Optimal control of an Allen-Cahn equation with singular potentials and dynamic boundary condition

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Abstract

In this paper, we investigate optimal control problems for Allen-Cahn equations with singular nonlinearities and a dynamic boundary condition involving singular nonlinearities and the Laplace-Beltrami operator. The approach covers both the cases of distributed controls and of boundary controls. The cost functional is of standard tracking type, and box constraints for the controls are prescribed. Parabolic problems with nonlinear dynamic boundary conditions involving the Laplace-Beltrami operation have recently drawn increasing attention due to their importance in applications, while their optimal control was apparently never studied before. In this paper, we first extend known well-posedness and regularity results for the state equation and then show the existence of optimal controls and that the control-to-state mapping is twice continuously Fréchet differentiable between appropriate function spaces. Based on these results, we establish the first-order necessary optimality conditions in terms of a variational inequality and the adjoint state equation, and we prove second-order sufficient optimality conditions.

1 Introduction

Let $\Omega \subset \mathbb{R}^N$, $2 \le N \le 3$, denote some open and bounded domain with smooth boundary Γ and outward unit normal $\mathbf{n}$, and let $T > 0$ be a given final time. We put $Q := \Omega \times (0,T)$ and $\Sigma := \Gamma \times (0,T)$, and we assume that $\beta_i \ge 0$, $1 \le i \le 6$, are given constants which do not all vanish. Moreover, we assume:

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(A1) There are given functions

$$\begin{aligned} &z_Q \in L^2(Q), \quad z_\Sigma \in L^2(\Sigma), \quad z_T \in H^1(\Omega), \quad z_{\Gamma,T} \in H^1(\Gamma), \\ &\widetilde{u}_1, \widetilde{u}_2 \in L^\infty(Q) \ \text{ with } \ \widetilde{u}_1 \le \widetilde{u}_2 \ \text{ a.e. in } \ Q, \\ &\widetilde{u}_{1_\Gamma}, \widetilde{u}_{2_\Gamma} \in L^\infty(\Sigma) \ \text{ with } \ \widetilde{u}_{1_\Gamma} \le \widetilde{u}_{2_\Gamma} \ \text{ a.e. in } \ \Sigma\,. \end{aligned}$$

We then consider the following (tracking type) optimal control problem:

(CP) Minimize

$$\begin{aligned} J((y,y_\Gamma),(u,u_\Gamma)) \ := \ & \frac{\beta_1}{2}\int_0^T\!\!\int_\Omega |y - z_Q|^2 \,\mathrm{d}x\,\mathrm{d}t \,+\, \frac{\beta_2}{2}\int_0^T\!\!\int_\Gamma |y_\Gamma - z_\Sigma|^2 \,\mathrm{d}\Gamma\,\mathrm{d}t \\ & + \frac{\beta_3}{2}\int_\Omega |y(\cdot,T) - z_T|^2 \,\mathrm{d}x \,+\, \frac{\beta_4}{2}\int_\Gamma |y_\Gamma(\cdot,T) - z_{\Gamma,T}|^2 \,\mathrm{d}\Gamma \\ & + \frac{\beta_5}{2}\int_0^T\!\!\int_\Omega |u|^2 \,\mathrm{d}x\,\mathrm{d}t \,+\, \frac{\beta_6}{2}\int_0^T\!\!\int_\Gamma |u_\Gamma|^2 \,\mathrm{d}\Gamma\,\mathrm{d}t \end{aligned} \tag{1.1}$$

subject to the parabolic initial-boundary value problem with nonlinear dynamic boundary condition

$$y_t - \Delta y + f'(y) = u \quad \text{a.e. in } Q, \tag{1.2}$$

$$\partial_t y_\Gamma - \Delta_\Gamma y_\Gamma + \partial_{\mathbf{n}} y + g'(y_\Gamma) = u_\Gamma, \quad y_{|\Gamma} = y_\Gamma, \quad \text{a.e. in } \Sigma, \tag{1.3}$$

$$y(\cdot,0) = y_0 \quad \text{a.e. in } \Omega, \qquad y_\Gamma(\cdot,0) = y_{0_\Gamma} \quad \text{a.e. on } \Gamma, \tag{1.4}$$

and to the control constraints

$$\begin{aligned} (u,u_\Gamma) \in \mathcal{U}_{\mathrm{ad}} := \big\{ & (w,w_\Gamma) \in L^2(Q) \times L^2(\Sigma) \,: \\ & \widetilde{u}_1 \le w \le \widetilde{u}_2 \quad \text{a.e. in } Q, \qquad \widetilde{u}_{1_\Gamma} \le w_\Gamma \le \widetilde{u}_{2_\Gamma} \quad \text{a.e. in } \Sigma \,\big\}\,. \end{aligned} \tag{1.5}$$

Here, y_0 and y_{0_Γ} are given initial data, Δ_Γ is the Laplace-Beltrami operator on Γ, and the functions f, g are given nonlinearities, while u, u_Γ play the roles of distributed or boundary controls, respectively. Note that we do not require u_Γ to be somehow the restriction of u on Γ; such a requirement would be much too restrictive for a control to satisfy.

We remark at this place that for the cost functional to be meaningful it would suffice to only assume that $z_T \in L^2(\Omega)$ and $z_{\Gamma,T} \in L^2(\Gamma)$. However, the higher regularity of z_T and z_{Γ_T} requested in **(A1)** will later be essential to be able to treat the adjoint state problem.

The system (1.2)–(1.4) is an initial-boundary value problem with nonlinear dynamic boundary condition for an Allen-Cahn equation. In this connection, the unknown y usually stands for the order parameter of an isothermal phase transition, typically the fraction of one of the involved phases. In such a situation it is physically meaningful to require y to attain values in the interval $[0,1]$ on both Ω and Γ. A standard technique to meet this requirement is to postulate that the first derivatives of the bulk potential f and of the surface potential g become singular at 0 and at 1. A typical form for such a potential is $f = f_1 + f_2$, where f_2 is smooth on $[0,1]$ and $f_1(y) = \alpha\,[y\ln(y) + (1-y)\ln(1-y)]$

with some $\alpha > 0$. Another possibility is to choose f_1 as the indicator function $I_{[0,1]}$ of the interval $[0,1]$; in this case f_1' has to be replaced by the subdifferential $\partial I_{[0,1]}$, and f becomes a *double obstacle* potential. In this case, (1.2) has to be understood as a differential inclusion or variational inequality. Similar choices can be made for the surface potential g.

There exists a vast literature on the well-posedness and asymptotic behaviour of the Allen-Cahn equation with the *no-flux boundary condition* $\partial_{\mathbf{n}} y = 0$ in place of (1.3). Also, the well-posedness and asymptotic behavior of the system (1.2)–(1.4) has been the subject of numerous papers (see [3] and the many references given there).

Moreover, distributed and boundary control problems for the Allen-Cahn equation with no-flux boundary conditions or boundary conditions of the third kind have been studied in a number of recent papers, in particular, for the case of the double obstacle potential. In this connection, we refer to [5] and [6]. Associated stationary, that is, elliptic MPEC problems have been studied in [9] (see also the monograph [14]), and the related Cahn-Hilliard case was recently analyzed in [10]. We also like mention the works [7], [8], [12] that treated optimal control problems for the Caginalp-type temperature-dependent generalization of the Allen-Cahn equation in the case of nonsingular potentials and standard boundary conditions; a thermodynamically consistent temperature-dependent model with singular potential of the above logarithmic type was the subject of [13].

The main novelty of the present paper is to study optimal control problems with singular potentials of the logarithmic type and dynamic boundary conditions of the form (1.3). In fact, while various types of dynamic boundary conditions have already been studied in connection with optimal control theory (see [11], for a recent example), it seems that dynamic boundary conditions involving the Laplace-Beltrami operator have not been considered before. One of the difficulties is that from the viewpoint of optimal control it does not make sense to postulate that the controls u and u_Γ satisfy $u_{|\Gamma} = u_\Gamma$.

The paper is organized as follows: in Section 2, we give a precise statement of the problem under investigation, and we derive some results concerning the state system (1.2)–(1.4) and a certain linear counterpart, which will be employed repeatedly in the later analysis. In Section 3, we then treat the optimal control problem, proving the existence of optimal controls and deriving the first-order necessary and the second-order sufficient optimality conditions. During the course of this analysis, we will make repeated use of the elementary Young's inequality

$$a\,b \,\le\, \gamma |a|^2 \,+\, \frac{1}{4\gamma}\,|b|^2 \quad \forall\, a, b \in \mathbb{R} \quad \forall\, \gamma > 0,$$

of Hölder's inequality, and of the fact that we have the continuous embeddings $H^1(\Omega) \subset L^p(\Omega)$, for $1 \le p \le 6$, and $H^2(\Omega) \subset L^\infty(\Omega)$ in three dimensions of space. In particular, we have

$$\|v\|_{L^p(\Omega)} \,\le\, \widetilde{C}_p \,\|v\|_{H^1(\Omega)} \quad \forall\, v \in H^1(\Omega), \tag{1.6}$$

$$\|v\|_{L^\infty(\Omega)} \,\le\, \widetilde{C}_\infty \,\|v\|_{H^2(\Omega)} \quad \forall\, v \in H^2(\Omega), \tag{1.7}$$

with positive constants $\widetilde{C}_p$, $1 \le p \le \infty$, that only depend on Ω.

2 General assumptions and the state equation

In this section, we formulate the general assumptions of the paper, and we state some results for the state system (1.2)-(1.4). To this end, we introduce the function spaces

$$
\begin{aligned}
&H := L^2(\Omega), \quad V := H^1(\Omega), \quad H_\Gamma := L^2(\Gamma), \quad V_\Gamma := H^1(\Gamma), \\
&\mathcal{H} := L^2(Q) \times L^2(\Sigma), \quad \mathcal{X} := L^\infty(Q) \times L^\infty(\Sigma), \\
&\mathcal{Y} := \big\{ (y, y_\Gamma) : \, y \in H^1(0,T;H) \cap C^0([0,T];V) \cap L^2(0,T;H^2(\Omega)), \\
&\qquad y_\Gamma \in H^1(0,T;H_\Gamma) \cap C^0([0,T];V_\Gamma) \cap L^2(0,T;H^2(\Gamma)), \quad y_\Gamma = y_{|\Gamma} \big\}, \qquad (2.1)
\end{aligned}
$$

which are Banach spaces when endowed with their natural norms. In the following, we denote the norm in a Banach space E by $\|\cdot\|_E$; for convenience, the norm of the space $H \times H \times H$ will also be denoted by $\|\cdot\|_H$. Identifying H with its dual space H^*, we have the Hilbert triplet $V \subset H \subset V^*$, with dense and compact embeddings. Analogously, we obtain the triplet $V_\Gamma \subset H_\Gamma \subset V_\Gamma^*$, with dense and compact embeddings. We make the following general assumptions:

(A2) $f = f_1 + f_2$ and $g = g_1 + g_2$, where $f_2, g_2 \in C^3[0,1]$, and where $f_1, g_1 \in C^3(0,1)$ are convex and satisfy the following conditions:

$$
\lim_{r \searrow 0} f_1'(r) = \lim_{r \searrow 0} g_1'(r) = -\infty, \quad \lim_{r \nearrow 1} f_1'(r) = \lim_{r \nearrow 1} g_1'(r) = +\infty. \qquad (2.2)
$$

$$
\exists \, M_1 \geq 0, \, M_2 > 0 \quad \text{such that} \quad |f_1'(r)| \leq M_1 + M_2 \, |g_1'(r)| \quad \forall \, r \in (0,1). \qquad (2.3)
$$

(A3) $y_0 \in V$, $y_{0\Gamma} \in V_\Gamma$, and we have $f_1(y_0) \in L^1(\Omega)$, $g_1(y_{0\Gamma}) \in L^1(\Gamma)$, and

$$
0 < y_0 < 1 \quad \text{a.e. in } \Omega, \qquad 0 < y_{0\Gamma} < 1 \quad \text{a.e. on } \Gamma. \qquad (2.4)
$$

Remark 1: The condition (2.2) is obviously satisfied if f_1 and g_1 are potentials of logarithmic type as those mentioned in Section 1, while (2.3) is needed for the existence result from [3] that will be used below.

To simplify notation, in the following we will denote the trace $y_{|\Gamma}$ (if it exists) of a function y on Γ by y_Γ without further comment. Now observe that set $\mathcal{U}_{\rm ad}$ is a bounded subset of $\mathcal{X}$. Hence, there exists a bounded open ball in $\mathcal{X}$ that contains $\mathcal{U}_{\rm ad}$. For later use it is convenient to fix such a ball once and for all, noting that any other such ball could be used instead. In this sense, the following assumption is rather a denotation:

(A4) $\mathcal{U}$ is a nonempty open and bounded subset of $\mathcal{X}$ containing $\mathcal{U}_{\rm ad}$, and the constant $R > 0$ satisfies

$$
\|u\|_{L^\infty(Q)} + \|u_\Gamma\|_{L^\infty(\Sigma)} \leq R \quad \forall \, (u, u_\Gamma) \in \mathcal{U}. \qquad (2.5)
$$

The following result follows as a special case from [3, Theorems 2.3–2.5 and Remark 4.5] if one puts (in the notation of [3]) $\beta = f_1'$, $\beta_\Gamma = g_1'$, $\pi = f_2'$, $\pi_\Gamma = g_2$ there.

