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Optimal boundary control of a phase field system modeling nonisothermal phase transitions

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Abstract

In this paper, we study an optimal control problem for a singular system of partial differential equations that models a nonisothermal phase transition with a nonconserved order parameter. The control acts through a third boundary condition for the absolute temperature and plays the role of the outside temperature. It is shown that the corresponding control-to-state mapping is well defined, and the existence of an optimal control and the first-order optimality conditions for a quadratic cost functional of Bolza type are established.

1 Introduction

Let $\Omega \subset I\!R^3$ be an open and bounded domain with smooth boundary Γ, and let $T > 0$ be given. We denote $Q_t = \Omega \times (0,t)\,,\ \Gamma_t = \partial\Omega \times (0,T)$, for any $t \in (0,T]$. We consider the following phase field system:

$$\mu(\theta)\chi_t = -F_1'(\chi) - \left(\frac{\beta_1}{\theta} + \beta_2\right) F_2'(\chi) - \frac{F_3'(\chi)}{\theta}\,, \qquad \text{in } Q_T\,, \tag{1.1}$$

$$C_V\theta_t + (\beta_1 F_2'(\chi) + F_3'(\chi))\chi_t - \Delta\theta = 0\,, \qquad \text{in } Q_T\,, \tag{1.2}$$

$$\frac{\partial\theta}{\partial n} + k\theta = u\,, \qquad \text{on } \Gamma_T\,, \tag{1.3}$$

$$\chi(\cdot,0) = \chi_0, \quad \theta(\cdot,0) = \theta_0\,, \qquad \text{in } \Omega\,. \tag{1.4}$$

This system constitutes a model for a nonisothermal phase transition occurring in the container Ω that is controlled by the outside temperature u. In this connection, θ stands for the (positive) absolute temperature, χ is a nonconserved order parameter that characterizes the phase transition, C_V, β_1, β_2, k are positive physical constants, and μ, F_1, F_2, F_3 are given nonlinearities. Typically, χ must attain values in $[0,1]$; for instance, if χ represents the liquid fraction in a melting-solidification process, then $\{\chi = 0\}$ characterizes the solid phase, $\{\chi = 1\}$ the liquid phase, and $\{0 < \chi < 1\}$ a mixture of both phases.

The system (1.1)–(1.4), as well as nonlocal versions thereof, has been extensively studied in recent years for the case of thermal insulation, i.e., if the boundary condition (1.3) is replaced by

$$\frac{\partial\theta}{\partial n} = 0\,, \qquad \text{on } \Gamma_T\,. \tag{1.3$'$}$$

In this connection, we refer to the papers [1, 2, 4, 6]. A very general case with boundary condition of the form (1.3) was recently studied in [3]. Notice, however, that the smoothness assumptions for the control u in [3] are stronger than in this paper, so that we have a weaker regularity of the temperature field θ. More precisely, we assume here that $u \in L^\infty(\Gamma_T)$ so that (1.2), (1.3) has to be understood in the weak sense; in particular, we only can expect that $\theta_t \in L^2(0,T;(H^1(\Omega))^*)$, while under the assumptions of [3] one obtains that $\theta_t \in L^2(Q_T)$. In this sense, also the wellposedness results stated below deserve some interest on their own right.

However, we do not strive for the largest possible generality in this paper, since we want to stress the control aspects. Notice also that (depending on the form of $\mu(\theta)$) Eq. (1.1) may become singular, so that the positivity of θ must be guaranteed. In addition, the typical form of the nonlinearity F_2 is given by

$$F_2(\chi) = \kappa\Big(\chi\log(\chi) + (1-\chi)\log(1-\chi)\Big)\,, \quad \kappa > 0\,, \tag{1.5}$$

which induces another singularity. In fact, it is then necessary to bound χ uniformly away from both 0 and 1.

We thus consider the following optimal control problem (which will be denoted by **(P)** in the following):

Minimize

$$J\,[u,(\chi,\theta)] := \int_0^T\!\!\int_\Gamma u^2(x,t)\,dx\,dt + \|\theta(\cdot,T)-\theta_T\|^2 + \|\chi(\cdot,T)-\chi_T\|^2, \tag{1.6}$$

subject to (1.1)–(1.4) (state equations) and to the pointwise control constraints

$$u \in \mathcal{U} := \{u \in L^\infty(\Gamma_T); \quad 0 < u_1 \le u(x,t) \le u_2 \quad \text{a.e. }\}\,. \tag{1.7}$$

Here, $u_1 > 0$, $u_2 > 0$ are given constants, $(\theta_T, \Gamma_T) \in L^2(\Omega)^2$ is the desired final state at time T, and $\|\cdot\|$ denotes the $L^2(\Omega)$ norm. Notice that the regularity results proved below will guarantee that $\chi,\theta \in C([0,T];L^2(\Omega))$, which implies that J is well defined.

It is the aim of this note to show that the optimal control problem **(P)** admits a solution pair $[u^*,(\chi^*,\theta^*)]$ and to derive the first-order optimality conditions. To this end, we first study in Section 2 the state system (1.1)–(1.4) for fixed $u \in \mathcal{U}$, showing the wellposedness. The technique used differs from the one employed in [1, 4, 6] for similar problems; indeed, we will reverse the order of arguments used there. In addition, we obtain new results for the state system itself. The concluding Section 3 is devoted to the existence of an optimal solution $[u^*,(\chi^*,\theta^*)]$ and to the derivation of first-order necessary conditions.

2 Wellposedness of the state system

The proof of existence and uniqueness of the solution of the state system (1.1)–(1.4) follows the ideas developed in [1, 6], but the order of arguments is reversed in the sense that we first derive a priori bounds for the solution and then treat a truncated system that coincides with the initial system inside these bounds.

We generally assume:

(H1) $\chi_0, \chi_T, \theta_0, \theta_T \in L^\infty(\Omega)$, and there is some $0 < \delta < 1$ such that $\delta \le \chi_0(x) \le 1 - \delta$, $\theta_0(x) \ge \delta$, for a.e. $x \in \Omega$.

