, m$  and  $y$ . The first consequence is that

$$\lambda_0 \hat{T} + \lambda(\hat{\theta}(\cdot, \hat{T}) - \theta_e, \hat{\theta}_t(\cdot, \hat{T}))_{L^2} = 0. \tag{122}$$

The second consequence is that, for all  $y$ , one has

$$\iint_Q \psi(y_t - \Delta y - m1_\omega) - \lambda(\hat{\theta}(\cdot, \hat{T}) - \theta_e, y(\cdot, \hat{T}))_{L^2} + (\eta, y(\cdot, 0))_{L^2} = 0 \tag{123}$$

and, after some computations, this leads to:

$$\begin{cases} -\psi_t - \Delta\psi = 0 & \text{in } \Omega \times (0, \hat{T}) \\ \psi = 0 & \text{on } \partial\Omega \times (0, \hat{T}) \\ \psi(\mathbf{x}, \hat{T}) = \lambda(\hat{\theta}(\mathbf{x}, \hat{T}) - \theta_e(\mathbf{x})) & \text{in } \Omega \end{cases} \tag{124}$$

and

$$\eta(\mathbf{x}) = \psi(\mathbf{x}, 0) \text{ in } \Omega, \tag{125}$$

Finally, we also have

$$\psi + \lambda_0 N \hat{h} = 0 \text{ in } \omega \times (0, \hat{T}). \tag{126}$$

We see from (122), (124) and (125) that  $\lambda$  cannot be zero. For, otherwise, we would also have  $\lambda_0 = 0, \psi \equiv 0$  and  $\eta = 0$ , which is impossible. The function  $t \mapsto \frac{1}{2} \|\hat{\theta}(\cdot, t) - \theta_e\|_{L^2}^2$  is non-increasing at  $t = \hat{T}$ ; consequently,  $(\hat{\theta}(\cdot, \hat{T}) - \theta_e, \hat{\theta}_t(\cdot, \hat{T}))_{L^2} \leq 0$ . It is immediate from (122) that, if the strict inequality holds, then  $\lambda_0 \neq 0$ . We can thus assume in this case that  $\lambda_0 = 1$  and (126) and (122) respectively become

$$\psi + N \hat{h} = 0 \text{ in } \omega \times (0, \hat{T}) \tag{127}$$

and

$$\hat{T} = -\lambda(\hat{\theta}(\cdot, \hat{T}) - \theta_e, \hat{\theta}_t(\cdot, \hat{T}))_{L^2}. \tag{128}$$

In this way, we obtain an optimality system similar to (115)–(119).

**Remark 11.** Let us consider again (121), where we assume that  $\hat{T} \in (0, T_0), \hat{h} \in \text{int } \mathcal{U}_{ad}$  and (113) is satisfied. We have already seen that, necessarily,  $(\hat{\theta}(\cdot, \hat{T}) - \theta_e, \hat{\theta}_t(\cdot, \hat{T}))_{L^2} \leq 0$ . If we have  $(\hat{\theta}(\cdot, \hat{T}) - \theta_e, \hat{\theta}_t(\cdot, \hat{T}))_{L^2} = 0$ , the identities (122) and (126) show that  $\lambda_0 = 0$  and

$$\psi = 0 \text{ in } \omega \times (0, \hat{T}).$$

But then  $\psi \equiv 0$ , because the solutions to systems of th kind (124) satisfy the unique continuation property, see for instance [16]. From (125), we also have  $\eta = 0$ . Taking into account the final condition satisfied by  $\psi$  and recalling that at least one multiplier must be nonzero, we deduce that

$$\hat{\theta}(\mathbf{x}, \hat{T}) = \theta_e(\mathbf{x}) \text{ in } \omega \times (0, \hat{T}).$$

But this is obviously absurd. Consequently,  $(\hat{\theta}(\cdot, \hat{T}) - \theta_e, \hat{\theta}_t(\cdot, \hat{T}))_{L^2} < 0$ . This shows that (114) is a reasonable assumption at least when  $\mathcal{U}_{ad} = L^2(\omega \times (0, T_0))$ .

*Proof of theorem 4.4.* Let us introduce  $S \in \mathbb{R}$ ,  $m \in L^2(\omega \times (0, T))$  and  $a \in \mathbb{R}_+$ , such that

$$T := \hat{T} + aS \in [0, T_0], \quad h := \hat{h} + am \in \mathcal{U}_{ad}, \quad \|\theta(\cdot, T) - \theta_e\|_{L^2}^2 = \delta^2 \quad (129)$$

and let  $(c, \theta, \mathbf{v})$  be a state associated to  $h$ .