Theorem 2.1 *Suppose that the general assumptions* **(A2)**, **(A3)** *are satisfied. Then we have:*
(i) *The state system* (1.2)–(1.4) *has for any pair* $(u, u_\Gamma) \in \mathcal{H}$ *a unique solution* $(y, y_\Gamma) \in \mathcal{Y}$ *such that*

$$0 < y < 1 \quad \text{a. e. in } Q, \qquad 0 < y_{0_\Gamma} < 1 \quad \text{a. e. on } \Sigma\,.$$

(ii) *Suppose that also* **(A4)** *is fulfilled. Then there is a positive constant* K_1^*, *which only depends on* Ω, T, y_0, y_{0_Γ}, f, g, *and* R, *such that for every* $(u, u_\Gamma) \in \mathcal{U}$ *the associated solution* $(y, y_\Gamma) \in \mathcal{Y}$ *satisfies*

$$\begin{aligned} \|(y, y_\Gamma)\|_{\mathcal{Y}} \;&=\; \|y\|_{H^1(0,T;H)\cap C^0([0,T];V)\cap L^2(0,T;H^2(\Omega))} \\ &\quad + \|y_\Gamma\|_{H^1(0,T;H_\Gamma)\cap C^0([0,T];V_\Gamma)\cap L^2(0,T;H^2(\Gamma))} \;\le\; K_1^*\,, \end{aligned} \tag{2.6}$$

$$\|f'(y)\|_{L^2(0,T;H)} \;+\; \|g'(y_\Gamma)\|_{L^2(0,T;H_\Gamma)} \;\le\; K_1^*\,. \tag{2.7}$$

Moreover, there is a positive constant K_2^*, *which only depends on* Ω, T, y_0, y_{0_Γ}, f, g, *and* R, *such that the following holds: whenever* $(u_1, u_{1_\Gamma}), (u_2, u_{2_\Gamma}) \in \mathcal{U}$ *are given and* $(y_1, y_{1_\Gamma}), (y_2, y_{2_\Gamma}) \in \mathcal{Y}$ *denote the associated solutions of the state system, then we have*

$$\begin{aligned} &\|y_1 - y_2\|^2_{C^0([0,T];H)} \;+\; \|\nabla(y_1 - y_2)\|^2_{L^2(Q)} \;+\; \|y_{1_\Gamma} - y_{2_\Gamma}\|^2_{C^0([0,T];H_\Gamma)} \\ &+ \|\nabla_\Gamma(y_{1_\Gamma} - y_{2_\Gamma})\|^2_{L^2(\Sigma)} \\ &\le\; K_2^* \left\{ \|u_1 - u_2\|^2_{L^2(0,T;H)} \;+\; \|u_{1_\Gamma} - u_{2_\Gamma}\|^2_{L^2(0,T;H_\Gamma)} \right\}. \end{aligned} \tag{2.8}$$

Remark 2: (i) It follows from Theorem 2.1, in particular, that the control-to-state mapping $\mathcal{S}$, $(u, u_\Gamma) \mapsto \mathcal{S}(u, u_\Gamma) := (y, y_\Gamma)$ is well defined as a mapping from $\mathcal{X}$ into $\mathcal{Y}$; moreover, $\mathcal{S}$ is Lipschitz continuous when viewed as a mapping from the subset $\mathcal{U}$ of $\mathcal{H}$ into the space $\big(C^0([0,T];H) \cap L^2(0,T;V)\big) \times \big(C^0([0,T];H_\Gamma) \cap L^2(0,T;V_\Gamma)\big)$.

(ii) Observe that we cannot expect y to be continuous in $\overline{Q}$, since both $\partial_t y_\Gamma$ and $\Delta_\Gamma y_\Gamma$ only belong to $L^2(\Sigma)$, so that also only $\partial_{\mathbf{n}} y_\Gamma \in L^2(\Sigma)$. However, we have $y \in L^2(0,T;C^0(\overline{\Omega}))$ and $y_\Gamma \in L^2(0,T;C^0(\Gamma))$.

The next result is concerned with a linear problem with dynamic boundary condition. It will later be needed to ensure the solvability of a number of linearized systems.

Theorem 2.2 *Suppose that functions* $(u, u_\Gamma) \in \mathcal{H}$, $c_1 \in L^\infty(Q)$, $c_2 \in L^\infty(\Sigma)$, $w_0 \in H^1(\Omega)$, *and* $w_{0_\Gamma} \in H^1(\Gamma)$ *are given. Then we have:*
(i) *The linear initial-boundary value problem*

$$w_t - \Delta w + c_1(x,t)\, w \;=\; u \quad \text{a. e. in } Q, \tag{2.9}$$

$$\partial_{\mathbf{n}} w + \partial_t w_\Gamma - \Delta_\Gamma w_\Gamma + c_2(x,t)\, w_\Gamma = u_\Gamma \quad \text{a. e. on } \Sigma, \tag{2.10}$$

$$w(\,\cdot\,,0) = w_0 \quad \text{a. e. in } \Omega, \qquad w_\Gamma(\,\cdot\,,0) = w_{0_\Gamma} \quad \text{a. e. on } \Gamma, \tag{2.11}$$

has a unique solution $(w, w_\Gamma) \in \mathcal{Y}$.

(ii) *There exists a constant* $\widehat{C} > 0$, *which only depends on* Ω, T, $\|c_1\|_{L^\infty(Q)}$, *and* $\|c_2\|_{L^\infty(\Sigma)}$, *such the the following holds: whenever* $w_0 = 0$ *and* $w_{0_\Gamma} = 0$ *then*

$$\|(w, w_\Gamma)\|_{\mathcal{Y}} \leq \widehat{C}\, \|(u, u_\Gamma)\|_{\mathcal{H}}\,. \tag{2.12}$$

Proof: We put $\beta(w) := \beta_\Gamma(w) := w$ and define the operators

$$\Pi(w)(x,t) := c_1(x,t)w(x,t) - w(x,t), \quad \Pi_\Gamma(w_\Gamma)(x,t) := c_2(x,t)w_\Gamma(x,t) - w_\Gamma(x,t).$$

With these definitions, we may rewrite the equations (2.9) and (2.10) in the form

$$w_t - \Delta w + \beta(w) + \Pi(w) = u, \tag{2.13}$$

$$\partial_{\mathbf{n}} w + \partial_t w_\Gamma - \Delta_\Gamma w_\Gamma + \beta_\Gamma(w_\Gamma) + \Pi_\Gamma(w_\Gamma) = u_\Gamma, \tag{2.14}$$

respectively. Since the functions β and β_Γ are strictly monotone increasing in $\mathbb{R}$, the system (2.11), (2.13), (2.14) has almost the same form as the system considered in Theorem 2.5 in [3], the only difference being that here Π, Π_Γ are linear and continuous operators while π, π_Γ in [3] were Lipschitz continuous functions. However, a closer inspection of the proof of Theorem 2.5 in [3] reveals that the argumentation used there carries over to the present situation with only minor and obvious modifications. Hence, the asserted existence result is valid.
Now let $w_0 = 0$ and $w_{0_\Gamma} = 0$. In the following, we denote by C_i, $i \in \mathbb{N}$, positive constants that only depend on the quantities mentioned in the assertion of (ii). Testing (2.13) by w_t yields for every $t \in (0, T]$ the inequality

$$\begin{aligned}
&\int_0^t\!\!\int_\Omega w_t^2 \,\mathrm{d}x\,\mathrm{d}t \,+\, \frac{1}{2}\,\|w(t)\|_V^2 \,+\, \int_0^t\!\!\int_\Gamma |\partial_t w_\Gamma|^2 \,\mathrm{d}\Gamma\,\mathrm{d}t \,+\, \frac{1}{2}\,\|w_\Gamma(t)\|_{V_\Gamma}^2 \\
&\leq \int_0^t\!\!\int_\Omega ((|c_1|+1)|w| \,+\, |u|)\,|w_t| \,\mathrm{d}x\,\mathrm{d}t \,+\, \int_0^t\!\!\int_\Gamma ((|c_2|+1)|w_\Gamma| \,+\, |u_\Gamma|)\,|\partial_t w_\Gamma| \,\mathrm{d}\Gamma\,\mathrm{d}t\,,
\end{aligned}$$

whence, using Young's inequality and the fact that $c_1 \in L^\infty(Q)$ and $c_2 \in L^\infty(\Sigma)$, we obtain

$$\begin{aligned}
&\int_0^t\!\!\int_\Omega w_t^2 \,\mathrm{d}x\,\mathrm{d}t \,+\, \|w(t)\|_V^2 \,+\, \int_0^t\!\!\int_\Gamma |\partial_t w_\Gamma|^2 \,\mathrm{d}\Gamma\,\mathrm{d}t \,+\, \|w_\Gamma(t)\|_{V_\Gamma}^2 \\
&\leq C_1 \Big(\int_0^t\!\!\int_\Omega (|w|^2 \,+\, |u|^2) \,\mathrm{d}x\,\mathrm{d}t \,+\, \int_0^t\!\!\int_\Gamma (|w_\Gamma|^2 \,+\, |u_\Gamma|^2) \,\mathrm{d}\Gamma\,\mathrm{d}t \Big)\,.
\end{aligned}$$

Gronwall's lemma then yields that

$$\|w\|_{H^1(0,T;H)\cap C^0([0,T];V)} \,+\, \|w_\Gamma\|_{H^1(0,T;H_\Gamma)\cap C^0([0,T];V_\Gamma)} \leq C_2\,\|(u, u_\Gamma)\|_{\mathcal{H}}\,. \tag{2.15}$$

Next, a comparison argument in (2.9) shows that also

$$\|\Delta w\|_{L^2(0,T;H)} \leq C_3\,\|(u, u_\Gamma)\|_{\mathcal{H}}\,. \tag{2.16}$$

Now we invoke [1, Theorem 3.1, p. 1.79] with the specifications

$$A = -\Delta, \quad g_0 = y_{|\Gamma}, \quad p = 2, \quad r = 0, \quad s = 3/2,$$

to conclude that

$$\int_0^T \|w(t)\|^2_{H^{3/2}(\Omega)}\,\mathrm{d}t \,\le\, C_4 \int_0^T \left(\|\Delta w(t)\|^2_H \,+\, \|w_\Gamma(t)\|^2_{V_\Gamma}\right)\,\mathrm{d}t, \tag{2.17}$$

whence it follows that

$$\|w\|_{L^2(0,T;H^{3/2}(\Omega))} \,\le\, C_5\,\|(u,u_\Gamma)\|_{\mathcal{H}}\,. \tag{2.18}$$

Hence, by the trace theorem, we have that

$$\|\partial_{\mathbf{n}} w\|_{L^2(0,T;H_\Gamma)} \,\le\, C_6\,\|(u,u_\Gamma)\|_{\mathcal{H}}\,, \tag{2.19}$$

so that, by comparison in the equation resulting from (2.10), we obtain

$$\|\Delta_\Gamma w_\Gamma\|_{L^2(\Sigma)} \,\le\, \|(u,u_\Gamma)\|_{\mathcal{H}} \tag{2.20}$$

and consequently

$$\|w_\Gamma\|_{L^2(0,T;H^2(\Gamma))} \,\le\, C_9\,\|(u,u_\Gamma)\|_{\mathcal{H}}\,. \tag{2.21}$$

Now, owing to standard elliptic estimates, we infer

$$\|w\|_{L^2(0,T;H^2(\Omega))} \,\le\, C_7\,\|(u,u_\Gamma)\|_{\mathcal{H}}\,. \tag{2.22}$$

This concludes the proof of the assertion. ∎

Remark 3: It follows from (ii) in Theorem 2.2 that for zero initial data the solution operator $(u,u_\Gamma)\mapsto(w,w_\Gamma)$ is a continuous linear mapping from $\mathcal{H}$ into $\mathcal{Y}$.