(H2) $F_1, F_3 \in C^2[0,1]$, $F_2 \in C^2(0,1)$, and it holds

$$\lim_{s \searrow 0} F_2'(s) = -\infty, \ \lim_{s \nearrow 1} F_2'(s) = +\infty \,. \tag{2.1}$$

(H3) $\mu \in C^1(0,\infty)$, and there is some $\hat{\mu} > 0$ such that

$$\mu(s) \ge \hat{\mu} \min\left\{1, \frac{1}{s}\right\} \quad \forall\ s > 0\,. \tag{2.2}$$

(H4) $u \in \mathcal{U} := \{u \in L^\infty(\Gamma_T); \quad u_1 \le u(x,t) \le u_2 \quad \text{a.e. } \}$,

with given constants $u_1 > 0$, $u_2 > 0$.

Remark 2.1 Condition (2.1) is satisfied if $\mu(s) = \hat{\mu} s^{-\alpha}$ with some $\hat{\mu} > 0$ and $0 \le \alpha \le 1$. Note that the case $\alpha = 1$ corresponds to the Caginalp phase field model, while $\alpha = 0$ gives the analogue of the Penrose–Fife model. Notice also that (2.2) is more general than the condition

$$\mu(s) \ge \hat{\mu}\left(1 + \frac{1}{s}\right), \quad \hat{\mu} > 0\,, \quad \forall\, s > 0\,, \tag{2.2$'$}$$

which was needed to derive the very general well-posedness results of [3].

2.1 A priori bounds

For what follows, we introduce the function $l \in C^1(0,\infty)$,

$$l(s) := \frac{1}{s\mu(s)} > 0 \qquad \text{for } s > 0\,.$$

To simplify notation, we assume without loss of generality that $\hat{\mu} = C_V = 1$, and we denote, for $0 < \chi < 1$,

$$h_1(\chi) := \beta_1 F_2'(\chi) + F_3'(\chi)\,, \quad h_2(\chi) := \beta_2 F_2'(\chi) + F_1'(\chi)\,.$$

Then, rearranging terms in (1.1) and substituting χ_t from (1.1) in (1.2), we may rewrite (1.1), (1.2) in the form

$$\chi_t = -l(\theta)[h_1(\chi) + h_2(\chi)\theta]\,, \tag{2.3}$$

$$\theta_t - \Delta\theta = l(\theta) h_1(\chi)[h_1(\chi) + h_2(\chi)\theta]\,. \tag{2.4}$$

We have the following result.

Proposition 2.2 *Suppose that* **(H1)**–**(H3)** *are fulfilled. For any* $\theta \in L^\infty(Q_T)$ *satisfying* $\theta(x,t) \ge \underline{\theta}$ *a.e. in* Q_T *for some* $\underline{\theta} > 0$, *there is a unique solution* $\chi \in L^\infty(Q_T)$ *to* (2.3) *such that* $\chi_t \in L^\infty(Q_T)$ *and* $\chi(x,0) = \chi_0(x)$ *for a.e.* $x \in \Omega$. *Moreover, there are constants* $0 < \underline{\chi} < \overline{\chi} < 1$, *which are independent of* θ, *such that*

$$\underline{\chi} \le \chi(x,t) \le \overline{\chi} \quad \text{a.e. in } Q_T\,. \tag{2.5}$$

Proof: There is some set $N \subset \Omega$ of zero measure such that $\theta(x,t) \ge \underline{\theta} > 0$ and $\chi_0(x) \in \mathbb{R}$ for every $x \in \Omega \setminus N$, and for any such x it follows that the initial value problem

$$\begin{aligned} \chi_t(x,t) &= l(\theta(x,t))\,[h_1(\chi(x,t)) + h_2(\chi(x,t))\theta(x,t)]\,, \quad \text{for a.e. } t \in (0,T)\,,\\ \chi(x,0) &= \chi_0(x)\,, \end{aligned} \tag{2.6}$$

has a unique local Carathéodory solution. Now observe that, owing to the general hypotheses **(H1)**–**(H3)**, there are constants $0 < \chi_1 < \chi_2 < 1$ such that $h_1 < 0$, $h_2 < 0$ on $(0,\chi_1]$, and $h_1 > 0$, $h_2 > 0$ on $[\chi_2, 1)$, respectively. Thus, $\chi_t(x,t) > 0$ whenever $\chi(x,t) \in (0,\chi_1]$, and $\chi_t(x,t) < 0$ whenever $\chi(x,t) \in [\chi_2, 1)$. Consequently, we must have

$$\underline{\chi} := \min\{\delta, \chi_1\} \le \chi(x,t) \le \overline{\chi} := \max\{1-\delta, \chi_2\}\,, \quad \text{a.e. in } Q_T\,.$$

From this we can infer that the solution to (2.6) exists in fact on the entire time interval $[0,T]$, and the assertion follows. ■

In order to obtain a priori bounds for the energy balance equation (2.1) (respectively, (2.4)) under the boundary condition (1.3), and in order to apply an iterative method to construct the solution to the system, we now replace in Eq. (2.4) the possibly unbounded term $l(\theta)$ by a truncation. To this end, let $0 < \varepsilon < 1$, and define

$$\varphi_\varepsilon(s) := \max\{\varepsilon, s\}\,, \quad l_\varepsilon(s) := \begin{cases} \dfrac{1}{\varphi_\varepsilon(s\mu(s))}\,, & \text{for } s > 0\,,\\ \varepsilon^{-1}\,, & \text{for } s \le 0\,. \end{cases} \tag{2.7}$$

Obviously, $0 < l_\varepsilon(s) \le \varepsilon^{-1}$ for all $s \in \mathbb{R}$, and thus $l_\varepsilon \in L^\infty(\mathbb{R})$. We now consider the truncated problem

$$\theta_t - \Delta\theta = l_\varepsilon(\theta) h_1(\chi)[h_1(\chi) + h_2(\chi)\theta]\,, \tag{2.8}$$

together with the boundary condition (1.3) and the initial condition (1.4) for θ. As usual, we call θ a (weak) variational solution to (2.8), (1.3), (1.4) if

$$\theta \in \mathcal{W} := \left\{\eta \in L^2(0,T;H^1(\Omega))\,;\, \eta_t \in L^2(0,T;(H^1(\Omega))^*)\right\}\,, \tag{2.9}$$

and

$$\begin{aligned} &\langle \theta_t(t), v\rangle + \int_\Omega \nabla\theta(t)\cdot\nabla v\,dx + \int_\Gamma (k\,\theta(t) - u(t))\,v\,d\sigma \\ &= \int_\Omega l_\varepsilon(\theta(t))\,h_1(\chi(t))\,[h_1(\chi(t)) + h_2(\chi(t))\,\theta(t)]\,v\,dx \\ &\qquad \forall\, v \in H^1(\Omega)\,, \quad \text{a.e. } t \in (0,T)\,, \end{aligned} \tag{2.10}$$

$$\theta(0) = \theta_0 \,, \tag{2.11}$$

where $\langle \cdot , \cdot \rangle$ denotes the dual pairing between $(H^1(\Omega))^*$ and $H^1(\Omega)$. We have the following result.

