ESAIM: COCV
Vol. 13, N° 4, 2007, pp. 750–775
DOI: 10.1051/cocv:2007028

ESAIM: Control, Optimisation and Calculus of Variations
www.esaim-cocv.org

SECOND-ORDER SUFFICIENT OPTIMALITY CONDITIONS FOR A SEMILINEAR OPTIMAL CONTROL PROBLEM WITH NONLOCAL RADIATION INTERFACE CONDITIONS *

Christian Meyer[1]

Abstract. We consider a control constrained optimal control problem governed by a semilinear elliptic equation with nonlocal interface conditions. These conditions occur during the modeling of diffuse-gray conductive-radiative heat transfer. After stating first-order necessary conditions, second-order sufficient conditions are derived that account for strongly active sets. These conditions ensure local optimality in an L^s-neighborhood of a reference function whereby the underlying analysis allows to use weaker norms than L^∞.

Mathematics Subject Classification. 49K20, 35J65, 80M50.

Received April 27, 2005. Revised May 2, 2006.
Published online July 20, 2007.

1. Introduction

In this paper, we investigate an optimal control problem that arises from the sublimation growth of semiconductor single crystals by the physical vapor transport (PVT) method. Possible semiconductor materials, produced with this method, are silicon carbide (SiC) or aluminum nitrite (AlN). They are used in numerous industrial applications, *e.g.* the production of optoelectronic devices such as blue and green LEDs and lasers. For the PVT method, polycrystalline powder is placed under a low-pressure inert gas atmosphere at the bottom of a cavity inside a crucible. The crucible is heated up to 2000 till 3000 K by induction. Due to the high temperatures and the low pressure, the powder sublimates and crystallizes at a single-crystalline seed located at the cooled top of the cavity, such that the desired single crystal grows into the reaction chamber. See [6] for more details.

Here, we focus on the conductive-radiative heat transfer in the growth apparatus. Therefore, we consider a simplified setup of the growth apparatus, shown in Figure 1, where Ω_s denotes the domain of the solid graphite crucible, whereas Ω_g is the domain of gas phase inside. A very important determining factor for the crystal's quality and growth rate is the temperature gradient inside the gas phase [9]. Since we do not consider the electromagnetic induction, we will optimize the temperature gradient in the gas phase Ω_g by directly controlling the heat source u in Ω_s.

Keywords and phrases. Optimal control, semilinear elliptic equations, nonlocal interface conditions, second-order sufficient optimality conditions.

* *Supported by the DFG Research Center* Matheon *"Mathematics for key technologies" in Berlin.*

[1] WIAS - Weierstrass Institute for Applied Analysis and Stochastics, Mohrenstr. 39, D-10117 Berlin, Germany;
cmeyer@math.tu-berlin.de

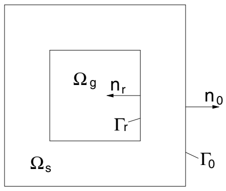

FIGURE 1. Exemplary domain for nonlocal radiative heat transfer.

The temperature y inside the growth apparatus arises as the solution of the conductive-radiative heat transfer problem in the growth apparatus. Accounting for radiative contributions is essential owing to the high temperatures. Thus, the problem is described by the stationary heat equation with radiation interface and boundary conditions on Γ_{r} and Γ_0, respectively. We take Ω_{s} to be entirely opaque, whereas Ω_{g} represents a transparent medium which does not interact with radiation. Furthermore, the radiative surfaces $\Gamma_0 := \partial\Omega$ and $\Gamma_{\mathrm{r}} := \overline{\Omega}_{\mathrm{s}} \cap \overline{\Omega}_{\mathrm{g}}$ are presumed to be diffuse-gray, *i.e.* the emissivity ε is independent of both the direction and the wavelength of the radiation. In particular, the local radiative heat exchange on Γ_0 can be modeled by the Boltzmann radiation condition with an external temperature y_0. Due to the heat exchange between points on Γ_{r}, we obtain an additional radiative heat flux on Γ_{r}, denoted by q_{r}.

In addition to the stationary semilinear heat equation with radiation interface and boundary conditions, we consider box constraints for the control function u. Thus, the optimal control problem, considered here, reads as follows:

$$
\text{(P)} \quad \begin{cases}
\text{minimize} \quad J(y,u) := \dfrac{1}{2}\displaystyle\int_{\Omega_{\mathrm{g}}} |\nabla y - z|^2 \,\mathrm{d}x + \dfrac{\nu}{2}\displaystyle\int_{\Omega_{\mathrm{s}}} u^2 \,\mathrm{d}x \\
\text{subject to} \quad -\mathrm{div}(\kappa_{\mathrm{s}} \nabla y) = u \quad \text{in } \Omega_{\mathrm{s}} \\
\qquad -\mathrm{div}(\kappa_{\mathrm{g}} \nabla y) = 0 \quad \text{in } \Omega_{\mathrm{g}} \\
\qquad \kappa_{\mathrm{g}} \left(\dfrac{\partial y}{\partial n_r}\right)_{\mathrm{g}} - \kappa_{\mathrm{s}} \left(\dfrac{\partial y}{\partial n_r}\right)_{\mathrm{s}} = q_{\mathrm{r}} \quad \text{on } \Gamma_{\mathrm{r}} \\
\qquad \kappa_{\mathrm{s}} \dfrac{\partial y}{\partial n_0} + \varepsilon\sigma\, |y|^3 y = \varepsilon\sigma\, y_0^4 \quad \text{on } \Gamma_0 \\
\text{and} \quad u_a \le u(x) \le u_b \quad \textit{a.e. } \text{in } \Omega_{\mathrm{s}},
\end{cases}
$$

where n_0 is the outward unit normal on Γ_0, and n_{r} is the unit normal on Γ_{r} facing outward with respect to Ω_{s} (*cf.* Fig. 1). Furthermore, z denotes the desired temperature gradient and $\nu > 0$ is a Tikhonov regularization parameter. In the state equation, σ represents the Boltzmann radiation constant, and κ_{s}, κ_{g} denote the thermal conductivities in Ω_{s}, Ω_{g}, respectively.

In contrast to the boundary condition on Γ_0, the radiative heat transfer on Γ_{r} is nonlocal. The corresponding mathematical model used here is described in detail in [10]. It provides the additional radiative heat flux q_{r} on Γ_{r} given by

$$
q_{\mathrm{r}} = (I - K)(I - (1-\varepsilon)K)^{-1}\varepsilon\, \sigma |y|^3 y := G\, \sigma |y|^3 y, \tag{1.1}
$$

where K is an integral operator representing the irradiation on Γ_{r}. The nonlocal operators K and G will be specified in Section 3. The nonlocal radiation on Γ_{r} represents the main characteristic of the problem, since the nonlinearity in the state equation in (P) is in general not monotone due to nonpositivity of G (see [10]).

Problem (P) has already been investigated by Meyer, Philip and Tröltzsch in [8], where first-order necessary conditions are proved. Based on these results, we establish second-order sufficient optimality conditions for (P). Due to the nonlinear interface and boundary conditions on Γ_{r} and Γ_0, (P) belongs to the class of semilinear elliptic optimal control problems. There are numerous publications which address second-order conditions for problems of such type. We only mention Casas, Tröltzsch and Unger [4], Bonnans [1], and Casas and Mateos [3]. Here, we consider conditions that are sufficient for local optimality of a reference function in an L^s-neighborhood, where s is not necessarily equal to ∞. To that end, we use a technique, introduced for the Navier-Stokes equations by Tröltzsch and Wachsmuth [12]. In case of the Navier-Stokes equations, the situation is, in some sense, easier, since the nonlinearity in the state equation is only of quadratic type. Hence, under certain assumptions on the objective functional, it is possible to avoid the well-known two-norm discrepancy (see [12] for details). This is even valid, if one allows for strongly active sets as introduced by Dontchev *et al.* [5]. However, in our case, one has to deal with a two-norm discrepancy when using strongly active control constraints. Therefore, we modify the proof of Tröltzsch and Wachsmuth and follow an approach by Casas, Tröltzsch and Unger [4], who consider a more general setting. This covers a class of optimal control problems with a semilinear elliptic state equation whose nonlinearity is monotone. However, although this is not the case here, main parts of the corresponding theory for second-order conditions can also be applied to (P).

The paper is organized as follows: After stating the mathematical setting in Section 2, we recall some results of [7, 8, 10], concerning the semilinear state equation and first-order conditions for (P), see Sections 3 and 4. Then, in Section 5, our main result, *i.e.* the second-order sufficient conditions, are stated. Section 6 is devoted to some auxiliary results that are needed for the proof of the second order-conditions, that is presented in Section 7.

2. The mathematical setting

Throughout this paper, we assume the following conditions on the domain Ω and on the quantities and functions occurring in (P):

Assumption 1. We assume that $\Omega \subset \mathbb{R}^3$ is a bounded simply connected domain with Lipschitz boundary Γ_0. The boundary of the simply connected subdomain $\overline{\Omega}_{\mathrm{g}} \subset \Omega$, denoted by Γ_{r}, is assumed to be a closed Lipschitz surface that is piecewise $C^{1,\delta}$. Notice that the distance of Γ_{r} to Γ_0 is positive. Then, Ω_{s} is defined by $\Omega_{\mathrm{s}} = \Omega \setminus \overline{\Omega}_{\mathrm{g}}$. The Boltzmann radiation constant is assumed to be positive, *i.e.* $\sigma \in \mathbb{R}^+$. For the thermal conductivity, we assume $\kappa \in L^\infty(\Omega)$ with

$$\kappa(x) = \begin{cases} \kappa_{\mathrm{s}}(x) & \text{in } \Omega_{\mathrm{s}} \\ \kappa_{\mathrm{g}}(x) & \text{in } \Omega_{\mathrm{g}} \end{cases}$$

and $\kappa(x) \geq \kappa_{\min} > 0$ *a.e.* on Ω. Furthermore, the emissivity $\varepsilon \in L^\infty(\Gamma_0 \cup \Gamma_{\mathrm{r}})$ is bounded by $1 \geq \varepsilon \geq \varepsilon_{\min} > 0$ *a.e.* on $\Gamma_0 \cup \Gamma_{\mathrm{r}}$.

Assumption 2. The desired temperature gradient z is given in $L^2(\Omega_{\mathrm{g}})$ and ν is a positive constant. For the box constraints, we assume $u_a, u_b \in L^t(\Omega_{\mathrm{s}})$, where t is a positive real number with $t \geq q'$ and some $q' \in [2, 4]$ that will be precised later in Section 5. Moreover, the bounds fulfill $0 \leq u_a(x) < u_b(x)$ *a.e.* in Ω_{s}. The external temperature y_0 is a function in $L^{16}(\Gamma_0)$ and fulfills $y_0 \geq \vartheta$ *a.e.* on Γ_0 with a positive constant ϑ.

Notice that, in this context, the assumption $u_a(x) \geq 0$ *a.e.* in Ω_{s} does not represent an additional restriction, since the heat sources in the application are always non-negative, as the crucible cannot be cooled. Throughout this article, we use the following notations:

Notation. We introduce the set of admissible controls by

$$U_{ad} := \{u \in L^t(\Omega_{\mathrm{s}}) \,|\, u_a(x) \leq u(x) \leq u_b(x) \;\; a.e. \text{ in } \Omega_{\mathrm{s}}\}.$$

The identity operator in the respective function spaces is denoted by I. Moreover, τ_{r} is the trace operator on Γ_{r}, whereas τ_0 denotes the trace on Γ_0. Throughout this paper, c is a generic constant and ψ denotes a generic function. Let W be a Banach space with its dual space W^*. Then, for $f \in W$ and $g \in W^*$, $\langle f\,,\, g\rangle$ denotes the associated pairing. Furthermore, for a given functional $j : W \to \mathbb{R}$ that is twice continuously

Fréchet differentiable, we denote the second derivative at $u \in W$ in the directions $h_1, h_2 \in W$ by $j''(u)[h_1, h_2]$. If $h_1 = h_2 = h$, then we write $j''(u)h^2$.

3. The semilinear state equations

In this section, we recall some results of Laitinen and Tiihonen [7], Tiihonen [10, 11], and Meyer, Philip and Tröltzsch [8]. First, we present some properties of the nonlocal radiation operator G and the integral operator K.