While it cannot be expected that the solution to the linear system (2.9)–(2.11) is bounded, we now establish a boundedness result for the solution to the nonlinear state system (1.2)–(1.4) that will be of key importance in the subsequent analysis. To this end, we need the following assumption:

(A5) $y_0 \in L^\infty(\Omega)$, $y_{0\Gamma} \in L^\infty(\Gamma)$, and it holds

$$\begin{aligned} 0 \,<\, \operatorname*{ess\,inf}_{x\in\Omega}\, y_0(x), \quad \operatorname*{ess\,sup}_{x\in\Omega}\, y_0(x) \,<\, 1, \\ 0 \,<\, \operatorname*{ess\,inf}_{x\in\Gamma}\, y_{0\Gamma}(x), \quad \operatorname*{ess\,sup}_{x\in\Gamma}\, y_{0\Gamma}(x) \,<\, 1\,. \end{aligned} \tag{2.23}$$

Lemma 2.3 *Suppose that the assumptions* **(A2)**–**(A5)** *are satisfied. Then there are constants* $0 < r_* \le r^* < 1$, *which only depend on* Ω, T, y_0, $y_{0\Gamma}$, f, g, *and* R, *such that we have: whenever* $(y,y_\Gamma) = \mathcal{S}(u,u_\Gamma)$ *for some* $(u,u_\Gamma)\in\mathcal{U}$ *then it holds*

$$r_* \le y \le r^* \ \text{ a.e. in } \ Q, \quad r_* \le y_\Gamma \le r^* \ \text{ a.e. in } \ \Sigma. \tag{2.24}$$

Proof: Let $(u,u_\Gamma)\in\mathcal{U}$ be arbitrary and $(y,y_\Gamma) = \mathcal{S}(u,u_\Gamma)$. Then we have

$$\|u\|_{L^\infty(Q)} \,+\, \|u_\Gamma\|_{L^\infty(\Sigma)} \,\le\, R.$$

By virtue of (2.2) and (2.23), there are constants $0 < r_* \le r^* < 1$ such that

$$r_* \le \min \left\{ \operatorname*{ess\,inf}_{x\in\Omega} y_0(x) \,, \operatorname*{ess\,inf}_{x\in\Gamma} y_{0\Gamma}(x) \right\}, \tag{2.25}$$

$$r^* \ge \max \left\{ \operatorname*{ess\,sup}_{x\in\Omega} y_0(x) \,, \operatorname*{ess\,sup}_{x\in\Gamma} y_{0\Gamma}(x) \right\}, \tag{2.26}$$

$$\max\{f'(r) + R \,, g'(r) + R\} \le 0 \quad \forall\, r \in (0, r_*), \tag{2.27}$$

$$\min\{f'(r) - R \,, g'(r) - R\} \ge 0 \quad \forall\, r \in (r^*, 1). \tag{2.28}$$

Now define $w := (y - r^*)^+$. Clearly, we have $w \in V$ and $w_{|\Gamma} \in V_\Gamma$. We put $w_\Gamma := w_{|\Gamma}$ and test (1.2) by w. Thanks to (2.26), we readily see that

$$\begin{aligned} 0 \;=\; & \frac{1}{2} \|w(T)\|_H^2 + \int_0^T \|\nabla w(t)\|_H^2 \,\mathrm{d}t \\ & + \frac{1}{2} \|w_\Gamma(T)\|_{H_\Gamma}^2 + \int_0^T \|\nabla_\Gamma w_\Gamma(t)\|_{H_\Gamma}^2 \,\mathrm{d}t + \Phi, \end{aligned}$$

where, owing to (2.27) and (2.28),

$$\Phi := \int_0^T \!\!\int_\Omega (f'(y) - u)\, w \,\mathrm{d}x \,\mathrm{d}t + \int_0^T \!\!\int_\Gamma (g'(y_\Gamma) - u_\Gamma)\, w_\Gamma \,\mathrm{d}\Gamma \,\mathrm{d}t \ge 0 \,.$$

In conclusion, $w = (y - r^*)^+ = 0$, i. e., $y \le r^*$, almost everywhere in Q and on Σ. The remaining inequalities follow similarly by testing (1.2) with $w := -(y - r_*)^-$. ∎

Observe that in view of **(A2)** and of Lemma 2.3, we may (by possibly choosing a larger K_1^*) assume that also

$$\max_{0\le i\le 3} \left\{ \max \left\{ \|f^{(i)}(y)\|_{L^\infty(Q)} \,, \|g^{(i)}(y_\Gamma)\|_{L^\infty(\Sigma)} \right\} \right\} \le K_1^* \,, \tag{2.29}$$

whenever $(y, y_\Gamma) = \mathcal{S}(u, u_\Gamma)$ for some $(u, u_\Gamma) \in \mathcal{U}$.

Remark 4: Lemma 2.3 entails that the singular components in the state equations of the control problem **(CP)** are only active in a domain of arguments where they behave like standard bounded smooth nonlinearities. As a consequence, we could use classical differentiability results to see that both f and g generate three times continuously differentiable Nemytskii operators on suitable subsets of $L^\infty(Q)$ and $L^\infty(\Sigma)$, respectively. From this point, it would in principle be possible to derive the subsequent differentiability results for the control-to-state mapping by using the implicit function theorem. A corresponding approach was taken in Chapter 5 in [16] for the case of standard Neumann boundary conditions not involving dynamic terms or the surface Laplacian. Here, we prefer a direct approach which, while being slighthly longer and possibly less elegant than the use of the implicit function theorem, has the advantage of yielding the explicit form of the corresponding derivatives directly.

With Lemma 2.3 at hand, we are now able to improve the stability estimate (2.8) from Theorem 2.1.

Lemma 2.4 *Suppose that the general assumptions* **(A2)**–**(A5)** *are satisfied. Then there is a constant* $K_3^* > 0$, *which only depends on* Ω, T, f, g, *and* R, *such that the following holds: whenever* $(u_1, u_{1\Gamma}), (u_1, u_{2\Gamma}) \in \mathcal{U}$ *are given and* $(y_1, y_{1\Gamma}), (y_2, y_{2\Gamma}) \in \mathcal{Y}$ *are the associated solutions to the state system* (1.2)–(1.4), *then we have*

$$\|(y_1, y_{1\Gamma}) - (y_2, y_{2\Gamma})\|_{\mathcal{Y}} \le K_3^* \, \|(u_1, u_{1\Gamma}) - (u_2, u_{2\Gamma})\|_{\mathcal{H}} \,. \tag{2.30}$$

Proof: In the following, we denote by C_i, $i \in \mathbb{N}$, positive constants that only depend on the quantities mentioned in the assertion. We subtract the state equations (1.2)–(1.4) corresponding to $((u_i, u_{i\Gamma}), (y_i, y_{i\Gamma}))$, $i = 1, 2$, from each other and multiply the equation resulting from (1.2) by $\partial_t(y_1 - y_2)$. Putting $u = u_1 - u_2$, $u_\Gamma = u_{1\Gamma} - u_{2\Gamma}$, $y = y_1 - y_2$, and $y_\Gamma = y_{1\Gamma} - y_{2\Gamma}$, we have for all $t \in [0, T]$ the estimate

$$\begin{aligned}
&\int_0^t \!\! \int_\Omega y_t^2 \, \mathrm{d}x \, \mathrm{d}s + \frac{1}{2} \int_\Omega |\nabla y(t)|^2 \, \mathrm{d}x + \int_0^t \!\! \int_\Gamma |\partial_t y_\Gamma|^2 \, \mathrm{d}\Gamma \, \mathrm{d}s + \frac{1}{2} \int_\Gamma |\nabla_\Gamma y_\Gamma(t)|^2 \, \mathrm{d}\Gamma \\
&\le \int_0^t \!\! \int_\Omega |f'(y_1) - f'(y_2)| \, |y_t| \, \mathrm{d}x \, \mathrm{d}s + \int_0^t \!\! \int_\Gamma |g'(y_{1\Gamma}) - g'(y_{2\Gamma})| \, |\partial_t y_\Gamma| \, \mathrm{d}\Gamma \, \mathrm{d}s \\
&\quad + \int_0^t \!\! \int_\Omega |u| \, |y_t| \, \mathrm{d}x \, \mathrm{d}s + \int_0^t \!\! \int_\Gamma |u_\Gamma| \, |\partial_t y_\Gamma| \, \mathrm{d}\Gamma \, \mathrm{d}s \,.
\end{aligned} \tag{2.31}$$

Now observe that Lemma 2.3 (see also (2.29)) and the mean value theorem imply that there is some constant $C_1 > 0$ such that

$$|f'(y_1) - f'(y_2)| \le C_1 \, |y| \quad \text{a. e. in } Q, \qquad |g'(y_{1\Gamma}) - g'(y_{2\Gamma})| \le C_1 \, |y_\Gamma| \quad \text{a. e. in } \Sigma \,.$$

Hence, it follows from Young's inequality and (2.8) that

$$\|y\|_{H^1(0,T;H) \cap C^0([0,T];V)} + \|y_\Gamma\|_{H^1(0,T;H_\Gamma) \cap C^0([0,T];V_\Gamma)} \le C_2 \, \|(u, u_\Gamma)\|_{\mathcal{H}} \,. \tag{2.32}$$

From this point we may continue as in the proof of Theorem 2.2 after proving the estimate (2.15): indeed, by the arguments used there, we can repeat the estimates (2.16) to (2.21) with (w, w_Γ) replaced by (y, y_Γ) to come to the conclusion that (2.30) is satisfied. This concludes the proof of the assertion. ∎

3 The optimal control problem

We now consider the optimal control problem **(CP)** under the general assumptions **(A1)**–**(A4)**.

3.1 Existence

We have the following existence result.

Theorem 3.1 *Suppose that the general assumptions* **(A1)**–**(A4)** *are fulfilled. Then the optimal control problem* **(CP)** *admits a solution.*

Proof: Let $\{(u_n, u_{n_\Gamma})\} \subset \mathcal{U}_{\rm ad}$ be a minimizing sequence for **(CP)**, and let $(y_n, y_{n_\Gamma}) = \mathcal{S}(u_n, u_{n_\Gamma})$, $n \in \mathbb{N}$. By virtue of the global estimates (2.6) and (2.24), we may assume (by possibly selecting a suitable subsequence again indexed by n) that there are functions $(\bar u, \bar u_\Gamma) \in \mathcal{X}$ and $(\bar y, \bar y_\Gamma) \in \mathcal{Y}$, such that

$$
\begin{aligned}
u_n &\to \bar u \quad \text{weakly-* in } L^\infty(Q),\\
u_{n_\Gamma} &\to \bar u_\Gamma \quad \text{weakly-* in } L^\infty(\Sigma),\\
y_n &\to \bar y \quad \text{weakly-* in } H^1(0,T;H) \cap L^\infty(0,T;V) \cap L^2(0,T;H^2(\Omega)) \cap L^\infty(Q),\\
y_{n_\Gamma} &\to \bar y_\Gamma \quad \text{weakly-* in } H^1(0,T;H_\Gamma) \cap L^\infty(0,T;V_\Gamma) \cap L^2(0,T;H^2(\Gamma)) \cap L^\infty(\Sigma)\,.
\end{aligned}
$$

In particular, we have

$$
\partial_{\mathbf{n}} y_n \to \partial_{\mathbf{n}} \bar y, \quad \Delta_\Gamma y_{n_\Gamma} \to \Delta_\Gamma \bar y_\Gamma, \quad \text{both weakly in } L^2(\Sigma).
$$

Clearly, $(\bar u, \bar u_\Gamma) \in \mathcal{U}_{\rm ad}$. Moreover, we infer from standard compact embedding results (cf. [15, Sect. 8, Cor. 4] that, in particular,

$$
y_n \to \bar y \quad \text{strongly in } C^0([0,T];H), \tag{3.1}
$$

$$
y_{n_\Gamma} \to \bar y_\Gamma \quad \text{strongly in } C^0([0,T];H_\Gamma). \tag{3.2}
$$

But then we can conclude from the Lipschitz continuity of f_2' and g_2' (see **(A2)**) that also

$$
\begin{aligned}
f_2'(y_n) &\to f_2'(\bar y) \quad \text{strongly in } C^0([0,T];H),\\
g_2'(y_{n_\Gamma}) &\to g_2'(\bar y_\Gamma) \quad \text{strongly in } C^0([0,T];H_\Gamma),
\end{aligned}
$$

while (2.7) and **(A2)** allow us to deduce that

$$
\begin{aligned}
f_1'(y_n) &\to \bar\xi \quad \text{weakly in } L^2(0,T;H),\\
g_1'(y_{n_\Gamma}) &\to \bar\xi_\Gamma \quad \text{weakly in } L^2(0,T;H_\Gamma).
\end{aligned}
$$

for some weak limits $\bar\xi$ and $\bar\xi_\Gamma$. Since f_1 and g_1 are convex (so that f_1' and g_1' are increasing), the weak convergences above, along with (3.1)–(3.2), imply that $\bar\xi = f_1'(\bar y)$ a.e. in Q and $\bar\xi_\Gamma = g_1'(\bar y_\Gamma)$ a.e. on Σ, due to the maximal monotonicity of the operators induced by f_1' on $L^2(Q)$ and g_1' on $L^2(\Sigma)$ (see, e.g., [1, Prop. 2.5, p. 27]). At this point, we may pass to the limit as $n \to \infty$ in the state system (1.2)–(1.4) (written for $(y_n, y_{n_\Gamma}), (u_n, u_{n_\Gamma})$, $n \in \mathbb{N}$) to conclude that $(\bar y, \bar y_\Gamma) = \mathcal{S}(\bar u, \bar u_\Gamma)$, that is, the pair $((\bar u, \bar u_\Gamma), (\bar y, \bar y_\Gamma))$ is admissible for **(CP)**. It then follows from the lower sequential semicontinuity of the cost functional J that $(\bar u, \bar u_\Gamma)$ is in fact an optimal control for **(CP)**. ∎

3.2 Differentiability of the control-to-state operator

Suppose now that $(\bar u, \bar u_\Gamma) \in \mathcal{U}_{\rm ad}$ is a local minimizer for **(CP)**, and let $(\bar y, \bar y_\Gamma) = \mathcal{S}(\bar u, \bar u_\Gamma)$ be the associated state. We consider for fixed $(h, h_\Gamma) \in \mathcal{X}$ the linearized system:

$$\xi_t - \Delta\xi + f''(\bar{y})\,\xi = h \quad \text{a.e. in } Q, \tag{3.3}$$

$$\partial_{\mathbf{n}}\xi + \partial_t\xi_\Gamma - \Delta_\Gamma\xi_\Gamma + g''(\bar{y}_\Gamma)\,\xi_\Gamma = h_\Gamma, \quad \xi_\Gamma = \xi_{|\Gamma}, \quad \text{a.e. on } \Sigma, \tag{3.4}$$

$$\xi(\cdot\,,0) = 0 \quad \text{a.e. in } \Omega, \qquad \xi_\Gamma(\cdot\,,0) = 0 \quad \text{a.e. on } \Gamma. \tag{3.5}$$

By Theorem 2.2 the system (3.3)–(3.5) admits for every $(h, h_\Gamma) \in \mathcal{H}$ (and thus, a fortiori, for every $(h, h_\Gamma) \in \mathcal{X}$) a unique solution $(\xi, \xi_\Gamma) \in \mathcal{Y}$, and the linear mapping $(h, h_\Gamma) \mapsto (\xi, \xi_\Gamma)$ is continuous from $\mathcal{H}$ into $\mathcal{Y}$ and thus also from $\mathcal{X}$ into $\mathcal{Y}$.
We have the following differentiability result.