Proposition 2.3 *There are constants $0 < \varepsilon_0 \le \delta_0 \,,\, \delta_1 > 0$, depending only on $\underline{\chi}, \overline{\chi}, u_1, u_2, \delta, \|\theta_0\|_{L^\infty(Q_T)}$, such that the following holds: whenever $\theta \in L^2(Q_T)$ is a variational solution to* (2.8), (1.3), (1.4) *for some $0 < \varepsilon \le \varepsilon_0$ and some $\chi \in L^\infty(Q_T)$ satisfying $\underline{\chi} \le \chi \le \overline{\chi}$ a.e. in Q_T, then*

$$0 < \delta_0 \le \theta \le \delta_1 \quad a.e. \ in \ Q_T \,. \tag{2.12}$$

In particular, $\theta \ge \varepsilon$ a.e. in Q_T, that is, θ satisfies Eq. (2.4).

Proof:

Step 1: Let $\varepsilon > 0$ and $\chi \in L^\infty(Q_T)$ with $\underline{\chi} \le \chi \le \overline{\chi}$ a.e. in Q_T be fixed, and let $\theta \in \mathcal{W} \cap L^\infty(Q_T)$ be an associated variational solution. Then $\theta_t - \Delta\theta + c_\varepsilon(x,t)\,\theta \ge 0$ in Q_T in the weak sense, where $c_\varepsilon = -l_\varepsilon(\theta)\,h_1(\chi)\,h_2(\chi) \in L^\infty(Q_T)$. Thus, we can infer from the maximum principle for parabolic equations that $\theta \ge \theta_1^\varepsilon$ a.e. in Q_T, where θ_1^ε is the strong solution to the problem

$$\theta^\varepsilon_{1,t} - \Delta\theta_1^\varepsilon + c(x,t)\theta_1^\varepsilon \ = \ 0 \quad \text{in } Q_T \,, \tag{2.13}$$

$$\frac{\partial \theta_1^\varepsilon}{\partial n} + k\,\theta_1^\varepsilon \ = \ u_1 \quad \text{on } \Gamma_T \,, \tag{2.14}$$

$$\theta_1^\varepsilon(x,0) \ = \ \theta_0(x) \quad \text{for a.e. } x \in \Omega \,, \tag{2.15}$$

which is positive a.e. in Q_T. Thus, $\theta > 0$ a.e. in Q_T.

Step 2: We now show that there is some $\overline{c} > 0$ that does not depend on $\varepsilon > 0$ such that

$$\frac{1}{\varphi_\varepsilon(\theta\mu(\theta))}[h_1^2(\chi) + h_1(\chi)h_2(\chi)\theta] \ge -\overline{c}\,\varphi_\varepsilon(\theta) \quad \text{a.e. in } Q_T \,. \tag{2.16}$$

Indeed, if $\theta \ge 1$ then it follows from $\hat{\mu} = 1$ that $\theta\,\mu(\theta) \ge \min\{1, \theta^{-1}\}\,\theta \ge 1$. Hence, $\varphi_\varepsilon(\theta\mu(\theta)) \ge 1$, so that the expression on the left-hand side of (2.16) is bounded from below by $-c_1\,\varphi_\varepsilon(\theta)$ for $c_1 := \max\limits_{\underline{\chi} \le \chi \le \overline{\chi}} |h_1(\chi)\,h_2(\chi)|$.

On the other hand, if $\theta < 1$ then $\theta \le \theta\,\mu(\theta)$, and thus $\theta \le \varphi_\varepsilon(\theta\,\mu(\theta))$. Therefore,

$$\frac{1}{\varphi_\varepsilon(\theta\,\mu(\theta))}[h_1^2(\chi) + h_1(\chi)\,h_2(\chi)\,\theta] \ge -\frac{h_2^2(\chi)\,\theta^2}{4\,\varphi_\varepsilon(\theta\,\mu(\theta))} \ge -c_2\,\varphi_\varepsilon(\theta)\,,$$

with $c_2 := \frac{1}{4} \max\limits_{\underline{\chi} \le \chi \le \overline{\chi}} h_2^2(\chi)$. Hence, (2.16) holds with the choice $\overline{c} = \max\{c_1, c_2\}$.

Step 3: Using the fact that $\varphi_\varepsilon(\theta) \le \theta + \varepsilon$ a.e., we conclude from (2.16) that $\theta_t - \Delta\theta + \overline{c}\,\theta \ge -\overline{c}\,\varepsilon$ in the weak sense. Hence, $\theta \ge \underline{\theta}^\varepsilon$ a.e. in Q_T, where $\underline{\theta}^\varepsilon$ solves

$$\underline{\theta}^\varepsilon_t - \Delta\underline{\theta}^\varepsilon + \overline{c}\,\underline{\theta}^\varepsilon \;=\; -\overline{c}\,\varepsilon \quad \text{in } Q_T\,, \tag{2.17}$$

$$\frac{\partial\underline{\theta}^\varepsilon}{\partial n} + k\,\underline{\theta}^\varepsilon \;=\; u_1 \quad \text{on } \Gamma_T\,, \tag{2.18}$$

$$\underline{\theta}^\varepsilon(x,0) \;=\; \delta \quad \text{for a.e. } x \in \Omega\,. \tag{2.19}$$

From the general regularity theory of linear parabolic problems we infer that $\underline{\theta}^\varepsilon$ is smooth. Moreover, we have $\underline{\theta}^\varepsilon \to \underline{\theta}^0$ uniformly on $\overline{Q_T}$ as $\varepsilon \searrow 0$, where $\underline{\theta}^0$ denotes the solution to (2.17)–(2.19) for $\varepsilon = 0$. Since $\min\limits_{(x,t)\in\overline{Q_T}} \underline{\theta}^0(x,t) =: 2\,\delta_0 > 0$, there is some $\hat{\varepsilon} > 0$ such that $\underline{\theta}^\varepsilon \ge \delta_0$ whenever $0 < \varepsilon < \hat{\varepsilon}$. Notice that $\delta_0\,,\,\hat{\varepsilon}$ only depend on $u_1, \delta, \underline{\chi}, \overline{\chi}$.