Definition 3.1. The integral operator K, representing the irradiation on Γ_r, is given by

$$(K\,y)(x) = \int\limits_{\Gamma_\mathrm{r}} \omega(x,z)\,y(z)\,\mathrm{d}s_z, \tag{3.1}$$

where the kernel ω is defined by

$$\omega(x,z) = \begin{cases} \Xi(x,z)\,\dfrac{[n_\mathrm{r}(z)\cdot(x-z)][n_\mathrm{r}(x)\cdot(z-x)]}{2|z-x|^3}, & \text{for } n=2 \\ \Xi(x,z)\,\dfrac{[n_\mathrm{r}(z)\cdot(x-z)][n_\mathrm{r}(x)\cdot(z-x)]}{\pi|z-x|^4}, & \text{for } n=3. \end{cases}$$

In this definition, x, z denote two points on Γ_r, and $n_\mathrm{r}(x)$ is the unit normal at x facing outward with respect to Ω_s. Here, Ξ represents the visibility factor which is given by

$$\Xi(x,z) = \begin{cases} 0 & \text{if } \overline{xz}\cap\Omega_\mathrm{g} \neq \emptyset, \\ 1 & \text{if } \overline{xz}\cap\Omega_\mathrm{g} = \emptyset, \end{cases}$$

with $\overline{xz}$ denotes the line segment between x and z.

In [11], it is proven that $\omega(x,z)$ has a singularity at x of type $|x-z|^{-(1-\delta)}$ in the two-dimensional and $|x-z|^{-2(1-\delta)}$ in the three-dimensional case, which is, in both cases, integrable. This is the key point to the following lemma derived in [11].

Lemma 3.2.

(i) *K maps $L^p(\Gamma_\mathrm{r})$ to $L^p(\Gamma_\mathrm{r})$ for all $1 \le p \le \infty$.*
(ii) *The operator $I-(1-\varepsilon)K\colon L^p(\Gamma_\mathrm{r}) \to L^p(\Gamma_\mathrm{r})$ is continuously invertible.*

With the help of Lemma 3.2, Tiihonen and Laitinen proved the following property of $G = (I-K)(I-(1-\varepsilon)K)^{-1}\varepsilon$ (*cf.* [10], Lem. 6 and [7], Lem. 8).

Lemma 3.3. *G is a bounded linear operator from $L^p(\Gamma_\mathrm{r})$ to itself for all $1 \le p \le \infty$.*

Notice that the kernel ω is symmetric and hence, K is formally self-adjoint. Therefore, we obtain that $G^* = \varepsilon(I-(1-\varepsilon)K)^{-1}(I-K)$ is also linear and bounded from $L^p(\Gamma_\mathrm{r})$ to $L^p(\Gamma_\mathrm{r})$ for all $1 \le p \le \infty$.

With these results at hand, Laitinen and Tiihonen derived the existence of solutions to the state equation in (P) that is given by

$$\begin{aligned} -\mathrm{div}(\kappa_\mathrm{s}\,\nabla y) &= u && \text{in } \Omega_\mathrm{s} \\ -\mathrm{div}(\kappa_\mathrm{g}\,\nabla y) &= 0 && \text{in } \Omega_\mathrm{g} \\ \kappa_\mathrm{g}\left(\frac{\partial y}{\partial n_r}\right)_\mathrm{g} - \kappa_\mathrm{s}\left(\frac{\partial y}{\partial n_r}\right)_\mathrm{s} &= G\,\sigma|y|^3 y && \text{on } \Gamma_\mathrm{r} \\ \kappa_\mathrm{s}\frac{\partial y}{\partial n_0} + \varepsilon\sigma\,|y|^3 y &= \varepsilon\sigma\,y_0^4 && \text{on } \Gamma_0. \end{aligned} \tag{3.2}$$

Notice that, G is in general non-positive, *i.e.* $v(x) \geq 0$ *a.e.* on Γ_r does not imply $(Gv)(x) \geq 0$ *a.e.* on Γ_r, and hence, the nonlinearity in (3.2) is not monotone. Therefore, Laitinen and Tiihonen used Brezis' existence theorem on the solution of equations with pseudomonotone operators to show the existence of solutions (see [7] for details). In the following, we consider y in the state space V that is defined by

$$V := \{v \in H^1(\Omega) \mid \tau_r\, v \in L^5(\Gamma_r),\ \tau_0\, v \in L^5(\Gamma_0)\}$$

where τ_r denotes the trace operator on Γ_r, whereas τ_0 is the trace on Γ_0. The space V is equipped with the norm

$$\|v\|_V = \|v\|_{H^1(\Omega)} + \|v\|_{L^5(\Gamma_r)} + \|v\|_{L^5(\Gamma_0)}.$$

Theorem 3.4 ([7], Th. 2)**.** *Under Assumption* 1*, the semilinear equation* (3.2) *admits a unique solution in* V *for every* $u \in H^1(\Omega_s)^*$ *and* $y_0 \in L^5(\Gamma_0)$.

In [8], it is shown that, if the right-hand side is sufficiently regular, solutions to (3.2) belong to the following function space

$$V^\infty := H^1(\Omega) \cap L^\infty(\Omega), \tag{3.3}$$

equipped with the norm

$$\|v\|_{V^\infty} = \|v\|_{H^1(\Omega)} + \|v\|_{L^\infty(\Omega)}.$$

Notice that $y \in V^\infty$ implies $\tau_r y \in L^\infty(\Gamma_r)$ and $\tau_0 y \in L^\infty(\Gamma_0)$ (see [8], Rem. 3.5).

Theorem 3.5 ([8], Th. 4.2)**.** *Suppose that Assumption* 1 *is fulfilled and* $u \in L^2(\Omega_s)$ *and* $y_0 \in L^{16}(\Gamma_0)$*. Then, there exists a constant* c *only depending on* Ω *such that the solution of* (3.2) *fulfills*

$$\|y\|_{L^\infty(\Omega)} + \|y\|_{L^\infty(\Gamma_r \cup \Gamma_0)} \leq c(1 + \|u\|_{L^2(\Omega_s)} + \|y_0\|^4_{L^{16}(\Gamma_0)}). \tag{3.4}$$

For a fixed $y_0 \in L^{16}(\Gamma_0)$, we introduce the control-to-state operator $S : L^2(\Omega_s) \to V^\infty$ that assigns y to u. The positivity of S is covered by the following maximum principle.

Theorem 3.6 ([8], Th. 4.3)**.** *Suppose that Assumption* 1 *is fulfilled and* $u(x) \geq 0$ *a.e. in* Ω_s *and* $y_0(x) \geq \vartheta > 0$ *a.e. on* Γ_0*. If* y *is the solution of* (3.2)*, then* $y(x) \geq \vartheta$ *holds a.e. on* Ω *and a.e. on* $\Gamma_r \cup \Gamma_0$.

The next theorem states the existence of an optimal solution for (P). It is also proven in [8] by rather standard arguments.

Theorem 3.7 ([8], Th. 5.2)**.** *Under the Assumptions* 1 *and* 2*, there exists an optimal control* $\bar{u} \in L^\infty(\Omega_s)$ *with associated state* $\bar{y} \in V^\infty$.

4. First-order necessary optimality conditions

The key point in the proof of first-order necessary optimality conditions is to show the differentiability of the control-to-state operator $S : u \mapsto y$. In preparation of a corresponding theorem, we consider the following linear equation We start with the following linear equation

$$\int_\Omega \kappa \nabla y \cdot \nabla v \,\mathrm{d}x + 4 \int_{\Gamma_0} \varepsilon\sigma\, |\bar{y}|^3 y\, v \,\mathrm{d}s = \langle \varphi\,,\, v\rangle_{H^1(\Omega)^*, H^1(\Omega)} \quad \forall\, v \in H^1(\Omega) \tag{4.1}$$

with a given $\varphi \in H^1(\Omega)^*$ and a fixed $\bar{y} \in V^\infty$ with $\bar{y} > 0$ *a.e.* in Ω. Notice that, in this section, the notation $\bar{y}$ does not necessarily refer to the optimal state, but to fixed, non negative, but otherwise arbitrary function in V^∞. It is easy to verify that the bilinear form in (4.1) is bounded and coercive in $H^1(\Omega)$. Therefore, the Lax-Milgram lemma implies that (4.1) admits solutions in $H^1(\Omega)$ for every right-hand side in $\varphi \in H^1(\Omega)^*$.

Thus, there exists a linear continuous operator $B_{\mathrm{d}}(\bar{y}) : H^1(\Omega)^* \to H^1(\Omega)$, mapping φ to y, such that the solution of (4.1) can be expressed as

$$y = B_{\mathrm{d}}(\bar{y})\, \varphi. \tag{4.2}$$

Next, we consider a slightly different equation:

$$\begin{aligned}\bar{a}[y, v] := \int_{\Omega} \kappa \nabla y \cdot \nabla v \,\mathrm{d}x + 4 \int_{\Gamma_{\mathrm{r}}} (G\, \sigma |\bar{y}|^3 y)\, v \,\mathrm{d}s + 4 \int_{\Gamma_0} \varepsilon\sigma\, |\bar{y}|^3 y\, v \,\mathrm{d}s \\ = \langle \varphi\,,\, v\rangle_{H^1(\Omega)^*, H^1(\Omega)} \quad \forall\, v \in H^1(\Omega).\end{aligned} \tag{4.3}$$

Since G is not positive, the bilinear form $\bar{a}$ is in general not coercive. Thus, the Lax-Milgram lemma cannot be applied. However, under a certain regularity assumption, one can employ the *Fredholm alternative* to show the unique existence of solutions to (4.3). To this aim, we transform (4.3) into

$$\int_{\Omega} \kappa \nabla y \cdot \nabla v \,\mathrm{d}x + 4 \int_{\Gamma_0} \varepsilon\sigma\, |\bar{y}|^3 y\, v \,\mathrm{d}s = \langle \varphi\,,\, v\rangle_{H^1(\Omega)^*, H^1(\Omega)} - 4 \int_{\Gamma_{\mathrm{r}}} (G\, \sigma |\bar{y}|^3 y) v \,\mathrm{d}s.$$

Moreover, analogously to B_{d}, we introduce the linear and continuous operator $B_{\mathrm{r}}(\bar{y}) : L^2(\Gamma_{\mathrm{r}}) \to H^1(\Omega)$ as solution operator to (4.1) if φ can be expressed by

$$\langle \varphi\,,\, v\rangle_{H^1(\Omega)^*, H^1(\Omega)} = \int_{\Gamma_{\mathrm{r}}} f_{\mathrm{r}}\, v \,\mathrm{d}s$$

with a function $f_{\mathrm{r}} \in L^2(\Gamma_{\mathrm{r}})$. Hence, (4.3) is equivalent to

$$y = B_{\mathrm{d}}(\bar{y})\, \varphi - B_{\mathrm{r}}(\bar{y})\, 4\, G\sigma |\bar{y}|^3 \tau_{\mathrm{r}} y. \tag{4.4}$$

Notice that it would be more appropriate to write $(G\sigma|\tau_{\mathrm{r}}\bar{y}|^3\, \tau_{\mathrm{r}} y)$ instead of $(G\sigma|\bar{y}|^3 \tau_{\mathrm{r}} y)$ in this context. However, for the purpose of readability, in all what follows, we suppress the trace in connection with $\bar{y}$ since it represents a fixed reference state. Applying the trace operator to (4.4) yields

$$\tau_{\mathrm{r}} y + 4\, \tau_{\mathrm{r}}\, B_{\mathrm{r}}(\bar{y})\, G\sigma |\bar{y}|^3 \tau_{\mathrm{r}} y = \tau_{\mathrm{r}} B_{\mathrm{d}}(\bar{y})\, \varphi. \tag{4.5}$$

To show the existence of solutions of this equation, we rely on the following assumption.

Assumption 3. $\lambda = -1$ is not an eigenvalue of

$$B(\bar{y})(\,\cdot\,) := 4\, \tau_{\mathrm{r}}\, B_{\mathrm{r}}(\bar{y})\, G\sigma |\bar{y}|^3 (\,\cdot\,), \tag{4.6}$$

with $B(\bar{y}) : L^2(\Gamma_{\mathrm{r}}) \to L^2(\Gamma_{\mathrm{r}})$.

Since $B_{\mathrm{r}}(\bar{y}) : L^2(\Gamma_{\mathrm{r}}) \to H^1(\Omega)$, we have that $\tau_{\mathrm{r}}\, B_{\mathrm{r}}(\bar{y}) : L^2(\Gamma_{\mathrm{r}}) \to H^{1/2}(\Gamma_{\mathrm{r}})$. Therefore, due to the compact embedding of $L^2(\Gamma_{\mathrm{r}})$ in $H^{1/2}(\Gamma_{\mathrm{r}})$, $B(\bar{y}) : L^2(\Gamma_{\mathrm{r}}) \to L^2(\Gamma_{\mathrm{r}})$ is a compact operator. Thus, thanks to Assumption 3, the theory of Fredholm operators ensures that $(I + B(\bar{y}))$ has a continuous inverse operator. Therefore, (4.5) admits a solution in $L^2(\Gamma_{\mathrm{r}})$, giving in turn the existence of solutions to (4.3) and thus the following result (*cf.* [8]).