Theorem 3.2 *Suppose that the assumptions* **(A2)**–**(A5)** *are satisfied. Then we have the following results:*

(i) *Let $(\bar{u}, \bar{u}_\Gamma) \in \mathcal{U}$ be arbitrary. Then the control-to-state mapping $\mathcal{S}$, viewed as a mapping from $\mathcal{X}$ into $\mathcal{Y}$, is Fréchet differentiable at $(\bar{u}, \bar{u}_\Gamma)$, and the Fréchet derivative $D\mathcal{S}(\bar{u}, \bar{u}_\Gamma)$ is given by $D\mathcal{S}(\bar{u}, \bar{u}_\Gamma)(h, h_\Gamma) = (\xi, \xi_\Gamma)$, where for any given $(h, h_\Gamma) \in \mathcal{X}$ the pair (ξ, ξ_Γ) denotes the solution to the linearized system* (3.3)–(3.5).

(ii) *The mapping $D\mathcal{S} : \mathcal{U} \to \mathcal{L}(\mathcal{X}, \mathcal{Y})$, $(\bar{u}, \bar{u}_\Gamma) \mapsto D\mathcal{S}(\bar{u}, \bar{u}_\Gamma)$ is Lipschitz continuous on $\mathcal{U}$ in the following sense: there is a constant $K_4^* > 0$ such that for all $(u, u_\Gamma), (\bar{u}, \bar{u}_\Gamma) \in \mathcal{U}$ and all $(h, h_\Gamma) \in \mathcal{X}$ it holds*

$$\|(D\mathcal{S}(u, u_\Gamma) - D\mathcal{S}(\bar{u}, \bar{u}_\Gamma))(h, h_\Gamma)\|_{\mathcal{Y}} \le K_4^* \,\|(u, u_\Gamma) - (\bar{u}, \bar{u}_\Gamma)\|_{\mathcal{H}} \,\|(h, h_\Gamma)\|_{\mathcal{H}}\,. \tag{3.6}$$

Proof: We first show (i). To this end, let $(\bar{u}, \bar{u}_\Gamma) \in \mathcal{U}$ be arbitrarily chosen, and let $(\bar{y}, \bar{y}_\Gamma) = \mathcal{S}(\bar{u}, \bar{u}_\Gamma) \in \mathcal{Y}$ denote the associated solution to the state system. Since $\mathcal{U}$ is an open subset of $\mathcal{X}$, there is some $\lambda > 0$ such that for any $(h, h_\Gamma) \in \mathcal{X}$ with $\|(h, h_\Gamma)\|_{\mathcal{X}} \le \lambda$ it holds $(\bar{u}, \bar{u}_\Gamma) + (h, h_\Gamma) \in \mathcal{U}$. In the following, we consider such variations $(h, h_\Gamma) \in \mathcal{X}$, and we denote by (y^h, y_Γ^h) the solution to the state system (1.2)–(1.4) associated with $(\bar{u}, \bar{u}_\Gamma) + (h, h_\Gamma)$. Moreover, we denote by (ξ^h, ξ_Γ^h) the unique solution to the linearized system (3.3)–(3.5) associated with (h, h_Γ). We also denote by C_i, $i \in \mathbb{N}$, positive constants that depend neither on the choice of $(h, h_\Gamma) \in \mathcal{X}$ with $\|(h, h_\Gamma)\|_{\mathcal{X}} \le \lambda$ nor on $t \in [0, T]$.
Now let

$$v^h := y^h - \bar{y} - \xi^h, \quad v_\Gamma^h := y_\Gamma^h - \bar{y}_\Gamma - \xi_\Gamma^h.$$

Obviously, we have $(v^h, v_\Gamma^h) \in \mathcal{Y}$. Since the linear mapping $(h, h_\Gamma) \mapsto (\xi^h, \xi_\Gamma^h)$ is by Theorem 2.2 (ii) continuous from $\mathcal{X}$ into $\mathcal{Y}$, it obviously suffices to show that there is an increasing function $G : [0, \lambda] \to [0, +\infty)$ which satisfies $\lim_{r \searrow 0} G(r)/r = 0$ and

$$\|(v^h, v_\Gamma^h)\|_{\mathcal{Y}} \le G\left(\|(h, h_\Gamma)\|_{\mathcal{H}}\right). \tag{3.7}$$

Apparently, v^h is a solution to the initial-boundary value problem

$$v_t^h - \Delta v^h + f'(y^h) - f'(\bar{y}) - f''(\bar{y})\,\xi^h = 0 \quad \text{a.e. in } Q, \tag{3.8}$$

$$\partial_{\mathbf{n}} v^h + \partial_t v_\Gamma^h - \Delta_\Gamma v_\Gamma^h + g'(y_\Gamma^h) - g'(\bar{y}_\Gamma) - g''(\bar{y}_\Gamma)\,\xi_\Gamma^h = 0 \quad \text{a.e. on } \Sigma, \tag{3.9}$$

$$v^h(\cdot, 0) = 0 \quad \text{a.e. in } \Omega \qquad v_\Gamma^h(\cdot, 0) = 0 \quad \text{a.e. on } \Gamma. \tag{3.10}$$

Next, we observe that it follows from Taylor's theorem and from the global estimate (2.24) (cf. also (2.29)) that almost everywhere on Q we have

$$f'(y^h) - f'(\bar{y})\,\xi^h \,=\, f''(\bar{y})\,v^h \,+\, \Phi^h, \tag{3.11}$$

with some function $\Phi^h \in L^\infty(Q)$ such that, almost everywhere in Q,

$$|\Phi^h| \,\le\, \frac{1}{2} \max_{r_* \le r \le r^*} |f^{(3)}(r)|\,|y^h - \bar{y}|^2 \,\le\, \frac{K_1^*}{2}\,|y^h - \bar{y}|^2\,. \tag{3.12}$$

By the same token, there is a function $\Phi_\Gamma \in L^\infty(\Sigma)$ such that, almost everywhere on Σ,

$$g'(y_\Gamma^h) - g'(\bar{y}_\Gamma)\,\xi_\Gamma^h \,=\, g''(\bar{y}_\Gamma)\,v_\Gamma^h \,+\, \Phi_\Gamma^h, \tag{3.13}$$

where

$$|\Phi_\Gamma^h| \,\le\, \frac{K_1^*}{2}\,|y_\Gamma^h - \bar{y}_\Gamma|^2\,. \tag{3.14}$$

Hence, with $c_1 := f''(\bar{y}) \in L^\infty(Q)$, $c_2 := g''(\bar{y}_\Gamma) \in L^\infty(\Sigma)$, $u := -\Phi^h \in L^2(Q)$, and $u_\Gamma := -\Phi_\Gamma^h \in L^2(\Sigma)$, we see that the system (3.8)–(3.10) satisfied by (v^h, v_Γ^h) has exactly the structure of the system (2.9)–(2.11). It therefore follows from (2.12) in Theorem 2.2 that

$$\|(v^h, v_\Gamma^h)\|_{\mathcal{Y}} \,\le\, C_1\,\|(\Phi^h, \Phi_\Gamma^h)\|_{\mathcal{H}}\,. \tag{3.15}$$

Now observe that, owing to the embedding $V \subset L^4(\Omega)$ and to (2.30) in Lemma 2.4, we have

$$\begin{aligned} \|\Phi^h\|_{L^2(Q)}^2 \,&\le\, C_2 \int_0^T \!\!\int_\Omega |y^h - \bar{y}|^4 \,\mathrm{d}x\,\mathrm{d}t \,=\, C_2 \int_0^T \|y^h(t) - \bar{y}(t)\|_{L^4(\Omega)}^4 \,\mathrm{d}t \\ &\le\, C_2\,T\,\|y^h - \bar{y}\|_{C^0([0,T];V)}^4 \,\le\, C_3\,\|(h, h_\Gamma)\|_{\mathcal{H}}^4\,. \end{aligned} \tag{3.16}$$

Similar reasoning shows that also

$$\|\Phi_\Gamma^h\|_{L^2(\Sigma)}^2 \,\le\, C_4\,\|(h, h_\Gamma)\|_{\mathcal{H}}^4\,.$$

In conclusion, (3.7) is satisfied for the function $G(r) = C_1(\sqrt{C_3} + \sqrt{C_4})\,r^2$, which concludes the proof of assertion (i).

Next, we show the validity of (ii). To this end, let $(\bar{u}, \bar{u}_\Gamma) \in \mathcal{U}$ be arbitrary, and let $(k, k_\Gamma) \in \mathcal{X}$ be such that $(\bar{u} + k, \bar{u}_\Gamma + k_\Gamma) \in \mathcal{U}$. We denote $(y^k, y_\Gamma^k) = \mathcal{S}(\bar{u} + k, \bar{u}_\Gamma + k_\Gamma)$ and $(\bar{y}, \bar{y}_\Gamma) = \mathcal{S}(\bar{u}, \bar{u}_\Gamma)$, and we assume that any $(h, h_\Gamma) \in \mathcal{X}$ with $\|(h, h_\Gamma)\|_{\mathcal{X}} = 1$ is given. It then suffices to show that there is some $L > 0$, independent of (h, h_Γ), $(\bar{u}, \bar{u}_\Gamma)$ and (k, k_Γ), such that

$$\|(\xi^k, \xi_\Gamma^k) - (\xi, \xi_\Gamma)\|_{\mathcal{Y}} \,\le\, L\,\|(k, k_\Gamma)\|_{\mathcal{H}}\,, \tag{3.17}$$

where $(\xi^k, \xi_\Gamma^k) = D\mathcal{S}(\bar{u} + k, \bar{u}_\Gamma + k_\Gamma)(h, h_\Gamma)$ and $(\xi, \xi_\Gamma) = D\mathcal{S}(\bar{u}, \bar{u}_\Gamma)(h, h_\Gamma)$. For this purpose, we denote in the following by K_i, $i \in \mathbb{N}$, positive constants that neither depend on $(\bar{u}, \bar{u}_\Gamma)$, (k, k_Γ), nor on the special choice of $(h, h_\Gamma) \in \mathcal{X}$ with $\|(h, h_\Gamma)\|_{\mathcal{X}} = 1$.

To begin with, observe that from part (i) it easily follows that $(w, w_\Gamma) := (\xi^k, \xi_\Gamma^k) - (\xi, \xi_\Gamma) \in \mathcal{Y}$ solves the initial-boundary value problem

$$w_t - \Delta w + f''(\bar{y})\, w = -\xi^k \,(f''(y^k) - f''(\bar{y})) \quad \text{a.e. in } Q, \tag{3.18}$$

$$\partial_{\mathbf{n}} w + \partial_t w_\Gamma - \Delta_\Gamma w_\Gamma + g''(\bar{y}_\Gamma)\, w_\Gamma = -\xi_\Gamma^k \,(g''(y_\Gamma^k) - g''(\bar{y}_\Gamma)) \quad \text{a.e. on } \Sigma, \tag{3.19}$$

$$w(\cdot\,, 0) = 0 \quad \text{a.e. in } \Omega, \qquad w_\Gamma(\cdot\,, 0) = 0 \quad \text{a.e. on } \Gamma. \tag{3.20}$$

Hence, it follows from Theorem 2.2 that

$$\|(w, w_\Gamma)\|_{\mathcal{Y}} \le K_1 \left(\|\xi^k \,(f''(y^k) - f''(\bar{y}))\|_{L^2(Q)} + \|\xi_\Gamma^k \,(g''(y_\Gamma^k) - g''(\bar{y}_\Gamma))\|_{L^2(\Sigma)} \right). \tag{3.21}$$

Now, by Taylor's theorem and (2.29), we have almost everywhere in Q (on Σ, respectively)

$$|f''(y^k) - f''(\bar{y})| \le K_1^* \,|y^k - \bar{y}| \quad \text{and} \quad |g''(y_\Gamma^k) - g''(\bar{y}_\Gamma)| \le K_1^* \,|y_\Gamma^k - \bar{y}_\Gamma|\,. \tag{3.22}$$

At this point, we recall that $\mathcal{U}$ is obviously a bounded subset of $\mathcal{H}$. Since $(\bar{u}+k, \bar{u}+k_\Gamma) \in \mathcal{U}$ and $\|(h, h_\Gamma)\|_{\mathcal{X}} = 1$, we thus can infer from (2.29) and from the estimate (2.12) in Theorem 2.2 that (ξ^k, ξ_Γ^k) is bounded in $\mathcal{Y}$ independently of (k, k_Γ), $(\bar{u}, \bar{u}_\Gamma)$, and the choice of $(h, h_\Gamma) \in \mathcal{X}$ with $\|(h, h_\Gamma)\|_{\mathcal{X}} = 1$. Using the embedding $V \subset L^4(\Omega)$ and Lemma 2.4, we therefore have

$$\begin{aligned}
\|\xi^k \,(f''(y^k) - f''(\bar{y}))\|_{L^2(Q)}^2 &\le K_2 \int_0^T \!\!\int_\Omega |\xi^k|^2 \,|y^k - \bar{y}|^2 \,\mathrm{d}x\,\mathrm{d}t \\
&\le K_2 \int_0^T \|\xi^k(t)\|_{L^4(\Omega)}^2 \,\|y^k(t) - \bar{y}(t)\|_{L^4(\Omega)}^2 \,\mathrm{d}t \\
&\le K_3 \,\|(y^k - \bar{y}, y_\Gamma^k - \bar{y}_\Gamma)\|_{\mathcal{Y}}^2 \le K_4 \,\|(k, k_\Gamma)\|_{\mathcal{H}}^2 .
\end{aligned} \tag{3.23}$$

Since an analogous estimate holds for the second summand in the bracket on the right-hand side of (3.21), the assertion follows. ∎

Remark 5: Notice that we could not establish Fréchet differentiability of $\mathcal{S}$ on $\mathcal{H}$; in fact, we only were able to show differentiability on the bounded subset $\mathcal{U}$ of $\mathcal{X}$. In particular, the boundedness of (u, u_Γ) in $\mathcal{X}$ was an indispensable prerequisite for proving Lemma 2.3 and the global estimate (2.29), which in turn was fundamental for the derivation of the differentiability result. This will below lead to a so-called *two-norm discrepancy* in the derivation of second-order sufficient optimality conditions, i. e., we will have to work with two different norms.