Step 4: To establish the global upper bound for θ, notice that, by Step 3, $\theta \ge \underline{\theta}^\varepsilon \ge \delta_0 > 0$ whenever $0 < \varepsilon \le \hat{\varepsilon}$. In particular, if $0 < \varepsilon \le \min\{\delta_0, \hat{\varepsilon}\}$, then $\theta \ge \varepsilon > 0$ and thus $\varphi_\varepsilon(\theta) = \theta$, so that, using **(H3)**,

$$l_\varepsilon(\theta) = (\theta\,\mu(\theta))^{-1} \le (\min\{\theta, 1\})^{-1} \le (\min\{\delta_0, 1\})^{-1} =: \tilde{\kappa}\,.$$

It thus follows from the maximum principle of parabolic equations that $\theta \le \tilde{\theta}$ a.e. in Q_T, where $\tilde{\theta}$ solves the problem

$$\tilde{\theta}_t - \Delta\tilde{\theta} - \tilde{\kappa} \max_{\underline{\chi}\le\chi\le\overline{\chi}} |h_1(\chi)\,h_2(\chi)|\,\tilde{\theta} \;=\; \tilde{\kappa} \max_{\underline{\chi}\le\chi\le\overline{\chi}} h_1^2(\chi) \quad \text{in } Q_T\,, \tag{2.20}$$

$$\frac{\partial\tilde{\theta}}{\partial n} + k\,\tilde{\theta} \;=\; u_2 \quad \text{on } \Gamma_T\,, \tag{2.21}$$

$$\tilde{\theta}(x,0) \;=\; \theta_0(x) \quad \text{for a.e. } x \in \Omega\,. \tag{2.22}$$

Putting $\delta_1 := \|\tilde{\theta}\|_{L^\infty(Q_T)}\,,\ \varepsilon_0 := \min\{\delta_0, \hat{\varepsilon}\}$, we have proved the assertion. ■

Remark 2.4 The truncation procedure was needed, since l may be unbounded on $(0,\infty)$. This is not the case if **(H3)** is replaced by the condition $\mu(\theta) \ge \theta^{-1}$, since then $l \in L^\infty(0,\infty)$.

2.2 Wellposedness of the State System

In this section, we are going to prove the following result.

Theorem 2.5 *Suppose that* **(H1)**–**(H4)** *are fulfilled. Then the system* (1.1)–(1.4) *admits for every* $u \in \mathcal{U}$ *a unique solution* (χ, θ) *such that*

$$\chi, \chi_t \in L^\infty(Q_T)\,, \quad \underline{\chi} \le \chi \le \overline{\chi} \quad \textit{a.e. in } Q_T\,, \quad (1.1) \textit{ holds a.e. in } Q_T\,, \tag{2.23}$$

$\theta \in \mathcal{W} \cap L^\infty(Q_T)$ *is a weak solution to* (1.2)–(1.4) *in the sense of* (2.13), (2.14) , (2.24)

$$0 < \gamma_1 \le \theta \le \gamma_2 \quad a.e. \ in \ Q_T\,, \tag{2.25}$$

with constants γ_1, γ_2 *that depend only on* $\delta, u_1, u_2, \|\theta_0\|_{L^\infty(\Omega)}$. *Moreover,* (χ, θ) *is the only solution to* (1.1)–(1.4) *that satisfies* (2.23), (2.24), *and*

$$\operatorname*{ess\,inf}_{Q_T} \theta(x,t) > 0\,. \tag{2.26}$$

Proof: Let $\underline{\chi}, \overline{\chi}$ and $\varepsilon_0, \delta_0, \delta_1$ be the positive constants introduced in Propositions 2.2 and 2.3, respectively. We fix $\varepsilon \in (0, \varepsilon_0]$, set $\rho(\theta) := \min\{\theta, \delta_1\}$, and choose some $\alpha > 0$ such that

$$l_\varepsilon(\theta)\, h_1(\chi)\, h_2(\chi) + \alpha > 0 \quad \text{for } \theta \ge 0\,, \quad \underline{\chi} \le \chi \le \overline{\chi}\,. \tag{2.27}$$

Now let $u \in \mathcal{U}$ be arbitrary, but fixed. We then consider the initial-boundary value problem

$$\chi_t = l_\varepsilon(\tilde{\theta})[h_1(\chi) + h_2(\chi)\, \tilde{\theta}] =: f(\chi, \tilde{\theta})\,, \quad \text{in } Q_T\,, \tag{2.28}$$

$$\begin{aligned} \theta_t - \Delta\theta + \alpha\,\theta \ &= \ l_\varepsilon(\tilde{\theta})\, h_1^2(\tilde{\chi}) + [l_\varepsilon(\tilde{\theta})\, h_1(\tilde{\chi})\, h_2(\tilde{\chi}) + \alpha]\, \rho(\tilde{\theta}) \\ &=: \ g(\tilde{\chi}, \tilde{\theta})\,, \quad \text{in } Q_T\,, \end{aligned} \tag{2.29}$$

$$\frac{\partial \theta}{\partial n} + k\,\theta = u\,, \quad \text{on } \Gamma_T\,, \tag{2.30}$$

$$\chi(\cdot, 0) = \chi_0\,, \quad \theta(\cdot, 0) = \theta_0\,, \quad \text{in } \Omega\,, \tag{2.31}$$

where $\tilde{\chi} \in L^2(Q_T)$ satisfies $\underline{\chi} \le \tilde{\chi} \le \overline{\chi}$ a.e. in Q_T, and where $\tilde{\theta} \in L^2(Q_T)$ fulfills

$$\gamma_1 \le \tilde{\theta} \le \gamma_2 \quad \text{a.e. in } Q_T\,, \tag{2.32}$$

with constants $0 < \gamma_1 < \gamma_2$, which will be defined below.