In view of (129),

$$\begin{aligned} 0 \leq \Phi(T, h) - \Phi(\hat{T}, \hat{h}) &= a \left( \hat{T}S + N \iint_{\omega \times (0, T_0)} \hat{h} m \right) \\ &+ \frac{a^2}{2} \left[ S^2 + N \iint_{\omega \times (0, T_0)} |m|^2 \right] \end{aligned}$$

for any small  $a > 0$ , whence

$$\hat{T}S + N \iint_{\omega \times (0, T_0)} \hat{h} m \geq 0. \quad (130)$$

As in the proof of theorem 3.2, we can write

$$(c, \theta, \mathbf{v}) = (\hat{c}, \hat{\theta}, \hat{\mathbf{v}}) + a(z, y, \mathbf{u}) + a(z'_a, y'_a, \mathbf{u}'_a)$$

with  $(z, y, \mathbf{u})$  and  $(z'_a, y'_a, \mathbf{u}'_a)$  solving systems respectively similar to (87) and (88), together with homogenous boundary and initial conditions. Arguing as we did in that proof, we see that  $(z, y, \mathbf{u}), (z'_a, y'_a, \mathbf{u}'_a) \in E_0$  and  $\|(z'_a, y'_a, \mathbf{u}'_a)\|_{E_0} \rightarrow 0$  as  $a \rightarrow 0^+$ . Moreover,

$$\begin{aligned} 0 &= \|\theta(\cdot, T) - \theta_e\|_{L^2}^2 - \delta^2 = \|(\theta(\cdot, T) - \hat{\theta}(\cdot, \hat{T})) + (\hat{\theta}(\cdot, \hat{T}) - \theta_e)\|_{L^2}^2 - \delta^2 \\ &= \|\theta(\cdot, T) - \hat{\theta}(\cdot, \hat{T})\|^2 + 2(\theta(\cdot, T) - \hat{\theta}(\cdot, \hat{T}), \hat{\theta}(\cdot, \hat{T}) - \theta_e)_{L^2} \end{aligned}$$

Taking into account that

$$\theta(\cdot, T) - \hat{\theta}(\cdot, \hat{T}) = ay(\cdot, \hat{T}) + a\hat{\theta}_t(\cdot, \hat{T})S + aO(a) \text{ in } L^2(\Omega)$$

where  $O(a) \rightarrow 0$ , we easily deduce that

$$-(\hat{\theta}(\cdot, \hat{T}) - \theta_e, \hat{\theta}_t(\cdot, \hat{T}))_{L^2} S = (\hat{\theta}(\cdot, \hat{T}) - \theta_e, y(\cdot, \hat{T}))_{L^2}. \quad (131)$$

Let us introduce  $\lambda \in \mathbb{R}$  with

$$-(\hat{\theta}(\cdot, \hat{T}) - \theta_e, \hat{\theta}_t(\cdot, \hat{T}))_{L^2} \lambda = \hat{T} \quad (132)$$

and let  $(\phi, \psi, \mathbf{w}) \in \hat{E}$  be the solution to (116).

Thanks to (114),  $\lambda$  is well defined. Furthermore,

$$\begin{aligned} \hat{T}S &= -(\hat{\theta}(\cdot, \hat{T}) - \theta_e, \hat{\theta}_t(\cdot, \hat{T}))_{L^2} \lambda S \\ &= (\lambda(\hat{\theta}(\cdot, \hat{T}) - \theta_e), y(\cdot, \hat{T}))_{L^2} \\ &= (\psi(\cdot, \hat{T}), y(\cdot, \hat{T}))_{L^2} \end{aligned}$$

and, using the equations and boundary and initial conditions satisfied by  $(\phi, \psi, \mathbf{w})$  and  $(z, y, \mathbf{u})$ , we see after some integrations by parts that

$$\hat{T}S = \iint_{\omega \times (0, T_0)} \psi m.$$

In view of (130), this yields

$$\iint_{\omega \times (0, T_0)} (\psi + N\hat{h})m \geq 0.$$



On the other hand, since  $\hat{T} \in (0, T_0)$  and  $\lambda$  is given by (132), the equality (118) is trivially satisfied. Consequently, the couple  $(\hat{T}, \hat{h})$ , the associate state  $(\hat{c}, \hat{\theta}, \hat{v})$ , the multiplier  $\lambda \in \mathbb{R}$  and the adjoint state  $(\phi, \psi, \mathbf{w})$  satisfy (115)–(119).

This ends the proof.  $\square$

**Remark 12.** The optimality system can be used to deduce iterative algorithms for the computation of an optimal  $(\hat{T}, \hat{k}, \hat{c}, \hat{\theta}, \hat{v})$ . This will be the goal of a forthcoming paper.

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Received October 2012; revised January 2013.

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