With Theorem 3.2 at hand, it is now straightforward to derive the standard variational inequality that optimal controls must satisfy: indeed, it follows from the quadratic form of J and from the chain rule that the reduced cost functional

$$\mathcal{J}(u, u_\Gamma) := J(\mathcal{S}(u, u_\Gamma), (u, u_\Gamma)) \tag{3.24}$$

is Fréchet differentiable at every $(\bar{u}, \bar{u}_\Gamma) \in \mathcal{U}$ with the Fréchet derivative

$$D\mathcal{J}(\bar{u}, \bar{u}_\Gamma) = D_{(y,y_\Gamma)} J(\mathcal{S}(\bar{u}, \bar{u}_\Gamma), (\bar{u}, \bar{u}_\Gamma)) \circ D\mathcal{S}(\bar{u}, \bar{u}_\Gamma) + D_{(u,u_\Gamma)} J(\mathcal{S}(\bar{u}, \bar{u}_\Gamma), (\bar{u}, \bar{u}_\Gamma))\,, \tag{3.25}$$

and, owing to the convexity of $\mathcal{U}_{\rm ad}$, we have for every minimizer $(\bar u, \bar u_\Gamma) \in \mathcal{U}_{\rm ad}$ of $\mathcal{J}$ in $\mathcal{U}_{\rm ad}$ that

$$D\mathcal{J}(\bar u, \bar u_\Gamma)(v - \bar u, v_\Gamma - \bar u_\Gamma) \,\geq\, 0 \quad \forall\, (v, v_\Gamma) \in \mathcal{U}_{\rm ad}\,. \tag{3.26}$$

Identification of the expressions in (3.25) from (1.1) and Theorem 3.2 yields the following result:

Corollary 3.3 *Let the assumptions* **(A1)**–**(A5)** *be satisfied, and let* $(\bar u, \bar u_\Gamma) \in \mathcal{U}_{\rm ad}$ *be an optimal control for the control problem* **(CP)** *with associated state* $(\bar y, \bar y_\Gamma) = \mathcal{S}(\bar u, \bar u_\Gamma) \in \mathcal{Y}$. *Then we have for every* $(v, v_\Gamma) \in \mathcal{U}_{\rm ad}$

$$\begin{aligned}
&\beta_1 \int_0^T \!\! \int_\Omega (\bar y - z_Q)\, \xi \,\mathrm{d}x\,\mathrm{d}t \,+\, \beta_2 \int_0^T \!\! \int_\Gamma (\bar y_\Gamma - z_\Sigma)\, \xi_\Gamma \,\mathrm{d}\Gamma\,\mathrm{d}t \\
&+ \beta_3 \int_\Omega (\bar y(\,\cdot\,,T) - z_T)\, \xi(\,\cdot\,,T) \,\mathrm{d}x \,+\, \beta_4 \int_\Gamma (\bar y_\Gamma(\,\cdot\,,T) - z_{\Gamma,T})\, \xi_\Gamma(\,\cdot\,,T) \,\mathrm{d}\Gamma \\
&+ \beta_5 \int_0^t \!\! \int_\Omega \bar u (v - \bar u) \,\mathrm{d}x\,\mathrm{d}t \,+\, \beta_6 \int_0^t \!\! \int_\Gamma \bar u_\Gamma (v_\Gamma - \bar u_\Gamma) \,\mathrm{d}\Gamma\,\mathrm{d}t \,\geq\, 0\,,
\end{aligned} \tag{3.27}$$

where $(\xi, \xi_\Gamma) \in \mathcal{Y}$ *is the unique solution to the linearized system* (3.3)–(3.5) *associated with* $(h, h_\Gamma) = (v - \bar u, v_\Gamma - \bar u_\Gamma)$.

3.3 First-order necessary optimality conditions

We are now in the position to derive the first-order necessary optimality conditions for the control problem **(CP)**.

Theorem 3.4 *Let the assumptions* **(A1)**–**(A5)** *be satisfied, and let* $(\bar u, \bar u_\Gamma) \in \mathcal{U}_{\rm ad}$ *be an optimal control for the control problem* **(CP)** *with associated state* $(\bar y, \bar y_\Gamma) = \mathcal{S}(\bar u, \bar u_\Gamma) \in \mathcal{Y}$. *Then the adjoint state system*

$$-\,p_t - \Delta p + f''(\bar y)\, p = \beta_1\,(\bar y - z_Q) \quad \text{a.\,e. in } Q, \tag{3.28}$$

$$\partial_{\mathbf{n}} p - \partial_t p_\Gamma - \Delta_\Gamma p_\Gamma + g''(\bar y_\Gamma)\, p_\Gamma = \beta_2\,(\bar y_\Gamma - z_\Sigma) \quad \text{a.\,e. on } \Sigma, \tag{3.29}$$

$$\begin{aligned}
p(\,\cdot\,,T) &= \beta_3(\bar y(\,\cdot\,,T) - z_T) \quad \text{a.\,e. in } \Omega, \\
p_\Gamma(\,\cdot\,,T) &= \beta_4\,(\bar y_\Gamma(\,\cdot\,,T) - z_{\Gamma,T}) \quad \text{a.\,e. on } \Gamma,
\end{aligned} \tag{3.30}$$

has a unique solution $(p, p_\Gamma) \in \mathcal{Y}$, *and for every* $(v, v_\Gamma) \in \mathcal{U}_{\rm ad}$ *we have*

$$\int_0^T \!\! \int_\Omega (p + \beta_5\,\bar u)(v - \bar u) \,\mathrm{d}x\,\mathrm{d}t \,+\, \int_0^T \!\! \int_\Gamma (p_\Gamma + \beta_6\,\bar u_\Gamma)(v_\Gamma - \bar u_\Gamma) \,\mathrm{d}\Gamma\,\mathrm{d}t \,\geq\, 0\,. \tag{3.31}$$

Proof: First observe that the system (3.28)–(3.30) is a linear backward-in-time parabolic initial-boundary value problem, which after the time transformation $t \mapsto T - t$ takes the form of the system (2.9)–(2.11) provided we put

$$\begin{aligned}
&c_1(x,t) := f''(\bar y(x, T-t)), \quad c_2(x,t) := g''(\bar y_\Gamma(x, T-t)), \\
&u(x,t) := \beta_1\,(\bar y - z_Q)(x, T-t), \quad u_\Gamma(x,t) := \beta_2\,(\bar y_\Gamma - z_\Sigma)(x, T-t), \\
&w_0(x) := \beta_3\,(\bar y(x,T) - z_\Gamma(x)), \quad w_{0_\Gamma}(x) = \beta_4\,(\bar y_\Gamma(x,T) - z_{\Gamma,T}(x))\,.
\end{aligned}$$

Obviously, $c_1 \in L^\infty(Q)$, $c_2 \in L^\infty(\Sigma)$, $u \in L^2(Q)$, $u_\Gamma \in L^2(\Sigma)$, $w_0 \in H^1(\Omega)$, and $w_{0_\Gamma} \in H^1(\Gamma)$. Hence, by virtue of Theorem 2.2, the transformed system admits a unique solution $(w, w_\Gamma) \in \mathcal{Y}$, so that $(p, p_\Gamma)(x,t) := (w, w_\Gamma)(x, T-t)$ is the unique solution to the adjoint system, and $(p, p_\Gamma) \in \mathcal{Y}$.
At this point, we may perform the standard calculation, using repeated integration by parts and the systems (3.3)–(3.5) and (3.28)–(3.30), which shows that

$$\begin{aligned}
&\beta_1 \int_0^T \int_\Omega (\bar y - z_Q)\, \xi \,\mathrm{d}x\,\mathrm{d}t \,+\, \beta_2 \int_0^T \int_\Gamma (\bar y_\Gamma - z_\Sigma)\, \xi_\Gamma \,\mathrm{d}\Gamma\,\mathrm{d}t \\
&+ \beta_3 \int_\Omega (\bar y(\,\cdot\,,T) - z_T)\, \xi(\,\cdot\,,T)\,\mathrm{d}x \,+\, \beta_4 \int_\Gamma (\bar y_\Gamma(\,\cdot\,,T) - z_{\Gamma,T})\, \xi_\Gamma(\,\cdot\,,T)\,\mathrm{d}\Gamma \\
&= \int_0^T \int_\Omega p\, h \,\mathrm{d}x\,\mathrm{d}t \,+\, \int_0^T \int_\Gamma p_\Gamma\, h_\Gamma \,\mathrm{d}\Gamma\,\mathrm{d}t\,, \qquad (3.32)
\end{aligned}$$

so that (3.31) follows from (3.27). ∎

Remark 6: (i) It follows from the above considerations that the Fréchet derivative $D\mathcal{J}(\bar u, \bar u_\Gamma) \in \mathcal{L}(\mathcal{X}, \mathcal{Y})$ can be identified with the pair $(p + \beta_5\,\bar u, p_\Gamma + \beta_6\,\bar u_\Gamma)$ in the sense that, with the standard inner product $(\,\cdot\,,\,\cdot\,)_{\mathcal{H}}$ in the Hilbert space $\mathcal{H}$, we have

$$D\mathcal{J}(\bar u, \bar u_\Gamma)(h, h_\Gamma) = ((p + \beta_5\,\bar u, p_\Gamma + \beta_6\,\bar u_\Gamma), (h, h_\Gamma))_{\mathcal{H}} \quad \forall\, (h, h_\Gamma) \in \mathcal{X}\,. \qquad (3.33)$$

(ii) If $\beta_5 > 0$ and $\beta_6 > 0$ then it follows from standard arguments that the condition (3.31) can be given a pointwise interpretation in the following sense: we have almost everywhere in Q (on Σ, respectively) that

$$\bar u(x,t) = \begin{cases} \widetilde u_2(x,t) & \text{if} \quad \widetilde u_2(x,t) < -\beta_5^{-1}\, p(x,t) \\ -\beta_5^{-1}\, p(x,t) & \text{if} \quad \widetilde u_1(x,t) \le -\beta_5^{-1}\, p(x,t) \le \widetilde u_2(x,t)\,, \\ \widetilde u_1(x,t) & \text{if} \quad \widetilde u_1(x,t) > -\beta_5^{-1}\, p(x,t) \end{cases}$$

$$\bar u_\Gamma(x,t) = \begin{cases} \widetilde u_{2_\Gamma}(x,t) & \text{if} \quad \widetilde u_{2_\Gamma}(x,t) < -\beta_6^{-1}\, p_\Gamma(x,t) \\ -\beta_6^{-1}\, p_\Gamma(x,t) & \text{if} \quad \widetilde u_{1_\Gamma}(x,t) \le -\beta_6^{-1}\, p_\Gamma(x,t) \le \widetilde u_{2_\Gamma}(x,t)\,, \\ \widetilde u_{1_\Gamma}(x,t) & \text{if} \quad \widetilde u_{1_\Gamma}(x,t) > -\beta_6^{-1}\, p_\Gamma(x,t) \end{cases} \qquad (3.34)$$

where $\widetilde u_1$, $\widetilde u_2$, $\widetilde u_{1_\Gamma}$, $\widetilde u_{2_\Gamma}$ represent the control constraints defined in **(A1)**.

3.4 The second-order Fréchet derivative of the control-to-state operator

Since the control problem **(CP)** is nonconvex, the first-order necessary optimality conditions established in the previous section are not sufficient. However, it is of utmost importance, e. g., for the numerical solution of **(CP)**, to derive sufficient optimality conditions. For this purpose, it is necessary to show that the control-to-state mapping is twice continuously Fréchet differentiable. We have the following result.