Arguing as in the proof of Proposition 2.2, we can infer that (2.28), (2.31) admits a unique solution $\chi \in L^\infty(Q_T)$ such that $\chi_t \in L^\infty(Q_T)$ and $\underline{\chi} \le \chi \le \overline{\chi}$ a.e. in Q_T. Moreover, it follows from the general theory of parabolic equations (cf. [5]) that the problem (2.29), (2.30), (2.31) has a weak solution $\theta \in \mathcal{W}$ that depends continuously on the data $\theta_0 \in L^2(\Omega)$, $u \in L^2(0,T; L^2(\Gamma))$, and on the right-hand side g (with respect to the topology of $L^2(0,T; (H^1(\Omega))^*)$). Now, by construction of α, the right-hand side of (2.29) is nonnegative. Hence, $\theta \ge \underline{\theta}$ a.e. in Q_T, where $\underline{\theta}$ is the (smooth) solution to the problem

$$\underline{\theta}_t - \Delta\underline{\theta} + \alpha\,\underline{\theta} \ = \ 0\,, \quad \text{in } Q_T\,, \tag{2.33}$$

$$\frac{\partial \underline{\theta}}{\partial n} + k\,\underline{\theta} \ = \ u_1\,, \quad \text{on } \Gamma_T\,, \tag{2.34}$$

$$\underline{\theta}(\cdot, 0) \ = \ \delta\,, \quad \text{in } \Omega\,, \tag{2.35}$$

which is positive. Consequently,

$$\theta \geq \gamma_1 := \min_{(x,t)\in\overline{Q_T}} \underline{\theta}(x,t) > 0 \quad \text{a.e. in } Q_T\,.$$

On the other hand, the right-hand side of (2.29) is bounded in the form

$$|g(\tilde{\chi},\tilde{\theta})| \leq \varepsilon^{-1} \max_{\underline{\chi}\leq\chi\leq\overline{\chi}} h_1^2(\chi) + \varepsilon^{-1} \max_{\underline{\chi}\leq\chi\leq\overline{\chi}} |h_1(\chi)\, h_2(\chi)|\, \delta_1 + \alpha\, \delta_1 =: \sigma\,.$$

Using the maximum principle once more, we find that $\theta \leq \overline{\theta}$, where $\overline{\theta}$ solves

$$\overline{\theta}_t - \Delta\overline{\theta} + \alpha\,\overline{\theta} \;=\; \sigma\,, \quad \text{in } Q_T\,, \tag{2.36}$$

$$\frac{\partial\overline{\theta}}{\partial n} + k\,\overline{\theta} \;=\; u_2\,, \quad \text{on } \Gamma_T\,, \tag{2.37}$$

$$\overline{\theta}(\cdot,0) \;=\; \|\theta_0\|_{L^\infty(\Omega)}\,, \quad \text{in } \Omega\,. \tag{2.38}$$

In conclusion, we have $\gamma_1 \leq \theta \leq \gamma_2$ a.e. in Q_T with $\gamma_2 := \|\overline{\theta}\|_{L^\infty(Q_T)}$.

Now let

$$M \;:=\; \Big\{(\tilde{\chi},\tilde{\theta}) \in C\left([0,T];L^2(\Omega)\right)^2; \quad \underline{\chi} \leq \chi \leq \overline{\chi} \quad \text{and} \\ \gamma_1 \leq \tilde{\theta} \leq \gamma_2 \quad \text{a.e. in } Q_T\Big\}\,. \tag{2.39}$$

Clearly, M is a nonempty and closed subset of $C([0,T];L^2(\Omega))^2$. Moreover, if $\mathcal{F}$ denotes the operator that assigns to each $(u,(\tilde{\chi},\tilde{\theta})) \in \mathcal{U}\times M$ the associated solution to (2.29)–(2.31), then $\mathcal{F}(u,\cdot)$ maps M into M for any fixed $u\in\mathcal{U}$. We now show that $\mathcal{F}(u,\cdot)$ is a contraction on M with respect to a suitably weighted norm on $C([0,T];L^2(\Omega))^2$. To this end, we show the following stability result.

Lemma 2.6 *Suppose that $(u^i,(\tilde{\chi}^i,\tilde{\theta}^i)) \in \mathcal{U}\times\mathcal{M}$, $i=1,2$, are given, and let $(\chi^i,\theta^i) = F(u^i,(\tilde{\chi}^i,\tilde{\theta}^i))$, $i=1,2$. Denote $\tilde{\chi} := \tilde{\chi}^1-\tilde{\chi}^2$, $\tilde{\theta} := \tilde{\theta}^1-\tilde{\theta}^2$, $u := u^1-u^2$, $\chi := \chi^1-\chi^2$, $\theta := \theta^1-\theta^2$. Then there is some constant $C>0$, depending only on $\underline{\chi},\overline{\chi},\gamma_1,\gamma_2,\varepsilon$, such that*

$$\|\chi(t)\|^2 + \|\theta(t)\|^2 + \int_0^t \|\nabla\theta(s)\|^2\,ds + \int_0^t\!\int_\Gamma \theta^2\,d\sigma\,ds + \int_0^t \|\theta(s)\|^2\,ds \\ \leq\; C\left(\int_0^t \left[\|\chi(s)\|^2 + \|\tilde{\chi}(s)\|^2 + \|\theta(s)\|^2 + \|\tilde{\theta}(s)\|^2 + \int_\Gamma u^2\,d\sigma\right] ds\right)\,. \tag{2.40}$$

Proof: The pair (χ,θ) satisfies the initial-boundary value problem

$$\chi_t = f(\chi^1,\tilde{\theta}^1) - f(\chi^2,\tilde{\theta}^2)\,, \quad \text{in } Q_T\,, \tag{2.41}$$

$$\theta_t - \Delta\theta + \alpha\,\theta = g(\tilde{\chi}^1,\tilde{\theta}^1) - g(\tilde{\chi}^2,\tilde{\theta}^2)\,, \quad \text{in } Q_T\,, \tag{2.42}$$

$$\frac{\partial\theta}{\partial n} + k\,\theta = u\,, \quad \text{on } \Gamma_T\,, \tag{2.43}$$

$$\chi(\cdot,0) = 0\,, \quad \theta(\cdot,0) = 0\,, \quad \text{in } \Omega\,, \tag{2.44}$$

where Eq. (2.41) holds a.e. in Q_T, while the equations for θ have to be understood in the weak sense (see (2.10), (2.12)).