Lemma 4.1. *Suppose that Assumption* 3 *is fulfilled and* $\bar{y} \in V^\infty$, $\bar{y} \geq \vartheta > 0$. *Then, to every* $\varphi \in H^1(\Omega)^*$, *there exists a unique solution* y *of* (4.3) *in* $H^1(\Omega)$ *that satisfies*

$$\|y\|_{H^1(\Omega)} \leq c\,\|\varphi\|_{H^1(\Omega)^*} \tag{4.7}$$

with a positive constant c. *Moreover, if the inhomogeneity* φ *is sufficiently smooth such that it can be expressed by*

$$\langle \varphi\,,\, v\rangle_{H^1(\Omega)^*, H^1(\Omega)} = \int_\Omega f_\Omega\, v\, \mathrm{d}x + \int_{\Gamma_\mathrm{r}} f_\mathrm{r}\, v\, \mathrm{d}s + \int_{\Gamma_0} f_0\, v\, \mathrm{d}s$$

with some functions $f_\Omega \in L^2(\Omega)$, $f_\mathrm{r} \in L^4(\Gamma_\mathrm{r})$, *and* $f_0 \in L^4(\Gamma_\mathrm{r})$, *then* (4.3) *admits a unique solution in* V^∞ *and the the following estimate*

$$\|y\|_{L^\infty(\Omega)} + \|y\|_{L^\infty(\Gamma_\mathrm{r}\cup\Gamma_0)} \leq c\,\big(\|f_\Omega\|_{L^2(\Omega)} + \|f_\mathrm{r}\|_{L^4(\Gamma_\mathrm{r})} + \|f_0\|_{L^4(\Gamma_0)}\big) \tag{4.8}$$

holds true with a constant c *only depending on* Ω.

Notice that we used the boundedness of $\bar{y}$ in V^∞ for (4.7), *i.e.* $\|\bar{y}\|_{V^\infty} \leq c$ with a constant only depending on Ω, which is guaranteed by Theorem 3.5 and [8], Lemma 5.1. In all what follows, we denote the solution operator associated to (4.3), mapping φ to y, by $\tilde{S}(\bar{y}) : H^1(\Omega)^* \to H^1(\Omega)$. An immediate consequence of Lemma 4.1 is the following theorem.

Theorem 4.2. *Under Assumptions* 1–3, $S : L^2(\Omega_\mathrm{s}) \to V^\infty$ *is twice continuously Fréchet-differenntiable at* $(\bar{y}, \bar{u})$. *Its first derivative, denoted by* $y = S'(\bar{u})h$, $h \in L^2(\Omega_\mathrm{s})$, *is given by*

$$\begin{aligned}
-\mathrm{div}(\kappa_\mathrm{s}\,\nabla y) &= h && \text{in } \Omega_\mathrm{s}\\
-\mathrm{div}(\kappa_\mathrm{g}\,\nabla y) &= 0 && \text{in } \Omega_\mathrm{g}\\
\kappa_\mathrm{s}\left(\frac{\partial y}{\partial n_r}\right)_\mathrm{s} - \kappa_\mathrm{g}\left(\frac{\partial y}{\partial n_r}\right)_\mathrm{g} + 4\,G(\sigma|\bar{y}|^3 y) &= 0 && \text{on } \Gamma_\mathrm{r}\\
\kappa_\mathrm{s}\frac{\partial y}{\partial n_0} + 4\,\varepsilon\sigma|\bar{y}|^3 y &= 0 && \text{on } \Gamma_0.
\end{aligned} \tag{4.9}$$

Moreover, the second derivative $w = S''(\bar{u})[h_1, h_2]$ *solves the equation*

$$\begin{aligned}
-\mathrm{div}(\kappa_\mathrm{s}\,\nabla w) &= 0 && \text{in } \Omega_\mathrm{s}\\
-\mathrm{div}(\kappa_\mathrm{g}\,\nabla w) &= 0 && \text{in } \Omega_\mathrm{g}\\
\kappa_\mathrm{s}\left(\frac{\partial w}{\partial n_r}\right)_\mathrm{s} - \kappa_\mathrm{g}\left(\frac{\partial w}{\partial n_r}\right)_\mathrm{g} + 4\,G(\sigma|\bar{y}|^3 w) &= -12\,G(\sigma|\bar{y}|\bar{y}\,y_1 y_2) && \text{on } \Gamma_\mathrm{r}\\
\kappa_\mathrm{s}\frac{\partial w}{\partial n_0} + 4\,\varepsilon\sigma|\bar{y}|^3 w &= -12\,\varepsilon\sigma|\bar{y}|\bar{y}\,y_1 y_2 && \text{on } \Gamma_0
\end{aligned} \tag{4.10}$$

with $y_i = S'(\bar{u})h_i$, $i = 1, 2$.

Proof. We follow the lines of [8], Theorem 7.1, where the Fréchet-differentiability of S is shown in detail. However, here we also need the second derivative of S, hence we shortly sketch the proof for convenience of the reader.

We reformulate (3.2) as

$$\begin{aligned} -\mathrm{div}(\kappa_{\mathrm{s}}\,\nabla\bar{y}) &= \bar{u} && \text{in } \Omega_{\mathrm{s}} \\ -\mathrm{div}(\kappa_{\mathrm{g}}\,\nabla\bar{y}) &= 0 && \text{in } \Omega_{\mathrm{g}} \\ \kappa_{\mathrm{g}}\left(\frac{\partial\bar{y}}{\partial n_r}\right)_{\mathrm{g}} - \kappa_{\mathrm{s}}\left(\frac{\partial\bar{y}}{\partial n_r}\right)_{\mathrm{s}} &= G\,\sigma|\bar{y}|^3\bar{y} && \text{on } \Gamma_{\mathrm{r}} \\ \kappa_{\mathrm{s}}\frac{\partial\bar{y}}{\partial n_0} + \lambda\,\bar{y} &= \varepsilon\sigma(y_0^4 - |\bar{y}|^3\bar{y}) + \lambda\,\bar{y} && \text{on } \Gamma_0, \end{aligned} \tag{4.11}$$

with some $\lambda > 0$ such that the bilinear form associated to the left-hand side in (4.11) is bounded an coercive in $H^1(\Omega)$. Thus, the Lax-Milgram lemma yields that (4.11) admits a solution in $H^1(\Omega)$ for every right-hand side in $H^1(\Omega)^*$. Moreover, in [8] it is shown that, if the right-hand side is sufficiently regular, *i.e.* in $L^2(\Omega_{\mathrm{s}})\times L^4(\Gamma_{\mathrm{r}})\times L^4(\Gamma_0)$, the solution is bounded in Ω and on $\Gamma_{\mathrm{r}}\cup\Gamma_0$. Thus, linear continuous operators $\tilde{B}_\Omega : L^2(\Omega) \to V^\infty$, $\tilde{B}_{\mathrm{r}} : L^4(\Gamma_{\mathrm{r}}) \to V^\infty$, and $\tilde{B}_0 : L^4(\Gamma_0) \to V^\infty$ exist such that (4.11) is equivalent to

$$0 = \bar{y} - \tilde{B}_{\Omega_{\mathrm{s}}}\,\bar{u} + \tilde{B}_{\mathrm{r}}\,(G(\sigma|\bar{y}|^3\bar{y})) - \tilde{B}_0\,(\lambda\,\bar{y} + \varepsilon\sigma\,y_0^4 - \varepsilon\sigma\,|\bar{y}|^3\bar{y}) =: T(\bar{y},\bar{u}), \tag{4.12}$$

with $T : V^\infty \times L^2(\Omega_{\mathrm{s}}) \to V^\infty$. Notice that, within this proof, we suppress the traces in arguments of operators with domain in $L^2(\Gamma_{\mathrm{r}})$ and $L^2(\Gamma_0)$, respectively, to improve the readability. Since $\Phi(y) = |y|^3y$ is twice Fréchet-differentiable in $L^\infty(\Gamma_{\mathrm{r}}\cup\Gamma_0)$ and $\tilde{B}_\Omega$, $\tilde{B}_{\mathrm{r}}$, and $\tilde{B}_0$ are linear continuous operators, the chain rule gives that T is twice continously differentiable from $V^\infty \times L^2(\Omega_{\mathrm{s}})$ to V^∞. Moreover, in [8] it is shown that, the equation $\frac{\partial T}{\partial y}(\bar{y},\bar{u})y = f$ with some $f \in V^\infty$ corresponds to a linear PDE with the same bilinear form as in (4.3). Hence, under Assumption 3, $\frac{\partial T}{\partial y}(\bar{y},\bar{u})$ is continuously invertible in V^∞. Therefore, the implicit function theorem gives that S is as smooth as T and hence, $y = S(u)$ is twice continuously differentiable at $\bar{u}$.

It remains to derive the particular form of $S'(\bar{u})$ and $S''(\bar{u})$. Substituting $\bar{y} = S(\bar{u})$ in (4.12) and differentiating in direction h yield

$$S'(\bar{u})h = \tilde{B}_{\Omega_{\mathrm{s}}}\,h - \tilde{B}_{\mathrm{r}}\,(G(4\sigma|S(\bar{u})|^3S'(\bar{u})h)) + \tilde{B}_0\,(\lambda\,S'(\bar{u})h - 4\varepsilon\sigma\,|S(\bar{u})|^3S'(\bar{u})h). \tag{4.13}$$

Now we replace $y = S'(\bar{u})h$ and $\bar{y} = S(\bar{u})$. Then, with the definitions of $\tilde{B}_\Omega$, $\tilde{B}_{\mathrm{r}}$, and $\tilde{B}_0$, (4.13) is equivalent to the linearized equation (4.9). For the second derivative, we rename $h_1 = h$ in (4.13) and differentiate both sides in direction h_2

$$\begin{aligned} S''(\bar{u})[h_1,h_2] = &- \tilde{B}_{\mathrm{r}}\,(G(12\sigma|S(\bar{u})|S(\bar{u})\,[S'(\bar{u})h_1,\,S'(\bar{u})h_2])) \\ &- \tilde{B}_{\mathrm{r}}\,(G(4\sigma|S(\bar{u})|^3\,S''(\bar{u})[h_1,\,h_2])) \\ &+ \tilde{B}_0\,(\lambda\,S''(\bar{u})[h_1,\,h_2] - 12\varepsilon\sigma\,|S(\bar{u})|S(\bar{u})\,[S'(\bar{u})h_1,\,S'(\bar{u})h_2]) \\ &- \tilde{B}_0\,(4\varepsilon\sigma\,|S(\bar{u})|^3\,S''(\bar{u})[h_1,\,h_2]). \end{aligned}$$

By setting $\bar{y} = S(\bar{u})$, $y_i = S'(\bar{u})h_i$, $i = 1,2$, and $w = S''(\bar{u})[h_1,h_2]$, the definitions of $\tilde{B}_\Omega$, $\tilde{B}_{\mathrm{r}}$, and $\tilde{B}_0$ imply (4.10). □

Remark 4.3. Clearly, the implicit function theorem also gives that $S : L^2(\Omega_{\mathrm{s}}) \to V^\infty$ is twice continuously Fréchet differentiable in a neighborhood of $\bar{u}$.