Theorem 3.5 *Assume that in addition to the general conditions* **(A1)**–**(A5)** *we have:*
(A6) $f, g \in C^4(0,1)$.
Then we have the following results:
(i) *The control-to-state operator* $\mathcal{S}$ *is at any* $(\bar u, \bar u_\Gamma) \in \mathcal{U}$ *twice Fréchet differentiable, and the second Fréchet derivative* $D^2\mathcal{S}(\bar u, \bar u_\Gamma) \in \mathcal{L}(\mathcal{X}, \mathcal{L}(\mathcal{X}, \mathcal{Y}))$ *is defined as follows: if* $(h, h_\Gamma), (k, k_\Gamma) \in \mathcal{X}$ *are arbitrary, then* $D^2\mathcal{S}(\bar u, \bar u_\Gamma)[(h, h_\Gamma), (k, k_\Gamma)] =: (\eta, \eta_\Gamma) \in \mathcal{Y}$ *is the unique solution to the initial-boundary value problem*

$$\eta_t - \Delta\eta + f''(\bar y)\,\eta = -f^{(3)}(\bar y)\,\phi\,\psi \quad \text{a. e in } Q, \tag{3.35}$$

$$\partial_{\mathbf{n}}\eta + \partial_t\eta_\Gamma - \Delta_\Gamma\eta_\Gamma + g''(\bar y_\Gamma)\,\eta_\Gamma = -g^{(3)}(\bar y_\Gamma)\,\phi_\Gamma\,\psi_\Gamma \quad \text{a. e. on } \Sigma, \tag{3.36}$$

$$\eta(\,\cdot\,,0) = 0 \quad \text{a. e. in } \Omega, \qquad \eta_\Gamma(\,\cdot\,,0) = 0 \quad \text{a. e. on } \Gamma, \tag{3.37}$$

where we have put

$$(\bar y, \bar y_\Gamma) = \mathcal{S}(\bar u, \bar u_\Gamma), \quad (\phi, \phi_\Gamma) = D\mathcal{S}(\bar u, \bar u_\Gamma)(h, h_\Gamma), \quad (\psi, \psi_\Gamma) = D\mathcal{S}(\bar u, \bar u_\Gamma)(k, k_\Gamma)\,. \tag{3.38}$$

(ii) *The mapping* $D^2\mathcal{S} : \mathcal{U} \to \mathcal{L}(\mathcal{X}, \mathcal{L}(\mathcal{X}, \mathcal{Y}))$, $(\bar u, \bar u_\Gamma) \mapsto D^2\mathcal{S}(\bar u, \bar u_\Gamma)$, *is Lipschitz continuous on* $\mathcal{U}$ *in the following sense: there exists a constant* $K_5^* > 0$ *such that for every* $(u, u_\Gamma), (\bar u, \bar u_\Gamma) \in \mathcal{U}$ *and all* $(h, h_\Gamma), (k, k_\Gamma) \in \mathcal{X}$ *it holds*

$$\begin{aligned} &\|(D^2\mathcal{S}(u, u_\Gamma) - D^2\mathcal{S}(\bar u, \bar u_\Gamma))[(h, h_\Gamma), (k, k_\Gamma)]\|_{\mathcal{Y}} \\ &\le K_5^*\,\|(u, u_\Gamma) - (\bar u, \bar u_\Gamma)\|_{\mathcal{H}}\,\|(h, h_\Gamma)\|_{\mathcal{H}}\,\|(k, k_\Gamma)\|_{\mathcal{H}}\,. \end{aligned} \tag{3.39}$$

Proof: We first prove part (i) of the assertion. To this end, let $(\bar u, \bar u_\Gamma) \in \mathcal{U}$ be fixed, $(h, h_\Gamma), (k, k_\Gamma) \in \mathcal{X}$ be arbitrary, and $(\bar y, \bar y_\Gamma), (\phi, \phi_\Gamma), (\psi, \psi_\Gamma) \in \mathcal{Y}$ be defined as in (3.38). Then, with

$$\begin{aligned} &c_1 := f''(\bar y) \in L^\infty(Q), \quad c_2 := g''(\bar y_\Gamma) \in L^\infty(\Sigma), \quad u := -f^{(3)}(\bar y)\,\phi\,\psi \in L^2(Q), \\ &u_\Gamma := -g^{(3)}(\bar y_\Gamma)\,\phi_\Gamma\,\psi_\Gamma \in L^2(\Sigma), \end{aligned}$$

the system (3.35)–(3.37) takes the form (2.9)–(2.11) and thus enjoys a unique solution $(\eta, \eta_\Gamma) \in \mathcal{Y}$. Moreover, by (2.12) we have the estimate

$$\|(\eta, \eta_\Gamma)\|_{\mathcal{Y}} \le \widehat{C}\left(\|f^{(3)}(\bar y)\,\phi\,\psi\|_{L^2(Q)} + \|g^{(3)}(\bar y_\Gamma)\,\phi_\Gamma\,\psi_\Gamma\|_{L^2(\Sigma)}\right). \tag{3.40}$$

In the remainder of the proof of part (i), we denote by C_i, $i \in \mathbb{N}$, positive constants that do not depend on the quantities (h, h_Γ), (k, k_Γ), and $(\bar u, \bar u_\Gamma)$. Using (2.29) and (2.30), and invoking the embedding $V \subset L^4(\Omega)$, we find that

$$\begin{aligned} &\|f^{(3)}(\bar y)\,\phi\,\psi\|^2_{L^2(Q)} \le K_1^{*2}\int_0^T\!\!\int_\Omega |\phi|^2\,|\psi|^2\,\mathrm{d}x\,\mathrm{d}t \le C_1\int_0^T \|\phi(t)\|^2_{L^4(\Omega)}\,\|\psi(t)\|^2_{L^4(\Omega)}\,\mathrm{d}t \\ &\le C_2\,\|\phi\|^2_{C^0([0,T];V)}\,\|\psi\|^2_{C^0([0,T];V)} \le C_3\,\|(h, h_\Gamma)\|^2_{\mathcal{H}}\,\|(k, k_\Gamma)\|^2_{\mathcal{H}}\,, \end{aligned} \tag{3.41}$$

where the validity of the last inequality can be seen as follows: by definition (recall (3.38)) (ϕ, ϕ_Γ) is the unique solution to the linear problem (3.3)–(3.5) with zero initial conditions,

and thus we can infer from Theorem 2.2 (see, in particular, (2.12)) that $\|(\phi,\phi_\Gamma)\|_{\mathcal{Y}} \leq \widehat{C}\,\|(h,h_\Gamma)\|_{\mathcal{H}}$. By the same token, we conclude that $\|(\psi,\psi_\Gamma)\|_{\mathcal{Y}} \leq \widehat{C}\,\|(k,k_\Gamma)\|_{\mathcal{H}}$. The asserted inequality therefore follows from the definition of the norm of the space $\mathcal{Y}$, and we obtain from similar reasoning that also

$$\|g^{(3)}(\bar y_\Gamma)\,\phi_\Gamma\,\psi_\Gamma\|_{L^2(\Sigma)} \,\leq\, C_4\,\|(h,h_\Gamma)\|_{\mathcal{H}}\,\|(k,k_\Gamma)\|_{\mathcal{H}}\,.$$

In particular, it follows that the bilinear mapping $\mathcal{X}\times\mathcal{X}\mapsto\mathcal{Y}$, $[(k,k_\Gamma),(h,h_\Gamma)]\mapsto(\eta,\eta_\Gamma)$, is continuous.

Now we prove the assertions concerning existence and form of the second Fréchet derivative. Since $\mathcal{U}$ is open, there is some $\lambda>0$ such that $(\bar u+k,\bar u_\Gamma+k_\Gamma)\in\mathcal{U}$ whenever $\|(k,k_\Gamma)\|_{\mathcal{X}}\leq\lambda$. In the following, we only consider such perturbations $(k,k_\Gamma)\in\mathcal{X}$. Then for $(y^k,y^k_\Gamma)=\mathcal{S}(\bar u+k,\bar u_\Gamma+k_\Gamma)$ the global estimates (2.6), (2.29), (2.30) are satisfied. Without loss of generality, we may also assume that

$$\max\left\{\|f^{(4)}(y^k)\|_{L^\infty(Q)}\,,\,\|g^{(4)}(y^k_\Gamma)\|_{L^\infty(\Sigma)}\right\}\,\leq\,K_1^*\quad\text{whenever }\ \|(k,k_\Gamma)\|_{\mathcal{X}}\,\leq\,\lambda\,. \tag{3.42}$$

After these preparations, we observe that it suffices to show that

$$\begin{aligned}
&\big\|D\mathcal{S}(\bar u+k,\bar u_\Gamma+k_\Gamma)-D\mathcal{S}(\bar u,\bar u_\Gamma)-D^2\mathcal{S}(\bar u,\bar u_\Gamma)(k,k_\Gamma)\big\|_{\mathcal{L}(\mathcal{X},\mathcal{Y})}\\
&=\sup_{\|(h,h_\Gamma)\|_{\mathcal{X}}=1}\big\|\big(D\mathcal{S}(\bar u+k,\bar u_\Gamma+k_\Gamma)-D\mathcal{S}(\bar u,\bar u_\Gamma)-D^2\mathcal{S}(\bar u,\bar u_\Gamma)(k,k_\Gamma)\big)\,(h,h_\Gamma)\big\|_{\mathcal{Y}}\\
&\leq\,G\left(\|(k,k_\Gamma)\|_{\mathcal{H}}\right)\,,
\end{aligned}\tag{3.43}$$

with an increasing function $G:(0,\lambda]\to(0,+\infty)$ that satisfies $\lim_{r\searrow0}G(r)/r=0$.

To this end, let $(h,h_\Gamma)\in\mathcal{X}$ be arbitrary with $\|h\|_{L^\infty(Q)}+\|h_\Gamma\|_{L^\infty(\Sigma)}=1$. We put $(\rho,\rho_\Gamma)=D\mathcal{S}(\bar u+k,\bar y_\Gamma+k_\Gamma)(h,h_\Gamma)$, define the pairs $(\phi,\phi_\Gamma),(\psi,\psi_\Gamma)\in\mathcal{Y}$ as in (3.38), and put

$$(w,w_\Gamma):=(\rho-\phi-\eta,\rho_\Gamma-\phi_\Gamma-\eta_\Gamma).$$

Then, according to (3.43), we need to show that

$$\|(w,w_\Gamma)\|_{\mathcal{Y}}\,\leq\,G\left(\|(k,k_\Gamma)\|_{\mathcal{H}}\right)\,. \tag{3.44}$$

Now, invoking the explicit expressions for the quantities defined above, it is easily seen that (w,w_Γ) is a solution to the linear initial-boundary value problem

$$w_t-\Delta w+f''(\bar y)\,w=\sigma\quad\text{a.e. in }\,Q, \tag{3.45}$$

$$\partial_{\mathbf{n}}w+\partial_t w_\Gamma-\Delta_\Gamma w_\Gamma+g''(\bar y_\Gamma)\,w_\Gamma=\sigma_\Gamma\quad\text{a.e. in }\,\Sigma, \tag{3.46}$$

$$w(\,\cdot\,,0)=0\quad\text{a.e. in }\,\Omega,\qquad w_\Gamma(\,\cdot\,,0)=0\quad\text{a.e. on }\,\Gamma, \tag{3.47}$$

where we have put

$$\begin{aligned}
\sigma&:=-\rho\left(f''(y^k)-f''(\bar y)\right)\,+\,f^{(3)}(\bar y)\,\phi\,\psi,\\
\sigma_\Gamma&:=-\rho_\Gamma\left(g''(y^k_\Gamma)-g''(\bar y_\Gamma)\right)\,+\,g^{(3)}(\bar y_\Gamma)\,\phi_\Gamma\,\psi_\Gamma\,.
\end{aligned}\tag{3.48}$$

In view of (2.29), and since it is easily checked that $(\sigma, \sigma_\Gamma) \in \mathcal{H}$, we may again invoke the estimate (2.12) in Theorem 2.2 to conclude that (3.44) is satisfied if only

$$\|(\sigma, \sigma_\Gamma)\|_{\mathcal{H}} \leq G\left(\|(k, k_\Gamma)\|_{\mathcal{H}}\right) . \tag{3.49}$$

Applying Taylor's theorem to f'', and recalling (3.38), we readily see that there is a function $\omega_f \in L^\infty(Q)$ such that

$$f''(y^k) - f''(\bar{y}) = f^{(3)}(\bar{y})\,(y^k - \bar{y} - \psi) + f^{(3)}(\bar{y})\,\psi + \omega_f\,(y^k - \bar{y})^2 \quad \text{a. e. in } Q\,. \tag{3.50}$$

Hence, we have that

$$\sigma = -\rho\, f^{(3)}(\bar{y})\,(y^k - \bar{y} - \psi) - \psi\, f^{(3)}(\bar{y})\,(\rho - \phi) - \rho\,\omega_f\,(y^k - \bar{y})^2\,. \tag{3.51}$$

Now recall that from the proofs of Fréchet differentiablity and of the Lipschitz continuity of the Fréchet derivative (see, in particular, the estimates (3.6)–(3.16) and (3.17)–(3.23), respectively) it follows that

$$\begin{aligned} \|(y^k - \bar{y} - \psi, y_\Gamma^k - \bar{y}_\Gamma - \psi_\Gamma)\|_{\mathcal{Y}} &\leq C_1\,\|(k, k_\Gamma)\|_{\mathcal{H}}^2\,, \\ \|(\rho - \phi, \rho_\Gamma - \phi_\Gamma)\|_{\mathcal{Y}} &\leq C_2\,\|(k, k_\Gamma)\|_{\mathcal{H}}\,. \end{aligned} \tag{3.52}$$

Moreover, we can infer from Lemma 2.4 that

$$\|(y^k - \bar{y}, y_\Gamma^k - \bar{y}_\Gamma)\|_{\mathcal{Y}} \leq K_3^*\,\|(k, k_\Gamma)\|_{\mathcal{H}}\,, \tag{3.53}$$

and it follows from Theorem 2.2 that ρ is bounded in $\mathcal{Y}$ by a positive constant that is independent of $(k, k_\Gamma), (h, h_\Gamma) \in \mathcal{X}$ with $\|(k, k_\Gamma)\|_{\mathcal{X}} \leq \lambda$ and $\|(h, h_\Gamma)\|_{\mathcal{X}} = 1$.
Finally, we conclude from Remark 3 that with a suitable constant $C_3 > 0$ it holds

$$\|(\psi, \psi_\Gamma)\|_{\mathcal{Y}} \leq C_3\,\|(k, k_\Gamma)\|_{\mathcal{H}}\,. \tag{3.54}$$