Now observe that f, g are globally Lipschitz continuous on $[\underline{\chi}, \overline{\chi}] \times [\gamma_1, \gamma_2]$, i.e., there is some $L_\varepsilon > 0$ such that

$$|f(\chi^1, \theta^1) - f(\chi^2, \theta^2)| + |g(\chi^1, \theta^1) - g(\chi^2, \theta^2)| \le L_\varepsilon \left(|\chi^1 - \chi^2| + |\theta^1 - \theta^2| \right)$$
$$\forall \, (\chi^1, \theta^1), (\chi^2, \theta^2) \in [\underline{\chi}, \overline{\chi}] \times [\gamma_1, \gamma_2] \, . \tag{2.45}$$

Now multiply (2.41) by χ and integrate over Q_t for $t > 0$. Then it follows from (2.45), using Young's inequality, that

$$\|\chi(t)\|^2 \le L_\varepsilon \int_0^t \left(3\|\chi(s)\|^2 + \|\tilde{\theta}(s)\|^2 \right) ds \, . \tag{2.46}$$

Next, we test the variational form of (2.42)–(2.44) by θ. Using Young's inequality and (2.45), we easily see that there is a constant $\tilde{C} > 0$, depending only on $\underline{\chi}, \overline{\chi}, \gamma_1, \gamma_2, \varepsilon$, such that

$$\|\theta(t)\|^2 + \int_0^t \|\nabla\theta(s)\|^2 \, ds + \int_0^t \|\theta(s)\|^2 \, ds + \int_0^t \int_\Gamma \theta^2 \, d\sigma \, ds$$
$$\le \tilde{C} \left(\int_0^t \left(\|\tilde{\chi}(s)\|^2 + \|\tilde{\theta}(s)\|^2 \right) ds + \int_0^t \int_\Gamma u^2 \, d\sigma \, ds \right) . \tag{2.47}$$

Combining (2.46) and (2.47), we obtain the assertion. ■

Proof of Theorem 2.5 (continued) Consider for $\omega > 0$ the norm

$$\|(\chi, \theta)\|_\omega := \max_{0 \le t \le T} e^{-\omega t} \left(\|\chi(t)\| + \|\theta(t)\| \right) , \tag{2.48}$$

which is equivalent to the standard norm of $C\Big([0, T]; L^2(\Omega)\Big)^2$. Multiplying (2.40) by $2e^{-2\omega t}$, we find that

$$e^{-2\omega t} \left(\|\chi(t)\| + \|\theta(t)\| \right)^2 \le 2 \, e^{-2\omega t} \left(\|\chi(t)\|^2 + \|\theta(t)\|^2 \right)$$
$$\le \frac{C}{\omega}(1 - e^{-2\omega T}) \max_{0 \le s \le t} e^{-2\omega s} \left(\|\chi(s)\|^2 + \|\tilde{\chi}(s)\|^2 + \|\theta(s)\|^2 + \|\tilde{\theta}(s)\|^2 \right)$$
$$+ 2 \, C \int_0^t \int_\Gamma u^2 \, d\sigma \, ds \, ,$$

whence

$$\|(\chi, \theta)\|_\omega^2 \le \frac{C}{\omega}(1 - e^{-2\omega T}) \left(\|(\chi, \theta)\|_\omega^2 + \|(\tilde{\chi}, \tilde{\theta})\|_\omega^2 \right)$$
$$+ 2 \, C \int_0^t \int_\Gamma u^2 \, d\sigma \, ds \, . \tag{2.49}$$

Choosing $\omega > 0$ appropriately large, it follows that there are constants $L_\omega \in (0,1)$, $C_\omega > 0$, which are independent of u, such that

$$\|(\chi,\theta)\|_\omega^2 \le L_\omega \|(\tilde\chi,\tilde\theta)\|_\omega^2 + C_\omega \int_0^t \int_\Gamma u^2 \, d\sigma \, ds\,. \tag{2.50}$$

In particular, the mapping $\mathcal{F}(u,\cdot)$ is a contraction on M (uniformly in $u \in M$) with respect to $\|\cdot\|_\omega$, and thus enjoys a unique fixed point $(\hat\chi,\hat\theta)$ in M, which in turn is the unique solution to the problem

$$\chi_t = l_\varepsilon(\theta)[h_1(\chi) + h_2(\chi)\,\theta]\,, \quad \text{in } Q_T\,, \tag{2.51}$$

$$\theta_t - \Delta\theta + \alpha\,\theta = l_\varepsilon(\theta)h_1^2(\chi) + [l_\varepsilon(\theta)h_1(\chi)\,h_2(\chi) + \alpha]\,\rho(\theta)\,, \tag{2.52}$$

together with the initial and boundary conditions (1.3), (1.4). Clearly, $\hat\chi, \hat\chi_t \in L^\infty(Q_T)$, while $\hat\theta \in \mathcal{W}$. Moreover, Proposition 2.3 implies that $\hat\theta \ge \varepsilon$ a.e. in Q_T, that is, $\varphi_\varepsilon(\hat\theta) = \hat\theta$, which implies that $(\hat\chi,\hat\theta)$ solves in fact Eq. (2.3). Also, we obviously have that

$$\hat\theta_t - \Delta\hat\theta + \alpha\,\hat\theta \le l_\varepsilon(\hat\theta)\,h_1(\hat\chi)\,[h_1(\hat\chi) + h_2(\hat\chi)\,\hat\theta] + \alpha\,\hat\theta$$

in the weak sense, and the same comparison argument as in Step 4 in the proof of Proposition 2.3 yields that $\hat\theta \le \delta_1$ a.e. in Q_T, and thus, $\rho(\hat\theta) = \hat\theta$. Therefore, $(\hat\chi,\hat\theta)$ solves also (2.4), and thus (1.1)–(1.4).