Next we derive first-order necessary optimaliy conditions to (P). To that end, we introduce the reduced objective functional by

$$j(u) := J(S(u),u) = \frac{1}{2}\,\|\nabla\,S(u) - z\|^2_{L^2(\Omega_{\mathrm{g}})} + \frac{\nu}{2}\,\|u\|^2_{L^2(\Omega_{\mathrm{s}})}. \tag{4.14}$$

Furthermore, we define the set of admissible controls by

$$U_{ad} := \{u \in L^2(\Omega) \,|\, u_a(x) \le u(x) \le u_b(x) \text{ a.e. in } \Omega_{\rm s}\}.$$

Due to Theorem 4.2 and the chain rule, we know that j is twice continuously Fréchet-differentiable from $L^2(\Omega_{\rm s})$ to $\mathbb{R}$. Thus, by standard arguments, an optimal solution $\bar u$ of (P) must satisfy the following variational inequality

$$j'(\bar u)(u - \bar u) \ge 0 \quad \forall\, u \in U_{ad}. \tag{4.15}$$

For the derivative of j, one obtains

$$j'(\bar u)h = (\nabla \bar y - z\,,\, \nabla y)_{L^2(\Omega_{\rm g})} + \nu(\bar u\,,\, h)_{L^2(\Omega_{\rm s})}, \tag{4.16}$$

with $\bar y = S(\bar u)$ and $y = S'(\bar u)h$. Now, let us transform (4.15) by introducing the adjoint state. Clearly, for every fixed $y \in H^1(\Omega)$, the bilinear form $\bar a$ in (4.3) can be seen as a linear and bounded functional on $H^1(\Omega)$. Thus, there is an operator $A \in \mathcal{L}(H^1(\Omega), H^1(\Omega)^*)$ with

$$\bar a[y, v] = \langle A\, y\,,\, v\rangle = \langle \varphi\,,\, v\rangle \quad \forall\, v \in H^1(\Omega) \quad \Leftrightarrow \quad A\, y = \varphi \quad \text{in } H^1(\Omega)^*.$$

The associated adjoint equation is given by $A^*\, p = g$ with some $g \in H^1(\Omega)^*$. Lemma 4.1 implies the existence of $A^{-1} \in \mathcal{L}(H^1(\Omega)^*, H^1(\Omega))$, giving in turn that A^* is continously invertible. Hence, it follows that the equation

$$\begin{aligned} \langle v\,,\, A^*\, p\rangle &= \langle A\, v\,,\, p\rangle = \bar a[v, p] \\ &= \int_\Omega \kappa \nabla p \cdot \nabla v \,\mathrm{d}x \;+\; 4 \int_{\Gamma_{\rm r}} \sigma\, |\bar y|^3\, (G^* p)\, v \,\mathrm{d}s + 4 \int_{\Gamma_0} \varepsilon\sigma\, |\bar y|^3\, p\, v \,\mathrm{d}s \\ &= \langle g, v\rangle_{H^1(\Omega)^*, H^1(\Omega)} \qquad \forall\, v \in H^1(\Omega) \end{aligned} \tag{4.17}$$

admits a unique solution $p \in H^1(\Omega)$ for every $g \in H^1(\Omega)^*$.

Lemma 4.4. *Suppose that Assumption* 3 *is fulfilled and let* $\bar y \in V^\infty$ *with* $\bar y \ge \vartheta > 0$ *be given. Then, to every* $g \in H^1(\Omega)^*$*, there exists a unique solution* p *of* (4.17) *in* $H^1(\Omega)$.

Now, let us choose a special inhomogeneity in (4.17) given by $\langle g\,,\, v\rangle = (\nabla \bar y - z\,,\, \nabla v)_{L^2(\Omega_{\rm g})}$ such that we obtain the *adjoint equation* associated to the state equation:

$$\int_\Omega \kappa \nabla p \cdot \nabla v \,\mathrm{d}x \;+\; 4 \int_{\Gamma_{\rm r}} \sigma\, |\bar y|^3\, (G^* p)\, v \,\mathrm{d}s + 4 \int_{\Gamma_0} \varepsilon\sigma\, |\bar y|^3\, p\, v \,\mathrm{d}s = \int_{\Omega_{\rm g}} (\nabla \bar y - z) \cdot \nabla v \,\mathrm{d}x \quad \forall\, v \in H^1(\Omega). \tag{4.18}$$

Note that, thanks to $\bar y \in V^\infty$ and $z \in L^2(\Omega_{\rm g})$ by Assumption 2, the right-hand side indeed defines an element of $H^1(\Omega)^*$. Formal integration by parts yields the PDE corresponding to (4.18):

$$\begin{aligned} \operatorname{div}(\kappa_{\rm g}\, \nabla p) &= \Delta \bar y - \operatorname{div} z && \text{in } \Omega_{\rm g} \\ \operatorname{div}(\kappa_{\rm s}\, \nabla p) &= 0 && \text{in } \Omega_{\rm s} \\ \kappa_{\rm s} \left(\frac{\partial p}{\partial n_{\rm r}}\right)_{\rm s} - \kappa_{\rm g} \left(\frac{\partial p}{\partial n_{\rm r}}\right)_{\rm g} + 4\sigma\, |\bar y|^3 G^* p &= -\frac{\partial \bar y}{\partial n_{\rm r}} + z \cdot n_{\rm r} && \text{on } \Gamma_{\rm r} \\ \kappa_s \frac{\partial p}{\partial n_0} + 4\varepsilon\sigma\, |\bar y|^3 p &= 0 && \text{on } \Gamma_0. \end{aligned} \tag{4.19}$$

Consider now the variational formulation associated to $y = S'(\bar{u})(u-\bar{u})$ with some $u \in L^2(\Omega_s)$, that is given by

$$\bar{a}[y,v] = (u-\bar{u}\,,\,v)_{L^2(\Omega_s)} \quad \forall\, v \in H^1(\Omega).$$

If we insert p, *i.e.* the solution of (4.18), as test function, then we obtain

$$(u-\bar{u}\,,\,p)_{L^2(\Omega_s)} = \bar{a}[y,p] = \langle A\,y\,,\,p\rangle = \langle y\,,\,A^*\,p\rangle = (\nabla\bar{y}-z\,,\,\nabla y)_{L^2(\Omega_g)}.$$

Inserting this into (4.16) and (4.15) gives

$$(p+\nu\,\bar{u}\,,\,u-\bar{u})_{L^2(\Omega_s)} \geq 0 \quad \forall\, u \in U_{ad}. \tag{4.20}$$

By standard arguments, a pointwise discussion of this inequality implies

$$\bar{u}(x) = \mathcal{P}_{ad}\left\{-\frac{1}{\nu}\,p(x)\right\}, \tag{4.21}$$

where $\mathcal{P}_{ad}(x)$ denotes the pointwise projection operator on $[u_a(x), u_b(x)]$. In this way, we have derived first-order necessary conditions to (P):

Theorem 4.5. *Suppose that Assumptions* 1–3 *are fulfilled and* $\bar{u}$ *is a locally optimal solution of* (P) *with associated state* $\bar{y}$. *Then, there exists an adjoint state* $p \in H^1(\Omega)$ *such that the adjoint equation* (4.19) *and the projection formula* (4.21) *are satisfied.*

5. Second-order sufficient conditions

This section is devoted to our main result, second-order sufficient optimality conditions for (P). First, we establish second-order conditions that require a rather large subspace where the second derivative of j must be positive definite. These conditions are very easy to prove. Then, we shrink this subspace and formulate another sufficient condition that is less restrictive than the first one. The associated proof is performed in Section 7.

In the following, the subspace, where $j''(\bar{u})$ is assumed to be positive definite, is called *critical cone*. The "large" critical cone is defined by

$$\tilde{C}(\bar{u}) := \left\{ u \in L^2(\Omega_s) \;\middle|\; \begin{array}{ll} u(x) \geq 0, & \text{where } \bar{u}(x) = u_a(x) \\ u(x) \leq 0, & \text{where } \bar{u}(x) = u_b(x) \end{array} \right\},$$

and hence does not account for strongly active sets.

Theorem 5.1. *Suppose that Assumptions* 1–3 *are fulfilled and that* $(\bar{y},\bar{u})$ *satisfy the first-order necessary optimality conditions. Assume further that a constant* $\tilde{\delta} > 0$ *exists such that*

$$j''(\bar{u})u^2 \geq \tilde{\delta}\,\|u\|^2_{L^2(\Omega_s)} \tag{5.1}$$

is satisfied for all $u \in \tilde{C}(\bar{u})$. *Then positive constants* $\tilde{\varepsilon} > 0$ *and* $\tilde{\sigma} > 0$ *exist, such that the quadratic growth condition*

$$j(u) \geq j(\bar{u}) + \tilde{\sigma}\,\|u-\bar{u}\|^2_{L^2(\Omega_s)} \tag{5.2}$$

holds true for all $u \in U_{ad}$ *with* $\|u-\bar{u}\|_{L^2(\Omega_s)} \leq \tilde{\varepsilon}$.

Proof. The proof follows standard arguments. A Taylor expansion of j at $\bar{u}$ yields for an arbitrary $u \in U_{ad}$

$$j(u) = j(\bar{u}) + j'(\bar{u})(u-\bar{u}) + \frac{1}{2}\, j''(\bar{u})(u-\bar{u})^2 + r_j^{(2)} \tag{5.3}$$

$$\geq j(\bar{u}) + \frac{\tilde{\delta}}{2}\,\|u-\bar{u}\|^2_{L^2(\Omega_{\mathrm{s}})} - |r_j^{(2)}| \tag{5.4}$$

where we used the variational inequality (4.15). Moreover, $u \in U_{ad}$ implies $(u-\bar{u}) \in \tilde{C}(\bar{u})$, hence (5.1) applies to $j''(\bar{u})(u-\bar{u})^2$. Since j is twice continuously Fréchet-differentiable from $L^2(\Omega_{\mathrm{s}})$ to $\mathbb{R}$, we have that

$$\frac{|r_j^{(2)}|}{\|u-\bar{u}\|^2_{L^2(\Omega_{\mathrm{s}})}} \to 0\ ,\ \text{if } \|u-\bar{u}\|_{L^2(\Omega_{\mathrm{s}})} \to 0. \tag{5.5}$$

Thus a constant $\tilde{\varepsilon}$ exists with $|r_j^{(2)}| \leq \tilde{\delta}/4\,\|u-\bar{u}\|^2_{L^2(\Omega_{\mathrm{s}})}$ for all $\|u-\bar{u}\|_{L^2(\Omega_{\mathrm{s}})} \leq \tilde{\varepsilon}$. Therefore, with $\tilde{\sigma} = \tilde{\delta}/4$, (5.4) implies (5.2). □

Next, we formulate less restrictive second-order sufficient conditions that consider strongly active sets. As mentioned in Section 1, in this case, we have to deal with a two-norm discrepancy. We establish a condition that gives local optimality in an L^s-neighborhood of a reference function, where s is not necessarily equal to ∞, but can be chosen smaller. This gives some flexibility in the choice of the neighborhood where local optimality of a reference function is obtained. However, a "larger" neighborhood corresponds to a "weaker" growth condition (see Th. 5.5).

We introduce the *strongly active set* as follows:

Definition 5.2. Let $\tau > 0$ be given. Then the strongly active set A_τ is defined by

$$A_\tau := \{x \in \Omega \,|\ |p(x) + \nu\,\bar{u}(x)| \geq \tau\},$$

where p is the adjoint state associated to $\bar{u}$, *i.e.* the solution of (4.19) with $\bar{y} = S(\bar{u})$.

Definition 5.3. Let a real number s be given with $2 \leq s \leq \infty$. Then, q is defined by

$$q := \begin{cases} 2s/(s+1), & \text{for } 2 \leq s < \infty \\ 2, & \text{for } s = \infty, \end{cases} \tag{5.6}$$

i.e. $q \in [4/3, 2]$, and q' is the corresponding conjugate exponent, *i.e.*

$$q' := \frac{q}{q-1} = \begin{cases} 2s/(s-1), & \text{for } 2 \leq s < \infty \\ 2, & \text{for } s = \infty. \end{cases} \tag{5.7}$$

Notice that the definition of q' implies $q' \in [2, 4]$ according to the condition on U_{ad} in Assumption 2. Moreover, (5.6) yields $q \in [4/3, 2]$. The corresponding "small" τ-*critical cone* is defined in a standard way (*cf.* Dontchev *et al.* [5]).

Definition 5.4. The critical cone belonging to (P) is given by

$$C_\tau(\bar{u}) := \left\{ u \in L^t(\Omega_{\mathrm{s}}) \;\middle|\; \begin{array}{ll} u(x) = 0, & a.e. \text{ in } A_\tau \\ u(x) \geq 0, & \text{where } \bar{u}(x) = u_a(x) \text{ and } x \notin A_\tau \\ u(x) \leq 0, & \text{where } \bar{u}(x) = u_b(x) \text{ and } x \notin A_\tau \end{array} \right\}. \tag{5.8}$$

Recall that t is the exponent in the regularity assumption on U_{ad} and satisfies $t \geq q'$ (*cf.* Assumption 2). Now, we are in the position to state second order sufficient conditions for (P) with respect to the reduced critical cone $C_\tau(\bar{u})$.

$$\text{(SSC)} \begin{cases} \textit{Let } \delta > 0 \text{ exist such that} \\ \qquad j''(\bar{u})\, u^2 \geq \delta\, \|u\|^2_{L^q(\Omega_{\rm s})} \quad \text{for all } u \in C_\tau(\bar{u}). \end{cases}$$

Notice that, by the definition of q, $j''(\bar{u})\, u^2 \geq \delta\, \|u\|^2_{L^2(\Omega_{\rm s})}$ for all $u \in C_\tau(\bar{u})$ immediately implies (SSC). In Section 7, we show that (SSC) is indeed sufficient for local optimality of $\bar{u}$.