After these preparations, and invoking Hölder's inequality and the embeddings $V \subset L^4(\Omega)$ and $V \subset L^6(\Omega)$, we can estimate as follows:

$$\begin{aligned} \|\sigma\|_{L^2(Q)}^2 &\leq C_4 \int_0^T \int_\Omega \left(|\rho|^2\,|y^k - \bar{y} - \psi|^2 + |\psi|^2\,|\rho - \phi|^2 + |\rho|^2\,|y^k - \bar{y}|^4\right) \mathrm{d}x\,\mathrm{d}t \\ &\leq C_4 \int_0^T \Big(\|\rho(t)\|_{L^4(\Omega)}^2 \|(y^k - \bar{y} - \psi)(t)\|_{L^4(\Omega)}^2 + \|\psi(t)\|_{L^4(\Omega)}^2 \|\rho(t) - \phi(t)\|_{L^4(\Omega)}^2 \Big) \mathrm{d}t \\ &\quad + C_4 \int_0^T \|\rho(t)\|_{L^6(\Omega)}^2\,\|y^k(t) - \bar{y}(t)\|_{L^6(\Omega)}^4\,\mathrm{d}t \\ &\leq C_5 \max_{0 \leq t \leq T} \left(\|\rho(t)\|_V^2\,\|(y^k - \bar{y} - \psi)(t)\|_V^2 + \|\psi(t)\|_V^2\,\|\rho(t) - \phi(t)\|_V^2 \right. \\ &\qquad \left. + \|\rho(t)\|_V^2\,\|y^k(t) - \bar{y}(t)\|_V^4 \right) \\ &\leq C_6\,\|(k, k_\Gamma)\|_{\mathcal{H}}^4\,. \end{aligned} \tag{3.55}$$

By the same reasoning, a similar estimate can be derived for $\|\sigma_\Gamma\|_{L^2(\Sigma)}$, which concludes the proof of the assertion (i).

Next, we prove the assertion (ii). To this end, suppose that $(\bar u, \bar u_\Gamma) \in \mathcal{U}$ and that (h, h_Γ) and (k, k_Γ) are arbitrarily chosen in $\mathcal{X}$, and let $(\delta, \delta_\Gamma) \in \mathcal{X}$ be arbitrary with $(\bar u + \delta, \bar u_\Gamma + \delta_\Gamma) \in \mathcal{X}$. In the following, we will denote by C_i, $i \in \mathbb{N}$, positive constants that do not depend on any of these quantities. We put

$$
\begin{aligned}
&(y^\delta, y_\Gamma^\delta) = \mathcal{S}(\bar u + \delta, \bar u_\Gamma + \delta_\Gamma), \quad (\bar y, \bar y_\Gamma) = \mathcal{S}(\bar u, \bar u_\Gamma), \quad (\phi, \phi_\Gamma) = D\mathcal{S}(\bar u, \bar u_\Gamma)(h, h_\Gamma),\\
&(\psi, \psi_\Gamma) = D\mathcal{S}(\bar u, \bar u_\Gamma)(k, k_\Gamma), \quad (\phi^\delta, \phi_\Gamma^\delta) = D\mathcal{S}(\bar u + \delta, \bar u_\Gamma + \delta_\Gamma)(h, h_\Gamma),\\
&(\psi^\delta, \psi_\Gamma^\delta) = D\mathcal{S}(\bar u + \delta, \bar u_\Gamma + \delta_\Gamma)(k, k_\Gamma), \quad (\eta, \eta_\Gamma) = D^2\mathcal{S}(\bar u, \bar u_\Gamma)[(h, h_\Gamma), (k, k_\Gamma)],\\
&(\eta^\delta, \eta_\Gamma^\delta) = D^2\mathcal{S}(\bar u + \delta, \bar u_\Gamma + \delta_\Gamma)[(h, h_\Gamma), (k, k_\Gamma)]\,.
\end{aligned}
$$

From the previous results, in particular, (2.30) and (3.6), we can infer that there is a constant $C_1 > 0$ such that

$$
\begin{aligned}
&\|(\phi, \phi_\Gamma)\|_{\mathcal{Y}} + \|(\phi^\delta, \phi_\Gamma^\delta)\|_{\mathcal{Y}} \le C_1 \, \|(h, h_\Gamma)\|_{\mathcal{H}},\\
&\|(\psi, \psi_\Gamma)\|_{\mathcal{Y}} + \|(\psi^\delta, \psi_\Gamma^\delta)\|_{\mathcal{Y}} \le C_1 \, \|(k, k_\Gamma)\|_{\mathcal{H}},\\
&\|(\eta, \eta_\Gamma)\|_{\mathcal{Y}} + \|(\eta^\delta, \eta_\Gamma^\delta)\|_{\mathcal{Y}} \le C_1 \, \|(h, h_\Gamma)\|_{\mathcal{H}} \, \|(k, k_\Gamma)\|_{\mathcal{H}},\\
&\|(y^\delta, y_\Gamma^\delta) - (\bar y, \bar y_\Gamma)\|_{\mathcal{Y}} \le C_1 \, \|(\delta, \delta_\Gamma)\|_{\mathcal{H}},\\
&\|(\phi^\delta, \phi_\Gamma^\delta) - (\phi, \phi_\Gamma)\|_{\mathcal{Y}} \le C_1 \, \|(\delta, \delta_\Gamma)\|_{\mathcal{H}} \, \|(h, h_\Gamma)\|_{\mathcal{H}},\\
&\|(\psi^\delta, \psi_\Gamma^\delta) - (\psi, \psi_\Gamma)\|_{\mathcal{Y}} \le C_1 \, \|(\delta, \delta_\Gamma)\|_{\mathcal{H}} \, \|(k, k_\Gamma)\|_{\mathcal{H}}\,.
\end{aligned}
\tag{3.56}
$$

Now observe that $(w, w_\Gamma) = (\eta^\delta, \eta_\Gamma^\delta) - (\eta, \eta_\Gamma)$ satisfies the linear initial-boundary value problem of the type (2.9)–(2.11)

$$
w_t - \Delta w + f''(\bar y)\, w = \sigma \quad \text{a.e. in } Q, \tag{3.57}
$$

$$
\partial_{\mathbf{n}} w + \partial_t w_\Gamma - \Delta_\Gamma w_\Gamma + g''(\bar y_\Gamma)\, w_\Gamma = \sigma_\Gamma \quad \text{a.e. on } \Sigma, \tag{3.58}
$$

$$
w(\cdot\,, 0) = 0 \quad \text{a.e. in } \Omega, \qquad w_\Gamma(\cdot\,, 0) = 0 \quad \text{a.e. on } \Gamma, \tag{3.59}
$$

where we have put

$$
\begin{aligned}
\sigma &= -\eta^\delta (f''(y^\delta) - f''(\bar y)) - (f^{(3)}(y^\delta)\, \phi^\delta\, \psi^\delta - f^{(3)}(\bar y)\, \phi\, \psi)\,,\\
\sigma_\Gamma &= -\eta_\Gamma^\delta (g''(y_\Gamma^\delta) - g''(\bar y_\Gamma)) - (g^{(3)}(y_\Gamma^\delta)\, \phi_\Gamma^\delta\, \psi_\Gamma^\delta - g^{(3)}(\bar y_\Gamma)\, \phi_\Gamma\, \psi_\Gamma)\,.
\end{aligned}
\tag{3.60}
$$

From Theorem 2.2 it follows that

$$
\|(w, w_\Gamma)\|_{\mathcal{Y}} \le \widehat{C} \, \|(\sigma, \sigma_\Gamma)\|_{\mathcal{H}}\,, \tag{3.61}
$$

so that it remains to show an estimate of the form

$$
\|(\sigma, \sigma_\Gamma)\|_{\mathcal{H}} \le C_2 \, \|(\delta, \delta_\Gamma)\|_{\mathcal{H}} \, \|(h, h_\Gamma)\|_{\mathcal{H}} \, \|(k, k_\Gamma)\|_{\mathcal{H}}\,. \tag{3.62}
$$

Moreover, we can infer from (2.30) and (3.6) that, almost everywhere in Q,

$$
|\sigma| \le K_1^* \, (|\eta^\delta|\, |y^\delta - \bar y| + |\phi^\delta|\, |\psi^\delta|\, |y^\delta - \bar y| + |\phi^\delta|\, |\psi^\delta - \psi| + |\psi|\, |\phi^\delta - \phi|)\,. \tag{3.63}
$$

Hence, by (3.56), and using Hölder's inequality and the embedding $V \subset L^4(\Omega)$,

$$\begin{aligned}
&\int_0^T \int_\Omega |\eta^\delta|^2 \, |y^\delta - \bar y|^2 \, \mathrm{d}x \, \mathrm{d}t \, \le \, \int_0^T \|\eta^\delta(t)\|^2_{L^4(\Omega)} \, \|(y^\delta - \bar y)(t)\|_{L^4(\Omega)} \, \mathrm{d}t \\
&\le \, C_3 \, \|\eta^\delta\|^2_{C^0([0,T];V)} \, \|y^\delta - \bar y\|^2_{C^0([0,T];V)} \, \le \, C_4 \, \|(\delta, \delta_\Gamma)\|^2_{\mathcal{H}} \, \|(h, h_\Gamma)\|^2_{\mathcal{H}} \, \|(k, k_\Gamma)\|^2_{\mathcal{H}} \,.
\end{aligned} \tag{3.64}$$

Similar reasoning yields

$$\|\phi^\delta(\psi^\delta - \psi)\|^2_{L^2(Q)} \, + \, \|\psi(\phi^\delta - \phi)\|^2_{L^2(Q)} \, \le \, C_5 \, \|(\delta, \delta_\Gamma)\|^2_{\mathcal{H}} \, \|(h, h_\Gamma)\|^2_{\mathcal{H}} \, \|(k, k_\Gamma)\|^2_{\mathcal{H}} \,. \tag{3.65}$$

Moreover, we invoke (3.56), Hölder's inequality, and the embeddings $V \subset L^4(\Omega)$ and $H^2(\Omega) \subset L^\infty(\Omega)$, to conclude that

$$\begin{aligned}
\int_0^T \int_\Omega |\phi^\delta|^2 \, |\psi^\delta|^2 \, |y^\delta - \bar y|^2 \, \mathrm{d}x \, \mathrm{d}t &\le \int_0^T \|(y^\delta - \bar y)(t)\|^2_{L^\infty(\Omega)} \, \|\phi^\delta(t)\|^2_{L^4(\Omega} \, \|\psi^\delta(t)\|^2_{L^4(\Omega)} \, \mathrm{d}t \\
&\le \, C_6 \, \|\phi^\delta\|^2_{C^0([0,T];V)} \, \|\psi^\delta\|^2_{C^0([0,T];V)} \, \|y^\delta - \bar y\|^2_{L^2(0,T;H^2(\Omega))} \\
&\le \, C_7 \, \|(\delta, \delta_\Gamma)\|^2_{\mathcal{H}} \, \|(h, h_\Gamma)\|^2_{\mathcal{H}} \, \|(k, k_\Gamma)\|^2_{\mathcal{H}} \,.
\end{aligned} \tag{3.66}$$

Finally, we can estimate $\|\sigma_\Gamma\|_{L^2(\Sigma)}$ deriving estimates similar to (3.63)–(3.66), which proves the validity of the required estimate (3.62). With this, the assertion is completely proved. ∎

3.5 Second-order sufficient optimality conditions

With Theorem 3.5 at hand, the road is paved to derive sufficient conditions for optimality. But, because the control-to-state operator $\mathcal{S}$ is not Fréchet differentiable on $\mathcal{H}$, we are faced with the two-norm discrepancy, which makes it impossible to establish second-order sufficient optimality conditions by means of the same simple arguments as in the finite-dimensional case or, e. g., in the proof of Theorem 4.23 on page 231 in [16]. It will thus be necessary to tailor the conditions in such a way as to overcome the two-norm discrepancy. At the same time, for practical purposes the conditions should not be overly restrictive. For such an approach, we follow the lines of Chapter 5 in [16], here. Since many of the arguments developed here are rather similar to those employed in [16], we can afford to be sketchy and refer the reader to [16] for full details.