Finally, if (χ,θ) is any solution to (1.1)–(1.4) that satisfies (2.23), (2.24), (2.26), then it follows from Proposition 2.2 that $\underline{\chi} \le \chi \le \overline{\chi}$ a.e. in Q_T, and Proposition 2.3 implies that (2.12) holds. But then in fact $(\chi,\theta) \in M$ and thus, $\chi = \hat\chi$, $\theta = \hat\theta$. This completes the proof of the theorem. ■

Remark 2.7 Observe that (2.50) implies the Lipschitz continuous dependence of the solution with respect to the control u. Indeed, if $u_1, u_2 \in \mathcal{U}$ are given, then it holds for the corresponding solutions (χ^1,θ^1), (χ^2,θ^2) the estimate

$$\|(\chi^1,\theta^1) - (\chi^2,\theta^2)\|_\omega^2 \le \frac{C_\omega}{1-L_\omega} \int_0^t \int_\Gamma |u_1 - u_2|^2 \, d\sigma \, ds\,. \tag{2.53}$$

3 The Optimal Control Problem

3.1 Existence of Optimal Controls

We now study the optimal control problem **(P)**. We first show the existence of optimal controls. To this end, let $\{u_n\} \subset \mathcal{U}$ be a minimizing sequence, and let $(\chi_n,\theta_n) \in M$ denote the solution of (1.1)–(1.4) associated with $u_n, n \in \mathbb{N}$. Clearly, $\{u_n\}$ is bounded in $L^\infty(Q_T), \{\chi_n\}, \{\chi_{n,t}\}$ are bounded in $L^\infty(Q_T)$, and $\{\theta_n\}$ is bounded in $\mathcal{W} \cap L^\infty(Q_T)$. Hence, for a subsequence, which is again indexed by n, we have the convergences

$$
\begin{aligned}
& u_n \to u^* \quad \text{weakly-star in } L^\infty(Q_T)\,, \\
& \chi_n \to \chi^*\,, \quad \chi_{n,t} \to \chi_t^*\,, \quad \text{weakly-star in } L^\infty(Q_T)\,, \\
& \theta_n \to \theta^*\,, \quad \text{weakly in } \mathcal{W} \text{ and weakly-star in } L^\infty(Q_T)\,.
\end{aligned} \tag{3.1}
$$

Since $\mathcal{W}$ is continuously embedded in $C([0,T;L^2(\Omega))$ and compactly embedded in $L^2(Q_T)$, we also have

$$
\theta_n \to \theta^*\,, \quad \text{weakly in } C([0,T];L^2(\Omega)) \text{ and strongly in } L^2(Q_T)\,. \tag{3.2}
$$

In particular, $\theta_n(T) \to \theta^*(T)$ weakly in $L^2(\Omega)$.

Next, we subtract Eq. (2.3) for $(\chi,\theta) = (\chi_n,\theta_n)$ from the equation for $(\chi,\theta) = (\chi^*,\theta^*)$ and multiply the resulting equation by $\chi_n - \chi^*$. Using the fact that $l_\varepsilon(\theta) = l(\theta)$ and $\rho(\theta) = \theta$ for both $\theta = \theta_n$ and $\theta = \theta^*$, and invoking (2.45), we can argue as in the derivation of Eq. (2.46) to conclude that, for any $t \ge 0$,

$$
\|\chi_n(t) - \chi^*(t)\|^2 \le L_\varepsilon \int\limits_0^t \Big(3\|\chi_n(s) - \chi^*(s)\|^2 + \|\theta_n(s) - \theta^*(s)\|^2\Big)\, ds\,,
$$

and thus (3.2) implies that

$$
\chi_n \to \chi^* \quad \text{strongly in } C([0,T];L^2(\Omega))\,. \tag{3.3}
$$

In particular, $\chi_n(T) \to \chi^*(T)$ weakly in $L^2(\Omega)$, and using the L^∞-bounds, we have

$$
l(\theta_n) \to l(\theta^*)\,,\; h_1(\chi_n) \to h_1(\chi^*)\,,\; h_2(\chi_n) \to h_2(\chi^*),\; \text{all strongly in } L^2(Q_T)\,.
$$

In consequence, (χ^*,θ^*) satisfies (2.3) a.e. in Q_T and thus, also (1.1). Moreover, it is a standard argument to conclude that (χ^*,θ^*) is a weak solution to (1.2)–(1.4) associated with $u = u^*$, i.e., we have

$$
\begin{aligned}
& \langle \theta_t^*(t), v\rangle + \int\limits_\Omega \nabla\theta^*(t)\cdot\nabla v\,dx + \int\limits_\Gamma (k\,\theta^*(t) - u^*(t))\, v\,d\sigma \\
= & \int\limits_\Omega (l(\theta^*(t))\,h_1(\chi^*(t)))\;[h_1(\chi^*(t)) + h_2(\chi^*(t))\,\theta^*(t)]\,v\,dx \\
& \qquad \forall\; v \in H^1(\Omega)\,, \quad \text{for a.e. } t \in (0,T)\,.
\end{aligned}
$$

Since (χ^*,θ^*) is uniquely determined, we conclude that the convergences (3.1), (3.2) hold for the entire sequence $\{(\chi_n,\theta_n)\}$ and not just for a subsequence. The weak lower semicontinuity of the cost functional J then shows that

$$
J[u^*,(\chi^*,\theta^*)] \le \liminf_{n\to\infty} J[u_n,(\chi_n,\theta_n)]\,,
$$

that is, $u^* \in \mathcal{U}$ is an optimal control with the associated state $(\chi^*,\theta^*) \in M$. The existence of an optimal control is thus shown.

3.2 Necessary Conditions of Optimality

In this section, we derive the first-order necessary conditions of optimality. To this end, suppose that $(u^*,(\chi^*,\theta^*)) \in \mathcal{U} \times M$ is optimal, and let $v \in L^\infty(\Gamma_T)$ be an admissible variation, i.e., $\exists \tau_0 > 0$ such that $u^\tau := u^* + \tau\, v \in \mathcal{U}$ for $0 \le \tau \le \tau_0$. We denote by $(\chi^\tau,\theta^\tau) \in M$ the unique solution to (1.1)–(1.4) associated with u^τ.