Theorem 5.5. *Suppose that Assumptions* 1–3 *are fulfilled and that* $s \in [2, \infty]$ *is given. Moreover, let* $(\bar{y}, \bar{u})$ *satisfy the first-order necessary optimality conditions for problem* (P) *and assume that condition* (SSC) *is fulfilled with some* $\delta > 0$, $\tau > 0$. *Then, there exist* $\bar{\varepsilon} > 0$ *and* $\bar{\sigma} > 0$ *such that*

$$j(u) \geq j(\bar{u}) + \bar{\sigma}\, \|u - \bar{u}\|^2_{L^q(\Omega_{\rm s})}, \tag{5.9}$$

with q *as defined in* (5.6), *holds for all* $u \in U_{ad}$ *with* $\|u - \bar{u}\|_{L^s(\Omega_{\rm s})} \leq \bar{\varepsilon}$.

Remark 5.6. Setting $s = \infty$, we obtain $q = 2$, and hence Theorem 5.5 gives an L^2-quadratic growth condition in an L^∞-neighborhood of $\bar{u}$. Choosing $s = 2$ and thus $q = 4/3$, we obtain $L^{4/3}$-quadratic growth of j in an L^2-neighborhood of $\bar{u}$. Therefore, in this case, an L^∞-neighborhood is not required for local optimality. As second-order sufficient conditions are important for the convergence theory of higher order optimization methods, as *e.g.* sequential quadratic programming methods, this can be used to guarantee convergence if numerical schemes do not provide a sufficient accuracy with respect to the L^∞-norm, which may happen for instance if the optimal control is discontinuous.

6. Auxiliary results

Before we are in the position to prove Theorem 5.5, we have to investigate the neighborhood of a stationary point, *i.e.* a fixed reference solution of (P). Based on these findings, we derive some results concerning the second derivative of j in Section 6.2 also needed for the proof of Theorem 5.5. Throughout this section, we assume that $(\bar{y}, \bar{u})$ is a fixed stationary point of problem (P). Therefore, we have that $\bar{u} \in U_{ad}$ and $(\bar{y}, \bar{u})$ satisfy the state equation (3.2). As before, this implies that $\|\bar{y}\|_{V^\infty}$ is bounded by a constant because of Theorem 3.5 and [8] Lemma 5.1. This property is used several times in the proofs presented above. Notice that Lemma 3.3 implies the boundedness of G and G^* from $L^p(\Gamma_{\rm r})$ to $L^p(\Gamma_{\rm r})$ for all $1 \leq p \leq \infty$, what is also used in the subsequent proofs.

6.1. The neighborhood of a stationary point

In all what follows, we denote by $\hat{u}$ an admissible control in a neighborhood of $\bar{u}$, *i.e.*. $\hat{u} \in B_\rho(\bar{u}) \cap U_{ad}$, where $B_\rho(\bar{u})$ denotes an open ball in $L^2(\Omega_{\rm s})$ of radius ρ around $\bar{u}$. Furthermore, we define $\hat{y} = S(\hat{u})$. Analogously to $\bar{y}$, we have the boundedness of $\|\hat{y}\|_{V^\infty}$ and $\hat{y}(x) \geq \vartheta > 0$ *a.e.* in Ω and *a.e.* on $\Gamma_{\rm r} \cup \Gamma_0$ (*cf.* Ths. 3.5 and 3.6, and [8], Lem. 5.1). Now, given some $\varphi \in H^1(\Omega)^*$, we consider the following linear equation

$$\int_\Omega \kappa \nabla y \cdot \nabla v \,\mathrm{d}x + 4 \int_{\Gamma_{\rm r}} (G\,\sigma |\hat{y}|^3 y) v \,\mathrm{d}s + 4 \int_{\Gamma_0} \varepsilon\sigma\, |\hat{y}|^3 y\, v \,\mathrm{d}s = \langle \varphi\,,\, v \rangle_{H^1(\Omega)^*, H^1(\Omega)} \quad \forall\, v \in H^1(\Omega), \tag{6.1}$$

which is equivalent to (4.3) with $\hat{y}$ instead of $\bar{y}$. Naturally, Assumption 3 does in general not imply that a similar conditions holds with $\hat{y}$ such that the existence of solutions to (6.1) is not immediately guaranteed. Notice further that the Fréchet differentiability of S from $L^2(\Omega_{\rm s})$ to V^∞ only gives the existence of $S'(\hat{u}) : L^2(\Omega_{\rm s}) \to V^\infty$ but does not imply that $\tilde{S}(\hat{y}) : H^1(\Omega)^* \to H^1(\Omega)$, *i.e.* the solution operator to (6.1), is well defined. To overcome these problems, let us consider the operator $A(\bar{y}) : L^2(\Gamma_{\rm r}) \to L^2(\Gamma_{\rm r})$ defined by

$$A(\bar{y}) := I + B(\bar{y}) = I + \tau_{\rm r} B_{\rm r}(\bar{y})\, G\sigma|\bar{y}|^3$$

with $B(\bar{y})$ as defined in Assumption 3 and $B_{\rm r}(\bar{y})$ as introduced before (4.4). Moreover, we set $\hat{y} = S(\hat{u})$ and define $A(\hat{y})$ analogously to $A(\bar{y})$. Due to Assumption 3, it is clear that $A(\bar{y})$ is continuously invertible. In the following, we will show that the same holds for $A(\hat{y})$ presumed that $\|\bar{u} - \hat{u}\|_{L^2(\Omega_{\rm s})}$ is sufficiently small. Then one can argue as in Section 4 to obtain the existence of solutions to (6.1) giving in turn the existence of an adjoint state in the neighborhood of a stationary point.

Lemma 6.1. *Let the Assumptions* 1–3 *be fulfilled. Assume further that* $\hat{u} \in B_\rho(\bar{u}) \cap U_{ad}$*. If* ρ *is chosen sufficiently small, then* $\tilde{S}(\hat{y})$ *exists as a linear and continuous operator from* $H^1(\Omega)^*$ *to* $H^1(\Omega)$*, i.e. equation* (6.1) *admits a unique solution in* $H^1(\Omega)$ *for every* $\varphi \in H^1(\Omega)^*$ *that can be estimated by*

$$\|y\|_{H^1(\Omega)} \le c\, \|\varphi\|_{H^1(\Omega)^*} \tag{6.2}$$

with a constant c *only depending on* Ω.

Proof. We start with the definition

$$\delta A := A(\hat{y}) - A(\bar{y}). \tag{6.3}$$

Applying both sides in (6.3) to an arbitrary $g \in L^2(\Gamma_{\rm r})$ yields

$$\begin{aligned} \delta A\, g &= A(\hat{y})\, g - A(\bar{y})\, g \\ &= \tau_{\rm r}\big(B_{\rm r}(\hat{y})\, G\sigma|\hat{y}|^3\, g - B_{\rm r}(\bar{y})\, G\sigma|\bar{y}|^3\, g\big). \end{aligned} \tag{6.4}$$

Next, we set $y_1 := B_{\rm r}(\hat{y})\, G\sigma|\hat{y}|^3\, g$ and $y_2 := B_{\rm r}(\bar{y})\, G\sigma|\bar{y}|^3\, g$. The definition of $B_{\rm r}(.) : L^2(\Gamma_{\rm r}) \to H^1(\Omega)$ implies that y_1 solves

$$\int_\Omega \kappa \nabla y_1 \cdot \nabla v \, {\rm d}x + 4 \int_{\Gamma_0} \varepsilon\sigma\, |\hat{y}|^3 y_1\, v \, {\rm d}s = \int_{\Gamma_{\rm r}} (G\sigma|\hat{y}|^3 g)\, v \, {\rm d}s \quad \forall\, v \in H^1(\Omega). \tag{6.5}$$

Note that the bilinear from in this equation is bounded and coercive because of $\hat{y} \in V^\infty$, $\hat{y}(x) \ge \vartheta > 0$ *a.e.* on Γ_0. Clearly, y_2 satisfies an analogous equation with $\bar{y}$ instead of $\hat{y}$ such that the difference $y_2 - y_1$ solves

$$\begin{aligned} &\int_\Omega \kappa \nabla (y_2 - y_1) \cdot \nabla v \, {\rm d}x + 4 \int_{\Gamma_0} \varepsilon\sigma\, |\bar{y}|^3 (y_2 - y_1)\, v \, {\rm d}s \\ &\quad = 4 \int_{\Gamma_0} \varepsilon\sigma \left(|\hat{y}|^3 - |\bar{y}|^3\right) y_1\, v \, {\rm d}s + \int_{\Gamma_{\rm r}} \big(G\sigma\big(|\bar{y}|^3 - |\hat{y}|^3\big) g\big)\, v \, {\rm d}s \quad \forall\, v \in H^1(\Omega). \end{aligned}$$

Because of the coercivity of the bilinear form, we can estimate

$$\begin{aligned} \|y_2 - y_1\|^2_{H^1(\Omega)} \le c\Big(&\int_{\Gamma_0} \varepsilon\sigma \left(|\hat{y}|^3 - |\bar{y}|^3\right) y_1\, (y_2 - y_1) \, {\rm d}s \\ &+ \int_{\Gamma_{\rm r}} \big(G\sigma\big(|\bar{y}|^3 - |\hat{y}|^3\big) g\big)\, (y_2 - y_1) \, {\rm d}s\Big) =: I_1 + I_2. \end{aligned} \tag{6.6}$$

For I_1, one obtains

$$I_1 \leq c \, \| \, |\hat{y}|^3 - |\bar{y}|^3 \|_{L^\infty(\Gamma_0)} \, \|y_1\|_{L^2(\Gamma_0)} \, \|y_2 - y_1\|_{L^2(\Gamma_0)}.$$

Thanks to the boundedness of $\bar{y}$ and $\hat{y}$, we can continue with

$$\begin{aligned} \| \, |\hat{y}|^3 - |\bar{y}|^3 \|_{L^\infty(\Gamma_0)} &= \|(\hat{y}^2 + |\hat{y}| \, |\bar{y}| + \bar{y}^2)(|\hat{y}| - |\bar{y}|)\|_{L^\infty(\Gamma_0)} \\ &\leq c \, \|\hat{y} - \bar{y}\|_{L^\infty(\Gamma_0)}. \end{aligned} \tag{6.7}$$

Moreover, since y_1 is the solution of (6.5), it is easy to see that $\|y_1\|_{L^2(\Gamma_0)} \leq c \, \|g\|_{L^2(\Gamma_\mathrm{r})}$. Hence, it follows

$$I_1 \leq c \, \|\hat{y} - \bar{y}\|_{V^\infty} \, \|g\|_{L^2(\Gamma_\mathrm{r})} \, \|y_2 - y_1\|_{H^1(\Omega)}.$$

A similar discussion yields

$$I_2 \leq c \, \|\hat{y} - \bar{y}\|_{V^\infty} \, \|g\|_{L^2(\Gamma_\mathrm{r})} \, \|y_2 - y_1\|_{H^1(\Omega)},$$

such that (6.6) gives

$$\|y_2 - y_1\|_{H^1(\Omega)} \leq c \, \|\hat{y} - \bar{y}\|_{V^\infty} \, \|g\|_{L^2(\Gamma_\mathrm{r})}.$$

Now, the definitions of y_1 and y_2 imply

$$\|A(\hat{y}) \, g - A(\bar{y}) \, g\|_{L^2(\Gamma_\mathrm{r})} = \|y_2 - y_1\|_{L^2(\Gamma_\mathrm{r})} \leq c \, \|\hat{y} - \bar{y}\|_{V^\infty} \, \|g\|_{L^2(\Gamma_\mathrm{r})}$$

for all $g \in L^2(\Gamma_\mathrm{r})$. In view of (6.4), this gives

$$\|\delta A\|_{\mathcal{L}(L^2(\Gamma_\mathrm{r}))} \leq c \, \|\hat{y} - \bar{y}\|_{V^\infty}. \tag{6.8}$$

Next, we consider the equation

$$A(\hat{y})g = f \quad \Leftrightarrow \quad \big(I - \underbrace{A(\bar{y})^{-1}(-\delta A)}_{=:\,T}\big)g = A(\bar{y})^{-1} f,$$

with some $f \in L^2(\Gamma_\mathrm{r})$. Here, we used that $A(\bar{y})$ is continuously invertible by Assumption 3. With (6.8), one obtains

$$\begin{aligned} \|T\|_{\mathcal{L}(L^2(\Gamma_\mathrm{r}))} &\leq \|A(\bar{y})^{-1}\|_{\mathcal{L}(L^2(\Gamma_\mathrm{r}))} \, \|\delta A\|_{\mathcal{L}(L^2(\Gamma_\mathrm{r}))} \\ &\leq c \, \|\hat{y} - \bar{y}\|_{V^\infty}. \end{aligned}$$

If $\|\hat{u} - \bar{u}\|_{L^2(\Omega_\mathrm{s})}$ is chosen sufficiently small, then the continuity of S implies $\|\hat{y} - \bar{y}\|_{V^\infty} < 1/c$ and hence

$$\|T\|_{\mathcal{L}(L^2(\Gamma_\mathrm{r}))} < 1.$$

Then, the theory of Neumann series yields that $I - T$ is continuously invertible giving in turn that $A(\hat{y})g = f$ admits a unique solution in $L^2(\Gamma_\mathrm{r})$ for all $f \in L^2(\Gamma_\mathrm{r})$. Now, together with the definition of $A(\hat{y})$, this implies the continuous invertibility of $I + B(\hat{y}) = I + \tau_\mathrm{r} B_\mathrm{r}(\hat{y}) \, G\sigma|\hat{y}|^3$ such that a condition analogous to Assumption 3 holds with $\hat{y}$. Then, an analogous discussion as before Lemma 4.1 gives the unique existence of solutions to

(6.1), *i.e.* $\tilde{S}(\hat{y}) : H^1(\Omega)^* \to H^1(\Omega)$ is well defined, provided that $\|\hat{u} - \bar{u}\|_{L^2(\Omega_s)}$ is sufficiently small. Finally, (6.2) follows from the boundedness of $\|\hat{y}\|_{V^\infty}$. □

Lemma 6.1 immediately implies the existence of $\tilde{S}(\hat{y})^* : H^1(\Omega)^* \to H^1(\Omega)$. Then, by the same arguments leading to Lemma 4.4, the following result is obtained.