To begin with, the quadratic cost functional J, viewed as a mapping on $\mathcal{Y} \times \mathcal{U}$, is obviously twice continuously Fréchet differentiable on $\mathcal{Y} \times \mathcal{U}$, and for any $((\bar y, \bar y_\Gamma), (\bar u, \bar u_\Gamma)) \in \mathcal{Y} \times \mathcal{U}$ and any $((v, v_\Gamma), (h, h_\Gamma)), ((w, w_\Gamma), (k, k_\Gamma)) \in \mathcal{Y} \times \mathcal{X}$ it holds

$$\begin{aligned}
&D^2 J((\bar y, \bar y_\Gamma), (\bar u, \bar u_\Gamma))[((v, v_\Gamma), (h, h_\Gamma)), ((w, w_\Gamma), (k, k_\Gamma))] \\
&= \beta_1 \int_0^T \int_\Omega v \, w \, \mathrm{d}x \, \mathrm{d}t \, + \, \beta_2 \int_0^T \int_\Gamma v_\Gamma \, w_\Gamma \, \mathrm{d}\Gamma \, \mathrm{d}t \, + \, \beta_3 \int_\Omega v(T) \, w(T) \, \mathrm{d}x \\
&\quad + \beta_4 \int_\Gamma v_\Gamma(T) \, w_\Gamma(T) \, \mathrm{d}\Gamma \, + \, \beta_5 \int_0^T \int_\Omega h \, k \, \mathrm{d}x \, \mathrm{d}t \, + \, \beta_6 \int_0^T \int_\Gamma h_\Gamma \, k_\Gamma \, \mathrm{d}\Gamma \, \mathrm{d}t \,.
\end{aligned} \tag{3.67}$$

Hence, it follows from Theorem 3.5 and from the chain rule that the reduced cost functional $\mathcal{J}$ is twice continuously Fréchet differentiable on $\mathcal{U}$. Now let $(\bar u, \bar u_\Gamma) \in \mathcal{U}$ be fixed and $(h, h_\Gamma), (k, k_\Gamma) \in \mathcal{X}$ be arbitrary. In accordance with our previous notation, we put

$$(\bar y, \bar y_\Gamma) = \mathcal{S}(\bar u, \bar u_\Gamma), \quad (\phi, \phi_\Gamma) = D\mathcal{S}(\bar u, \bar u_\Gamma)(h, h_\Gamma), \quad (\psi, \psi_\Gamma) = D\mathcal{S}(\bar u, \bar u_\Gamma)(k, k_\Gamma),$$
$$(\eta, \eta_\Gamma) = D^2\mathcal{S}(\bar u, \bar u_\Gamma)[(h, h_\Gamma), (k, k_\Gamma)]\,.$$

Then a straightforward calculation resembling that carried out on page 241 in [16], using the chain rule as main tool, yields the equality

$$\begin{aligned} D^2\mathcal{J}(\bar u, \bar u_\Gamma)[(h, h_\Gamma), (k, k_\Gamma)] \,&=\, D_{(y,y_\Gamma)}J((\bar y, \bar y_\Gamma), (\bar u, \bar u_\Gamma))(\eta, \eta_\Gamma) \\ &+ D^2J((\bar y, \bar y_\Gamma), (\bar u, \bar u_\Gamma))[((\phi, \phi_\Gamma), (h, h_\Gamma))\,,\, ((\psi, \psi_\Gamma), (k, k_\Gamma))]\,. \end{aligned} \tag{3.68}$$

Now observe that the first summand of the right-hand side of (3.68) is equal to the expression

$$\begin{aligned} &\beta_1 \int_0^T \!\! \int_\Omega (\bar y - z_Q)\, \eta \,\mathrm{d}x\,\mathrm{d}t \,+\, \beta_2 \int_0^T \!\! \int_\Gamma (\bar y_\Gamma - z_\Sigma)\, \eta_\Gamma \,\mathrm{d}\Gamma\,\mathrm{d}t \\ &+ \beta_3 \int_\Omega (\bar y(T) - z_T)\, \eta(T)\,\mathrm{d}x \,+\, \beta_4 \int_\Gamma (y_\Gamma(T) - z_{\Gamma,T})\, \eta_\Gamma(T)\,\mathrm{d}\Gamma \end{aligned} \tag{3.69}$$

and that (η, η_Γ) solves a system of the form (3.3)–(3.5), with h replaced by $-f^{(3)}(\bar y)\phi\psi \in L^2(Q)$ and h_Γ replaced by $-g^{(3)}(\bar y_\Gamma)\phi_\Gamma\psi_\Gamma \in L^2(\Sigma)$. Since the calculation leading to the identity (3.32) also works for right-hand sides in $L^2(Q) \times L^2(\Sigma)$, we can infer that

$$\begin{aligned} &D_{(y,y_\Gamma)}J((\bar y, \bar y_\Gamma), (\bar u, \bar u_\Gamma))(\eta, \eta_\Gamma) \\ &= -\int_0^T \!\! \int_\Omega p\, f^{(3)}(\bar y)\, \phi\, \psi \,\mathrm{d}x\,\mathrm{d}t \,-\, \int_0^T \!\! \int_\Gamma p_\Gamma\, g^{(3)}(\bar y_\Gamma)\, \phi_\Gamma\, \psi_\Gamma \,\mathrm{d}\Gamma\,\mathrm{d}t\,, \end{aligned} \tag{3.70}$$

where $(p, p_\Gamma) \in \mathcal{Y}$ is the adjoint state associated with $((\bar y, \bar y_\Gamma), (\bar u, \bar u_\Gamma))$. Summarizing, we have thus shown that it holds the representation formula

$$\begin{aligned} D^2\mathcal{J}(\bar u, \bar u_\Gamma)[(h, h_\Gamma), (h, h_\Gamma)] \,&=\, \int_0^T \!\! \int_\Omega (\beta_1 - p\, f^{(3)}(\bar y))\, |\phi|^2 \,\mathrm{d}x\,\mathrm{d}t \\ &+ \int_0^T \!\! \int_\Gamma (\beta_2 - p_\Gamma\, g^{(3)}(\bar y_\Gamma))\, |\phi_\Gamma|^2 \,\mathrm{d}\Gamma\,\mathrm{d}t \,+\, \beta_3 \int_\Omega |\phi(T)|^2 \,\mathrm{d}x \,+\, \beta_4 \int_\Gamma |\phi_\Gamma(T)|^2 \,\mathrm{d}\Gamma \\ &+ \beta_5\, \|h\|^2_{L^2(Q)} \,+\, \beta_6\, \|h_\Gamma\|^2_{L^2(\Sigma)}\,. \end{aligned} \tag{3.71}$$

Equality (3.71) gives rise to hope that, under appropriate conditions, $D^2\mathcal{J}(\bar u, \bar u_\Gamma)$ might be a positive definite operator on a suitable subset of the space $\mathcal{H}$. To formulate such a condition, assume that $(\bar u, \bar u_\Gamma) \in \mathcal{U}_{\mathrm{ad}}$ is a given control with associated state $(\bar y, \bar y_\Gamma) = \mathcal{S}(\bar u, \bar u_\Gamma) \in \mathcal{Y}$ and adjoint state $p \in \mathcal{Y}$ satisfying (3.28)–(3.30). We then introduce for fixed $\tau > 0$ the *set of strongly active constraints for* $(\bar u, \bar u_\Gamma)$ by

$$\begin{aligned} A_\tau(\bar u, \bar u_\Gamma) \,:=\, &\{(x,t) \in Q :\, |p(x,t) + \beta_5\, \bar u(x,t)| > \tau\} \\ &\cup \{(x,t) \in \Sigma :\, |p_\Gamma(x,t) + \beta_6\, \bar u_\Gamma(x,t)| > \tau\}\,. \end{aligned} \tag{3.72}$$

Apparently it follows from (3.31) that, depending on the signs of $p(x,t) + \beta_5\,\bar u(x,t)$ and of $p_\Gamma(x,t) + \beta_6\,\bar u_\Gamma(x,t)$, the control values $\bar u(x,t)$ and $\bar u_\Gamma(x,t)$, respectively, attain one of the constraint values. We now define the $\tau-$ *critical cone* $C_\tau(\bar u, \bar u_\Gamma)$ to be the set of all $(h, h_\Gamma) \in \mathcal{X}$ such that

$$h(x,t) \begin{cases} = 0 & \text{if} \quad (x,t) \in A_\tau(\bar u, \bar u_\Gamma) \\ \geq 0 & \text{if} \quad \bar u(x,t) = \widetilde u_1(x,t) \ \text{ and } \ (x,t) \notin A_\tau(\bar u, \bar u_\Gamma) \\ \leq 0 & \text{if} \quad \bar u(x,t) = \widetilde u_2(x,t) \ \text{ and } \ (x,t) \notin A_\tau(\bar u, \bar u_\Gamma) \end{cases} ,$$

$$h_\Gamma(x,t) \begin{cases} = 0 & \text{if} \quad (x,t) \in A_\tau(\bar u, \bar u_\Gamma) \\ \geq 0 & \text{if} \quad \bar u_\Gamma(x,t) = \widetilde u_{1_\Gamma}(x,t) \ \text{ and } \ (x,t) \notin A_\tau(\bar u, \bar u_\Gamma) \\ \leq 0 & \text{if} \quad \bar u_\Gamma(x,t) = \widetilde u_{2_\Gamma}(x,t) \ \text{ and } \ (x,t) \notin A_\tau(\bar u, \bar u_\Gamma) \end{cases} . \tag{3.73}$$

After these preparations, we can formulate the second-order sufficient optimality condition as follows:

There exist constants $\delta > 0$ and $\tau > 0$ such that

$$D^2\mathcal{J}[(\bar u, \bar u_\Gamma)\,[(h, h_\Gamma), (h, h_\Gamma)] \ \geq \ \delta\,\|(h, h_\Gamma)\|^2_{\mathcal{H}} \quad \forall\,(h, h_\Gamma) \in C_\tau(\bar u, \bar u_\Gamma)\,,$$

where $D^2\mathcal{J}[(\bar u, \bar u_\Gamma)\,[(h, h_\Gamma), (h, h_\Gamma)]$ is given by (3.71) with $(\bar y, \bar y_\Gamma) = \mathcal{S}(\bar u, \bar u_\Gamma)$, $(\phi, \phi_\Gamma) = D\mathcal{S}(\bar u, \bar u_\Gamma)(h, h_\Gamma)$ and the associated adjoint state (p, p_Γ). (3.74)

The following result resembles Theorem 5.17 in [16].

Theorem 3.6 *Suppose that the assumptions* **(A1)**–**(A6)** *are satisfied, and assume that the triple* $(\bar u, \bar u_\Gamma) \in \mathcal{U}_{\rm ad}$, $(\bar y, \bar y_\Gamma) = \mathcal{S}(\bar u, \bar u_\Gamma) \in \mathcal{Y}$ *and* $(p, p_\Gamma) \in \mathcal{Y}$ *fulfills the first-order necessary optimality conditions* (3.28)–(3.31). *Moreover, assume that the condition* (3.74) *is fulfilled. Then there are constants* $\varepsilon > 0$ *and* $\sigma > 0$ *such that*

$$\begin{aligned} &\mathcal{J}(u, u_\Gamma) \ \geq \ \mathcal{J}(\bar u, \bar u_\Gamma) \ + \ \sigma\,\|(u - \bar u, u_\Gamma - \bar u_\Gamma)\|^2_{\mathcal{H}} \\ &\text{whenever } \ (u, u_\Gamma) \in \mathcal{U}_{\rm ad} \ \text{ and } \ \|(u, u_\Gamma) - (\bar u, \bar u_\Gamma)\|_{\mathcal{X}} \ \leq \ \varepsilon\,. \end{aligned} \tag{3.75}$$

In particular, $(\bar u, \bar u_\Gamma)$ *is locally optimal in the sense of* $\mathcal{X}$.

Proof: The proof closely resembles that of Theorem 5.17 in [16], and therefore we can refer to [16]. We only indicate one argument that needs a bit more explanation. To this end, let $(u, u_\Gamma) \in \mathcal{U}_{\rm ad}$ be arbitrary. Since $\mathcal{J}$ is twice continuously Fréchet differentiable in $\mathcal{U}$, it follows from Taylor's theorem with integral remainder (see, e. g., Theorem 8.14.3 on page 186 in [4]) that

$$\begin{aligned} \mathcal{J}(u, u_\Gamma) - \mathcal{J}(\bar u, \bar u_\Gamma) \ = \ DJ(\bar u, \bar u_\Gamma)(v, v_\Gamma) \ + \ \frac{1}{2}\,D^2\mathcal{J}(\bar u, \bar u_\Gamma)[(v, v_\Gamma), (v, v_\Gamma)] \\ + R^{\mathcal{J}}((u, u_\Gamma), (\bar u, \bar u_\Gamma))\,, \end{aligned} \tag{3.76}$$

with the remainder

$$
\begin{aligned}
&R^{\mathcal{J}}((u,u_\Gamma),(\bar u,\bar u_\Gamma))\\
&= \int_0^1 (1-s)\left(D^2\mathcal{J}(\bar u+sv,\bar u_\Gamma+sv_\Gamma)-D^2\mathcal{J}(\bar u,\bar u_\Gamma)\right)[(v,v_\Gamma),(v,v_\Gamma)]\,\mathrm{d}s\,.
\end{aligned}
\tag{3.77}
$$

A lengthy but straightforward calculation, based on the representation formulas (3.67)–(3.69) as well as on the Lipschitz estimates (2.30), (3.6), and (3.39), reveals that

$$
\begin{aligned}
\left|R^{\mathcal{J}}((u,u_\Gamma),(\bar u,\bar u_\Gamma))\right| &\le C_1\int_0^1 (1-s)\,s\,\|(v,v_\Gamma)\|_{\mathcal{H}}^3\mathrm{d}s\\
&\le C_2\,\|(v,v_\Gamma)\|_{\mathcal{X}}\,\|(v,v_\Gamma)\|_{\mathcal{H}}^2\,,
\end{aligned}
\tag{3.78}
$$

with global constants $C_1>0$ and $C_2>0$ that do not depend on the choice of $(u,u_\Gamma)\in\mathcal{U}_{\rm ad}$. From this point, we can argue along exactly the same lines as on pages 292–294 in the proof of Theorem 5.17 in [16] to conclude the validity of the assertion. ∎

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