Now observe that the state system (2.3), (2.4), (1.3), (1.4) is, owing to the a priori estimates shown in the previous section and due to the differentiability assumptions made in **(H2)**, in fact a nonsingular initial-boundary value problem with continuously differentiable right-hand side. It is then a standard argument (which can be omitted here) to show that the solution operator $S : u \mapsto (\chi,\theta)$ admits a directional derivative $D_v S(u^*) = (\xi,\eta)$ at u^* in the direction v in the sense of L^2, that is, we have

$$\left\| \frac{\chi^\tau - \chi^*}{\tau} - \xi \right\|_{L^2(Q_T)} + \left\| \frac{\theta^\tau - \theta^*}{\tau} - \eta \right\|_{L^2(Q_T)} \to 0 \quad \text{as } \tau \searrow 0\,. \tag{3.4}$$

The directional derivative (ξ,η) is defined as follows: if we denote the right-hand sides of (2.3) and (2.4) by $\tilde{f}(\chi,\theta)$ and $\tilde{g}(\chi,\theta)$ respectively, and extend them from $[\underline{\chi},\overline{\chi}] \times [\gamma_1,\gamma_2]$ onto $\mathbb{R}^2$ as continuously differentiable and bounded functions having bounded first derivatives on $\mathbb{R}^2$, then (ξ,η) solves the linear initial-boundary value problem

$$\xi_t = \tilde{f}_\chi(\chi^*,\theta^*)\,\xi + \tilde{f}_\theta(\chi^*,\theta^*)\,\eta \quad \text{in } Q_T\,, \tag{3.5}$$

$$\eta_t - \Delta\eta = \tilde{g}_\chi(\chi^*,\theta^*)\,\xi + \tilde{g}_\theta(\chi^*,\theta^*)\,\eta \quad \text{in } Q_T\,, \tag{3.6}$$

$$\frac{\partial\eta}{\partial n} + k\,\eta = v\,, \quad \text{on } \Gamma_T\,, \tag{3.7}$$

$$\eta(x,0) = \xi(x,0) = 0 \quad \text{for a.e. } x \in \Omega\,. \tag{3.8}$$

Clearly, we have $\xi, \xi_t \in L^\infty(Q_T)$, $\eta \in \mathcal{W} \cap L^\infty(Q_T)$.

We now introduce the *adjoint system*

$$q_t^* = -\tilde{f}_\chi(\chi^*,\theta^*)\,q^* - \tilde{g}_\chi(\chi^*,\theta^*)\,p^* \quad \text{in } Q_T\,, \tag{3.9}$$

$$p_t^* + \Delta p^* = -\tilde{f}_\theta(\chi^*,\theta^*)\,q^* - \tilde{g}_\theta(\chi^*,\theta^*)\,p^* \quad \text{in } Q_T\,, \tag{3.10}$$

$$\frac{\partial p^*}{\partial n} + k\,p^* = 0 \quad \text{on } \Gamma_T\,, \tag{3.11}$$

$$q^*(x,T) = -(\chi^*(x,T) - \chi_T(x))\,, \quad p^*(x,T) = -(\theta^*(x,T) - \theta_T(x))\,, \quad \text{for a.e. } x \in \Omega\,. \tag{3.12}$$

Again, (3.10)–(3.12) has to be understood in the weak sense.

By virtue of the boundedness properties of the partial derivatives of $\tilde{f}$ and $\tilde{g}$, we easily conclude that the linear backwards-in-time problem (3.9)–(3.12) admits a unique solution (p^*,q^*) such that

$$q^*, q_t^* \in L^\infty(Q_T)\,,\ p^* \in \mathcal{W} \cap L^\infty(Q_T)\,. \tag{3.13}$$

Moreover, since $(u^*, (\chi^*, \theta^*)) \in \mathcal{U} \times M$ is optimal for the cost functional J, we must have

$$\lim_{\tau \searrow 0} \frac{J(u^\tau, (\chi^\tau, \theta^\tau)) - J(u^*(\chi^*, \theta^*))}{\tau} \geq 0\,,$$

which, by definition of (ξ, η), results in the inequality

$$\int_0^T \int_\Gamma u^* \, v \, d\sigma \, dt + \int_\Omega (\theta^*(T) - \theta_T) \; \eta(T) \, dx + \int_\Omega (\chi^*(T) - \chi_T) \; \xi(T) \, dx \geq 0\,. \quad (3.14)$$

Finally, we eliminate the auxiliary variables (ξ, η) using the adjoint system. To this end, we test (3.5) by q^*, (3.6) by p^*, (3.9) by ξ and (3.10) by η, and add the four resulting equations. It then follows that

$$\int_\Omega (\theta^*(T) - \theta_T) \; \eta(T) \, dx + \int_\Omega (\chi^*(T) - \chi_T) \; \xi(T) \, dx = -\int_0^T \int_\Gamma p^* \, v \, d\sigma \, dt\,.$$

In conclusion, we have proved the following result.

Theorem 3.1 *Under the general hypotheses* **(H1)**–**(H4)***, the optimal control problem* **(P)** *admits a solution. Moreover, if* $(u^*, (\chi^*, \theta^*))$ *is an optimal pair, then there exist functions* (p^*, q^*) *such that* $q^*, q^*_t \in L^\infty(Q_T)$, $p^* \in \mathcal{W} \cap L^\infty(Q_T)$, *such that the following optimality system is satisfied:*

Eqs. (1.1)–(1.4) *for* $(u^*, (\chi^*, \theta^*))$, *Eqs.* (3.9)–(3.12) *for* (p^*, q^*), *as well as*

$$\int_0^T \int_\Gamma (u^* \, v - p^* \, v) \, d\sigma \, dt \geq 0\,, \quad \textit{for all admissible variations } v \in L^\infty(\Gamma_T)\,. \quad (3.15)$$

Remark 3.2 Notice that the Hamiltonian of the system,

$$\begin{aligned} H(u; (q,p), (\chi, \theta)) := & \int_\Omega q \, \tilde{f}(\chi, \theta) \, dx - \int_\Omega \nabla p \cdot \nabla \theta \, dx \\ & + \int_\Omega p \, \tilde{g}(\chi, \theta) \, dx - \int_\Gamma (k \, \theta - u) \, p \, d\sigma - \frac{1}{2} \int_\Gamma u^2 \, d\sigma\,, \end{aligned} \quad (3.16)$$

is concave with respect to the control u. Thus, (3.15) is equivalent to saying that

$$H(u^*; (q^*, p^*), (\chi^*, \theta^*)) = \max_{u \in \mathcal{U}} H(u; (q^*, p^*), (\chi^*, \theta^*))\,. \quad (3.17)$$

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