Lemma 6.2. *Under the assumptions of Lemma* 6.1*, the equation*

$$\int_\Omega \kappa \nabla \hat{p} \cdot \nabla v \, \mathrm{d}x \; + \; 4 \int_{\Gamma_r} \sigma \, |\hat{y}|^3 \, (G^* \hat{p}) \, v \, \mathrm{d}s + 4 \int_{\Gamma_0} \varepsilon\sigma \, |\hat{y}|^3 \, \hat{p} \, v \, \mathrm{d}s = \langle g, v \rangle_{H^1(\Omega)^*, H^1(\Omega)} \quad \forall \, v \in H^1(\Omega) \tag{6.9}$$

admits a unique solution $\hat{p} \in H^1(\Omega)$ *for every* $g \in H^1(\Omega)^*$*. Moreover, the estimate*

$$\|\hat{p}\|_{H^1(\Omega)} \leq c \, \|g\|_{H^1(\Omega)^*}$$

holds true with a constant c *only depending on* Ω*.*

With the previous results at hand, embedding theorems for $\dim(\Omega) \leq 3$ immediately give the follwoing lemma.

Lemma 6.3. *Suppose that Assumptions of Lemma* 6.1 *are fulfilled. Let* $\hat{p}$ *denote the solution of the adjoint equation* (6.9) *with*

$$\langle g \, , \, v \rangle = \int_{\Omega_g} (\nabla \hat{y} - z) \cdot \nabla v \, \mathrm{d}x$$

as inhomogeneity. Then, there exists a positive constant c *such that*

$$\|\hat{p}\|_{L^4(\Gamma_r \cup \Gamma_0)} \leq c$$

holds true.

Remark 6.4. Clearly, the same holds for the adjoint state associated to $\bar{y}$, *i.e.* the solution of (4.18) such that we have $\|p\|_{L^4(\Gamma_r \cup \Gamma_0)} \leq c$.

Now, let $h \in L^t(\Omega_s)$ be given such that $\bar{u} + h \in U_{ad}$ and define

$$\hat{u} := \bar{u} + \theta \, h \tag{6.10}$$

with a fixed, but arbitrary $\theta \in (0, 1)$. Clearly, if $\|h\|_{L^2(\Omega_s)}$ is sufficiently small, then $\hat{u}$ as defined in (6.10) satisfies the assumptions of Lemma 6.1. Moreover, we define

$$y := S'(\bar{u})h, \quad \text{and} \quad \eta := S'(\hat{u})h.$$

Then, the Taylor expansion for $\hat{y} = S(\hat{u}) = S(\bar{u} + \theta \, h)$ is given by

$$\hat{y} = S(\bar{u}) + \theta \, S'(\bar{u})h + r_S^{(1)} = \bar{y} + \theta \, y + r_S^{(1)}, \tag{6.11}$$

where the remainder term satisfies

$$\|r_S^{(1)}\|_{H^1(\Omega)} \leq \psi(\|h\|_{L^2(\Omega_s)}) \, \|h\|_{L^2(\Omega_s)} \tag{6.12}$$

due to the Fréchet diffrentiability of S. Here and in the following, $\psi : \mathbb{R}^+ \to \mathbb{R}^+$ denotes a generic function with $\psi(x) \to 0$ for every $x \downarrow 0$. In addition to (6.11), we have

$$S'(\bar{u} + \theta\, h) = S'(\bar{u}) + \theta\, S''(\bar{u})h + r_{S'}^{(1)} \tag{6.13}$$

with a remainder term $r_{S'}^{(1)}$. If one applies both sides of (6.13) to h, then

$$\eta = S'(\bar{u} + \theta\, h)h = S'(\bar{u})h + \theta\, S''(\bar{u})h^2 + r_{S'}^{(1)}h = y + \theta\, w + \tilde{r}_S^{(2)} \tag{6.14}$$

is obtained, where w is defined by $w = S''(\bar{u})h^2$, *i.e.* the solution of (4.10) with $h_1 = h_2 = h$. Moreover, $\tilde{r}_S^{(2)}$ is defined by $\tilde{r}_S^{(2)} := r_{S'}^{(1)}h$.

Lemma 6.5. *Assume that q is a fixed real number, chosen according to Definition* 5.3, *i.e.* $q \in [4/3, 2]$. *Then, if $\bar{u} + h \in U_{ad}$ and $\|h\|_{L^2(\Omega_s)}$ is sufficiently small,*

$$\|\tilde{r}_S^{(2)}\|_{H^1(\Omega)} \le \psi(\|h\|_{L^2(\Omega_s)})\, \|h\|_{L^q(\Omega_s)}$$

holds true.

Proof. Since S is twice Fréchet differentiable, we have

$$\|r_{S'}^{(1)}\|_{\mathcal{L}(L^2(\Omega_s),V^\infty)} \le \psi(\|h\|_{L^2(\Omega_s)})\, \|h\|_{L^2(\Omega_s)}.$$

Therefore, we obtain

$$\begin{aligned}\|\tilde{r}_S^{(2)}\|_{H^1(\Omega)} &\le \|r_{S'}^{(1)}\|_{\mathcal{L}(L^2(\Omega_s),V^\infty)}\, \|h\|_{L^2(\Omega_s)} \le \psi(\|h\|_{L^2(\Omega_s)})\, \|h\|^2_{L^2(\Omega_s)} \\ &\le \psi(\|h\|_{L^2(\Omega_s)})\, \|h\|_{L^{q'}(\Omega_s)} \|h\|_{L^q(\Omega_s)} \le c\, \psi(\|h\|_{L^2(\Omega_s)})\, \|h\|_{L^q(\Omega_s)},\end{aligned}$$

since $\|h\|_{L^{q'}(\Omega_s)} \le c\, \|h\|_{L^t(\Omega_s)} \le c\, \|u_b - u_a\|_{L^t(\Omega_s)}$ because of $\bar{u} + h \in U_{ad}$ and $q' \le t$ by Assumption 2. □

If we consider y as a function in $H^1(\Omega)$, it can be treated as the solution of (4.3) with

$$\langle \varphi\, ,\, v\rangle = \int_{\Omega_s} h\, v \,\mathrm{d}x$$

on the right-hand side. Moreover, embedding theorems for $\dim(\Omega) \le 3$ give that, $h \in L^r(\Omega_s)$ can be identified with an element of $H^1(\Omega)^*$, if $r \ge 6/5$. In this way, estimate (4.7) in Lemma 4.1 yields the following result.

Lemma 6.6. *Let the Assumptions* 1–3 *be fulfilled and q be given according to Definition* 5.3 *such that* $q \in [4/3, 2]$. *Then, the solution of* (4.9) *is estimated by*

$$\|y\|_{H^1(\Omega)} \le c\, \|h\|_{L^q(\Omega_s)} \tag{6.15}$$

with a constant c only depending on Ω.

Remark 6.7. Notice that Lemma 6.6 is also valid if $q \ge 6/5$. However, as we will see in Section 7, it is not necessary to consider the case $q < 4/3$ here (*cf.* (7.8)). The same also holds for the following results in this and the next section.

Similarly to Lemma 6.6, if we consider $w = S''(\bar{u})h^2$ as solution of (4.3) with

$$\langle \varphi\, ,\, v\rangle = -12 \int_{\Gamma_r} (G\sigma\, |\bar{y}|\bar{y}\, y^2)\, v \,\mathrm{d}s - 12 \int_{\Gamma_0} \varepsilon\sigma\, |\bar{y}|\bar{y}\, y^2\, v \,\mathrm{d}s,$$

we obtain:

Lemma 6.8. *Suppose that Assumptions* 1–3 *are fulfilled and* q *is given according to Definition* 5.3. *Then the solution of* (4.10) *with* $h_1 = h_2 = h$ *satisfies*

$$\|w\|_{H^1(\Omega)} \leq c\,\|h\|^2_{L^q(\Omega_s)}, \tag{6.16}$$

with a constant c *only depending on* Ω.

Proof. In this case, (4.7) implies

$$\|w\|_{H^1(\Omega)} \leq c\,\|\varphi\|_{H^1(\Omega)^*} \leq c\,(\|G\sigma\,|\bar{y}|\bar{y}\,y^2\|_{L^2(\Gamma_r)} + \|\varepsilon\sigma\,|\bar{y}|\bar{y}\,y^2\|_{L^2(\Gamma_0)}), \tag{6.17}$$

where y is as above defined by $y = S'(\bar{u})h$. The first addend on the right-hand side is estimated by

$$\|G\sigma\,|\bar{y}|\bar{y}\,y^2\|_{L^2(\Gamma_r)} \leq c\,\|G\|_{\mathcal{L}(L^2(\Gamma_r))}\|\bar{y}\|^2_{L^\infty(\Gamma_r)}\|y^2\|_{L^2(\Gamma_r)}.$$

Due to dim $(\Omega) \leq 3$, the embedding theorems imply for two arbitrary functions $v_1, v_2 \in H^1(\Omega)$:

$$\begin{aligned}\|v_1\,v_2\|_{L^2(\Gamma_r)} &\leq (\,\|v_1^2\|_{L^2(\Gamma_r)}\,\|v_2^2\|_{L^2(\Gamma_r)}\,)^{1/2} = \|v_1\|_{L^4(\Gamma_r)}\,\|v_2\|_{L^4(\Gamma_r)}\\ &\leq c\,\|v_1\|_{H^1(\Omega)}\,\|v_2\|_{H^1(\Omega)}.\end{aligned} \tag{6.18}$$

Thus, with $v_1\,v_2 = y^2$, (6.15) yields

$$\|G\sigma\,|\bar{y}|\bar{y}\,y^2\|_{L^2(\Gamma_r)} \leq c\,\|h\|^2_{L^q(\Omega_s)}. \tag{6.19}$$

Analogously, we obtain for the second addend in (6.17)

$$\|\varepsilon\sigma\,|\bar{y}|\bar{y}\,y^2\|_{L^2(\Gamma_0)} \leq c\,\|h\|^2_{L^q(\Omega_s)}. \tag{6.20}$$

Inserting (6.19) and (6.20) in (6.17) finally gives the assertion. □

With the previous findings, we can derive an estimation for the difference between p and $\hat{p}$, *i.e.* the solutions of (4.17) and (6.9) with the special inhomogeneities

$$\int_{\Omega_g} (\nabla\bar{y} - z)\cdot\nabla v\,\mathrm{d}x \quad \text{and} \quad \int_{\Omega_g} (\nabla\hat{y} - z)\cdot\nabla v\,\mathrm{d}x,$$

respectively.

Lemma 6.9. *Let the assumptions of Lemma* 6.1 *be fulfilled and* p *and* $\hat{p}$ *be the adjoint states associated to* $\bar{y}$ *and* $\hat{y}$ *respectively. Then*

$$\|\hat{p} - p\|_{H^1(\Omega)} \leq \psi(\|h\|_{L^2(\Omega_s)})$$

holds true.

Proof. According to the definition of p and $\hat{p}$, the difference of both solves equation (4.17) with the following right-hand side

$$\langle g\,,\,v\rangle = \int_{\Omega_g} \nabla(\hat{y} - \bar{y})\cdot\nabla v\,\mathrm{d}x + 4\int_{\Gamma_r} \sigma(|\bar{y}|^3 - |\hat{y}|^3)(G^*\hat{p})\,v\,\mathrm{d}s + 4\int_{\Gamma_0} \varepsilon\,\sigma(|\bar{y}|^3 - |\hat{y}|^3)\,\hat{p}\,v\,\mathrm{d}s.$$

This inhomogeneity is estimated as follows: thanks to (6.18), one obtains for the L^2-norm of the second addend

$$\begin{aligned}\|(|\bar y|^3 - |\hat y|^3)(G^*\hat p)\|_{L^2(\Gamma_r)} &\le \|(G^*\hat p)\|_{L^4(\Gamma_r)} \, \| \, |\bar y|^3 - |\hat y|^3 \, \|_{L^4(\Gamma_r)} \\ &\le c \, \| \, |\bar y|^3 - |\hat y|^3 \, \|_{L^4(\Gamma_r)},\end{aligned} \tag{6.21}$$

where Lemma 6.3 was used for the boundedness of $G^*\hat p$. Arguing as in (6.7), we arrive at

$$\| |\bar y|^3 - |\hat y|^3 \|_{L^4(\Gamma_r)} \le \|\bar y^2 + |\bar y| \, |\hat y| + \hat y^2\|_{L^\infty(\Gamma_r)} \|\bar y - \hat y\|_{L^4(\Gamma_r)} \le c \, \|\theta \, y + r_S^{(1)}\|_{L^4(\Gamma_r)},$$

since $\bar y$ and $\hat y$ are bounded in V^∞ as mentioned before. With $\theta \le 1$, inserting this into (6.21) yields

$$\begin{aligned}\|(|\bar y|^3 - |\hat y|^3)(G^*\hat p)\|_{L^2(\Gamma_r)} &\le c \, \|y\|_{L^4(\Gamma_r)} + \|r_S^{(1)}\|_{L^4(\Gamma_r)} \\ &\le c \, \big(1 + \psi(\|h\|_{L^2(\Omega_s)})\big) \|h\|_{L^2(\Omega_s)} = \psi(\|h\|_{L^2(\Omega_s)})\end{aligned} \tag{6.22}$$

thanks to (6.15) and (6.12). Analogously, $\|\varepsilon\sigma(|\bar y|^3 - |\hat y|^3)\hat p\|_{L^2(\Gamma_0)}$ is estimated. For the remaining part of the inhomogeneity, it follows

$$\begin{aligned}\|\hat y - \bar y\|_{H^1(\Omega_g)} &\le \|y\|_{H^1(\Omega)} + \|r_S^{(1)}\|_{H^1(\Omega)} \\ &\le c \, \|h\|_{L^q(\Omega_s)} + \psi(\|h\|_{L^2(\Omega_s)}) \|h\|_{L^2(\Omega_s)} = \psi(\|h\|_{L^2(\Omega_s)}).\end{aligned} \tag{6.23}$$

Since Lemma 6.2 implies

$$\|\hat p - p\|_{H^1(\Omega)} \le c \, \|g\|_{H^1(\Omega)^*} \le c \, \big(\|\hat y - \bar y\|_{H^1(\Omega_g)} + \|(|\bar y|^3 - |\hat y|^3)(G^*\hat p)\|_{L^2(\Gamma_r)} + \|(|\bar y|^3 - |\hat y|^3) \, \hat p)\|_{L^2(\Gamma_0)}\big),$$

inserting (6.23) together with (6.22) into this estimate gives the assertion. □

6.2. The second derivative of j

Now, we turn to the second derivative of the reduced objective functional. Due to the chain rule, the second derivative is given by

$$j''(\bar u)[h_1 \, , \, h_2] = (\nabla y_1 \, , \, \nabla y_2)_{L^2(\Omega_g)} + (\nabla \bar y - z \, , \, \nabla w)_{L^2(\Omega_g)} + \nu(h_1 \, , \, h_2)_{L^2(\Omega_s)},$$

with $y_i = S'(\bar u)h_i$, $i = 1, 2$, and $w = S''(\bar u)[h_1, h_2]$ defined by (4.10). Now inserting p as test function in the weak formulation of (4.10) and, on the other hand, choosing w as test function in the variational formulation of (4.17) with $(\nabla \bar y - z \, , \, \nabla v)_{L^2(\Omega_g)}$ and then subtracting both equations yield

$$(\nabla \bar y - z \, , \, \nabla w)_{L^2(\Omega_g)} = - 12 \int_{\Gamma_r} (G\sigma \, |\bar y| \bar y \, y_1 \, y_2) p \, \mathrm{d}s - 12 \int_{\Gamma_0} \varepsilon\sigma \, |\bar y| \bar y \, y_1 \, y_2 \, p \, \mathrm{d}s.$$

Hence, one obtains

$$j''(\bar u)[h_1 \, , \, h_2] = (\nabla y_1 \, , \, \nabla y_2)_{L^2(\Omega_g)} + \nu(h_1 \, , \, h_2)_{L^2(\Omega_s)} - 12 \Big(\int_{\Gamma_r} (G\sigma \, |\bar y| \bar y \, y_1 y_2) p \, \mathrm{d}s + \int_{\Gamma_0} \varepsilon\sigma \, |\bar y| \bar y \, y_1 \, y_2 \, p \, \mathrm{d}s \Big). \tag{6.24}$$

Lemma 6.10. *Let the Assumptions* 1–3 *be fulfilled and y be defined by $y = S'(\bar u)h$. Then*

$$\Big| \int_{\Gamma_r} (G\sigma \, |\bar y| \bar y \, y^2) p \, \mathrm{d}s \Big| + \Big| \int_{\Gamma_0} \varepsilon\sigma \, |\bar y| \bar y \, y^2 \, p \, \mathrm{d}s \Big| \le c \, \|h\|^2_{L^q(\Omega_s)}$$

holds true with a positive constant c independent of h and a fixed but arbitrary $q \in [4/3, 2]$.

Proof. The $\Gamma_{\rm r}$-integral is estimated as follows

$$\Big|\int_{\Gamma_{\rm r}} (G\sigma\,|\bar y|\bar y\,y^2)p\,{\rm d}s\Big| \le \|p\|_{L^2(\Gamma_{\rm r})}\,\|G\sigma\,|\bar y|\bar y\,y^2\|_{L^2(\Gamma_{\rm r})}$$
$$\le c\,\|y\|^2_{L^2(\Gamma_{\rm r})} \le c\,\|h\|^2_{L^q(\Omega_{\rm s})}, \tag{6.25}$$

where we used Remark 6.4, (6.18), (6.15), and the boundedness of $\bar y$ in V^∞. Analogously, we obtain for the integral over Γ_0:

$$\Big|\int_{\Gamma_0} \varepsilon\sigma\,|\bar y|\bar y\,y^2\,p\,{\rm d}s\,\Big| \le c\,\|h\|^2_{L^q(\Omega_{\rm s})}.$$

Together with (6.25), this yields the assertion. □

Based on the previous results, we are now able to show the desired property of the second order remainder term of j. We recall the Taylor expansion of j given by

$$j(\bar u + h) = j(\bar u) + j'(\bar u)\,h + \frac{1}{2}\,j''(\bar u)\,h^2 + r_j^{(2)}, \tag{6.26}$$

where the remainder term fulfills (5.5) since j is twice Fréchet differentiable from $L^2(\Omega_{\rm s})$ to $\mathbb{R}$. Using the results of Section 6.1, we show the following lemma that includes (5.5) as a special case.

Lemma 6.11. *Let Assumptions* 1–3 *be fulfilled and q be given according to Definition* 5.3*, i.e.* $q \ge 4/3$*. Then, the remainder term* $r_j^{(2)}$ *satisfies*

$$\frac{|r_j^{(2)}|}{\|h\|^2_{L^q(\Omega_{\rm s})}} \to 0 \tag{6.27}$$

for all h with $\bar u + h \in U_{ad}$ *and* $\|h\|_{L^2(\Omega_{\rm s})} \to 0$.

Proof. This rather technical essentially benefits from the fact that the control appears only linearly in the state equation and quadratically in the objective functional. Consequently, it vanishes in the expression for the remainder term $r_j^{(2)}$ as we will see below. Thus, $r_j^{(2)}$ only depends on the solutions of the state equation, its linearization and the adjoint equation. Consequently, one can employ the smoothing properties of the respective PDE solution operators to estimate $r_j^{(2)}$, especially Lemmas 6.6 and 6.8 of the previous section. First, we prove the assertion for $4/3 \le q \le 2$. At the end we show, that (6.27) also holds for every $q \ge 2$.

(i) Taylor expansion of j:
With (6.26) at hand, one obtains for $r_j^{(2)}$

$$\begin{aligned} r_j^{(2)} &= j(\bar u + h) - j(\bar u) - j'(\bar u)h - \frac{1}{2}j''(\bar u)h^2 \\ &= \int_0^1 j'(\bar u + \beta\,h)h\,{\rm d}\beta - j'(\bar u)h - \frac{1}{2}j''(\bar u)h^2 \\ &= \int_0^1\int_0^\beta \big(j''(\bar u + \theta\,h)h^2 - j''(\bar u)h^2\big)\,{\rm d}\theta\,{\rm d}\beta = \int_0^1\int_0^\beta \rho_j\,{\rm d}\theta\,{\rm d}\beta. \end{aligned} \tag{6.28}$$

with $\rho_j := j''(\bar u + \theta\, h)h^2 - j''(\bar u)h^2$. Notice that $j'(\bar u + \beta\, h)$ and $j''(\bar u + \theta\, h)$ are well defined thanks to the chain rule and Remark 4.3. Inserting (6.24) in the definition of ρ_j yields

$$\begin{aligned}\rho_j =& \|\nabla\eta\|^2_{L^2(\Omega_g)} - \|\nabla y\|^2_{L^2(\Omega_g)}\\ &- 12\int_{\Gamma_r} (G\sigma\,|\hat y|\hat y\,\eta^2)\hat p\,\mathrm{d}s + 12\int_{\Gamma_r} (G\sigma\,|\bar y|\bar y\,y^2)p\,\mathrm{d}s\\ &- 12\int_{\Gamma_0} \varepsilon\sigma\,|\hat y|\hat y\,\eta^2\,\hat p\,\mathrm{d}s + 12\int_{\Gamma_0} \varepsilon\sigma\,|\bar y|\bar y\,y^2\,p\,\mathrm{d}s,\end{aligned} \tag{6.29}$$

where $\hat y$, $\hat p$, y, and η are defined as in Section 6.1, *i.e.* in particular $\hat y = S(\hat u) = S(u + \theta\, h)$ and $\eta = S'(u + \theta\, h)h$. Notice that, as indicated above, h does not directly appear in (6.29). Hence, ρ_j only depends on "smooth" PDE solutions. Straightforward computation shows that the first addend in (6.29) can be expressed as

$$\|\nabla\eta\|^2_{L^2(\Omega_g)} - \|\nabla y\|^2_{L^2(\Omega_g)} = J''(\hat y,\hat u)(\eta,h)^2 - J''(\bar y,\bar u)(y,h)^2 =: \rho_J.$$

(ii) Estimation of ρ_J:
With (6.14) and $\theta \le 1$, we find for ρ_J

$$\begin{aligned}|\rho_J| &= \big|\,\|\nabla\eta\|^2_{L^2(\Omega_g)} - \|\nabla y\|^2_{L^2(\Omega_g)}\big| \le \big|\,\|\eta\|^2_{H^1(\Omega)} - \|y\|^2_{H^1(\Omega)}\big|\\ &\le \big|\,\|y + \theta\, w + \tilde r^{(2)}_S\|^2_{H^1(\Omega)} - \|y\|^2_{H^1(\Omega)}\big|\\ &\le 2\,\|w\|_{H^1(\Omega)}\|y\|_{H^1(\Omega)} + 2\,\|\tilde r^{(2)}_S\|_{H^1(\Omega)}\|y\|_{H^1(\Omega)}\\ &\quad + 2\,\|w\|_{H^1(\Omega)}\|\tilde r^{(2)}_S\|_{H^1(\Omega)} + \|\tilde r^{(2)}_S\|^2_{H^1(\Omega)} + \|w\|^2_{H^1(\Omega)},\end{aligned} \tag{6.30}$$

where Lemma 6.5 holds for $\|\tilde r^{(2)}_S\|_{H^1(\Omega)}$. Moreover, Lemmas 6.6 and 6.8 give

$$\|y\|_{H^1(\Omega)} \le c\,\|h\|_{L^q(\Omega_s)} \quad\text{and}\quad \|w\|_{H^1(\Omega)} \le c\,\|h\|^2_{L^q(\Omega_s)}.$$

Therefore, (6.30) results in

$$|\rho_J| \le \psi(\|h\|_{L^2(\Omega_s)})\,\|h\|^2_{L^q(\Omega_s)}, \tag{6.31}$$

where $\psi : \mathbb{R} \to \mathbb{R}$ again denotes a generic function with $\psi(x) \to 0$ for every $x \downarrow 0$. Notice that the assumption $q \le\ 2$ implies $\|h\|_{L^q(\Omega_s)} \le c\,\|h\|_{L^2(\Omega_s)}$. This is used for instance in the estimate $\|w\|_{H^1(\Omega)} \le \varphi(\|h\|_{L^2(\Omega_s)})\,\|h\|_{L^q(\Omega_s)}$.

(iii) Estimation of the boundary integrals:
Next, we estimate the difference of the integrals over Γ_r in (6.29):

$$\begin{aligned}&\Big|\int_{\Gamma_r} (G\sigma\,|\hat y|\hat y\,\eta^2)\hat p\,\mathrm{d}s - \int_{\Gamma_r} (G\sigma\,|\bar y|\bar y\,y^2)p\,\mathrm{d}s\Big|\\ &\qquad\le \Big|\int_{\Gamma_r} \big(G\sigma\,(|\hat y|\hat y\,\eta^2 - |\bar y|\bar y\,y^2)\big)\hat p\,\mathrm{d}s\Big| + \Big|\int_{\Gamma_r} (G\sigma\,|\bar y|\bar y\,y^2)(\hat p - p)\,\mathrm{d}s\Big| =: J_1 + J_2.\end{aligned} \tag{6.32}$$

Together with (6.18), Lemma 6.6 and 6.9 yield for the second addend

$$\begin{aligned} J_2 &\leq \|G\sigma|\bar{y}|\bar{y}\, y^2\|_{L^2(\Gamma_r)}\, \|\hat{p}-p\|_{L^2(\Gamma_r)} \\ &\leq \sigma\, \|G\|_{\mathcal{L}(L^2(\Gamma_r))}\, \|\bar{y}\|^2_{L^\infty(\Gamma_r)} \|y^2\|_{L^2(\Gamma_r)}\, \|\hat{p}-p\|_{H^1(\Omega)} \\ &\leq c\, \psi(\|h\|_{L^2(\Omega_s)})\, \|y\|^2_{H^1(\Omega)} \leq c\, \psi(\|h\|_{L^2(\Omega_s)})\, \|h\|^2_{L^q(\Omega_s)}. \end{aligned} \tag{6.33}$$

Notice that the additional assumption in Lemma 6.9, *i.e.* $\hat{u} \in B_\rho(\bar{u})$ with sufficiently small ρ, is automatically fulfilled if $\|h\|_{L^2(\Omega_s)}$ tends to zero. Using the Taylor expansion (6.14), the first addend is transformed into

$$J_1 = \Big| \int_{\Gamma_r} \big(G\sigma\, (|\hat{y}|\hat{y}\, (y + \theta\, w + \tilde{r}_S^{(2)})^2 - |\bar{y}|\bar{y}\, y^2)\big) \hat{p}\, \mathrm{d}s \Big| \leq I_1 + I_2$$

with

$$I_1 := \Big| \int_{\Gamma_r} \sigma\, (|\hat{y}|\hat{y} - |\bar{y}|\bar{y}) y^2\, (G^*\hat{p})\, \mathrm{d}s \Big|$$

and

$$I_2 := \Big| \int_{\Gamma_r} \sigma\, |\hat{y}|\hat{y}\, (G^*\hat{p})\, \big(2\theta\, y\, w + 2\, \tilde{r}_S^{(2)}\, y + 2\theta\, w\, \tilde{r}_S^{(2)} + (\tilde{r}_S^{(2)})^2 + \theta^2\, w^2\big)\, \mathrm{d}s \Big|.$$

We continue with

$$\begin{aligned} I_1 &\leq \sigma\, \|y^2\|_{L^2(\Gamma_r)}\, \|(|\hat{y}_h|\hat{y} - |\bar{y}|\bar{y})\, G^*\hat{p}\|_{L^2(\Gamma_r)} \\ &\leq \sigma\, \|y^2\|_{L^2(\Gamma_r)}\, \|G^*\|_{\mathcal{L}(L^4(\Gamma_r))}\, \|\hat{p}\|_{L^4(\Gamma_r)} \|\, |\hat{y}|\hat{y} - |\bar{y}|\bar{y}\, \|_{L^4(\Gamma_r)}, \end{aligned} \tag{6.34}$$

where we used (6.18) for the last inequality. Now, we argue similarly to the derivation of (6.22): thanks to $\bar{u}, \hat{u} \in U_{ad}$, the maximum principle in Theorem 3.6 implies $\bar{y}, \hat{y} \geq \vartheta > 0$. Thus, together with the Taylor expansion (6.11)

$$|\hat{y}|\hat{y} - |\bar{y}|\bar{y} = \hat{y}^2 - \bar{y}^2 = (\hat{y}+\bar{y})(\hat{y}-\bar{y}) = (\hat{y}+\bar{y})(\theta\, y + r_S^{(1)})$$

holds true. Hence, Lemma 6.6 and (6.12) yield

$$\begin{aligned} \|\, |\hat{y}|\hat{y} - |\bar{y}|\bar{y}\, \|_{L^4(\Gamma_r)} &\leq \|\hat{y}+\bar{y}\|_{L^\infty(\Gamma_r)}\, (\|y\|_{L^4(\Gamma_r)} + \|r_S^{(1)}\|_{L^4(\Gamma_r)}) \\ &\leq c\, (1 + \psi(\|h\|_{L^2(\Omega_s)}))\|h\|_{L^2(\Omega_s)} = \psi(\|h\|_{L^2(\Omega_s)}). \end{aligned}$$

Therefore, by applying Lemma 6.6 to $\|y\|^2_{L^2(\Gamma_r)}$ and Lemma 6.3 to $\|\hat{p}\|_{L^4(\Gamma_r)}$, (6.34) results in

$$I_1 \leq \psi(\|h\|_{L^2(\Omega_s)})\, \|h\|^2_{L^q(\Omega_s)}. \tag{6.35}$$

Using again (6.18) and Lemma 6.3, the integral I_2 is estimated as follows:

$$\begin{aligned}
I_2 &\leq \|\sigma\,|\hat{y}|\hat{y}\,G^*\,\hat{p}\|_{L^2(\Gamma_\mathrm{r})}\big(2\|yw\|_{L^2(\Gamma_\mathrm{r})}+2\|\tilde{r}_S^{(2)}y\|_{L^2(\Gamma_\mathrm{r})}+2\|w\tilde{r}_S^{(2)}\|_{L^2(\Gamma_\mathrm{r})}\\
&\qquad\qquad+\|(\tilde{r}_S^{(2)})^2\|_{L^2(\Gamma_\mathrm{r})}+\|w^2\|_{L^2(\Gamma_\mathrm{r})}\big)\\
&\leq \sigma\|\hat{y}\|^2_{L^\infty(\Omega_\mathrm{s})}\|G^*\|_{\mathcal{L}(L^2(\Gamma_\mathrm{r}))}\|\hat{p}\|_{L^2(\Gamma_\mathrm{r})}\\
&\quad\big(2\,\|w\|_{L^4(\Gamma_\mathrm{r})}\|y\|_{L^4(\Gamma_\mathrm{r})}+2\,\|\tilde{r}_S^{(2)}\|_{L^4(\Gamma_\mathrm{r})}\|y\|_{L^4(\Gamma_\mathrm{r})}+2\,\|w\|_{L^4(\Gamma_\mathrm{r})}\|\tilde{r}_S^{(2)}\|_{L^4(\Gamma_\mathrm{r})}\\
&\quad+\|\tilde{r}_S^{(2)}\|^2_{L^4(\Gamma_\mathrm{r})}+\|w\|^2_{L^4(\Gamma_\mathrm{r})}\big)\\
&\leq c\,\big(2\,\|w\|_{H^1(\Omega)}\|y\|_{H^1(\Omega)}+2\,\|\tilde{r}_S^{(2)}\|_{H^1(\Omega)}\|y\|_{H^1(\Omega)}+2\,\|w\|_{H^1(\Omega)}\|\tilde{r}_S^{(2)}\|_{H^1(\Omega)}\\
&\qquad+\|\tilde{r}_S^{(2)}\|^2_{H^1(\Omega)}+\|w\|^2_{H^1(\Omega)}\big).
\end{aligned}$$

The expression on the right-hand side in the last inequality is the same as in (6.30). Hence, we argue as before and obtain

$$I_2 \leq \psi(\|h\|_{L^2(\Omega_\mathrm{s})})\,\|h\|^2_{L^q(\Omega_\mathrm{s})}.$$

Together with (6.35), this implies $J_1 \leq \psi(\|h\|_{L^2(\Omega_\mathrm{s})})\,\|h\|^2_{L^q(\Omega_\mathrm{s})}$. If we insert this and (6.33) in (6.32), then

$$\Big|\int_{\Gamma_\mathrm{r}}(G\sigma\,|\hat{y}|\hat{y}\,\eta^2)\hat{p}\,\mathrm{d}s-\int_{\Gamma_\mathrm{r}}(G\sigma\,|\bar{y}|\bar{y}\,y^2)p\,\mathrm{d}s\Big| \leq \psi(\|h\|_{L^2(\Omega_\mathrm{s})})\,\|h\|^2_{L^q(\Omega_\mathrm{s})} \tag{6.36}$$

is obtained. An analogous discussion for the difference of the integrals over Γ_0 in (6.29) gives

$$\Big|\int_{\Gamma_0}(\varepsilon\sigma\,|\hat{y}|\hat{y}\,\eta^2)\hat{p}\,\mathrm{d}s-\int_{\Gamma_0}(\varepsilon\sigma\,|\bar{y}|\bar{y}\,y^2)p\,\mathrm{d}s\Big| \leq \psi(\|h\|_{L^2(\Omega_\mathrm{s})})\,\|h\|^2_{L^q(\Omega_\mathrm{s})}.$$

Hence, by inserting this estimate together with (6.36) and (6.31) in (6.29), we end up with

$$|\rho_j| \leq \psi(\|h\|_{L^2(\Omega_\mathrm{s})})\,\|h\|^2_{L^q(\Omega_\mathrm{s})}.$$

For the remainder term $r_j^{(2)}$, we finally obtain

$$\begin{aligned}
\Big|r_j^{(2)}\Big| &\leq \int_0^1\int_0^\beta|\rho_j|\,\mathrm{d}\theta\,\mathrm{d}\beta \leq \psi(\|h\|_{L^2(\Omega_\mathrm{s})})\,\|h\|^2_{L^q(\Omega_\mathrm{s})}\int_0^1\int_0^\beta\mathrm{d}\theta\,\mathrm{d}\beta\\
&\leq \psi(\|h\|_{L^2(\Omega_\mathrm{s})})\,\|h\|^2_{L^q(\Omega_\mathrm{s})},
\end{aligned} \tag{6.37}$$

with $4/3 \leq q \leq 2$. Due to $\|h\|^2_{L^q(\Omega_\mathrm{s})} \leq c\,\|h\|^2_{L^r(\Omega_\mathrm{s})}$ for every $r \geq q$, (6.37) clearly holds for every $q \geq 4/3$. □

Remark 6.12. As already indicated in Remark 6.7, if we assume that $t \geq 6$, *i.e.* $u_a, u_b \in L^6(\Omega_\mathrm{s})$, then Lemma 6.11 would also hold for $6/5 \leq q < 4/3$. However, in view of the interpolation inequality (7.8), it is meaningless to consider the case $q \in [6/5, 4/3)$ here.

7. Proof of Theorem 5.5

With the results of Section 6 at hand, it is straightforward to apply the theory developed by Casas, Tröltzsch, and Unger in [4] to proof the main result. For convenience of the reader, we present the rather technical arguments. As in the proof of Theorem 5.1, we start with the Taylor expansion of the reduced objective functional

$$j(u) = j(\bar{u}) + j'(\bar{u})(u-\bar{u}) + \frac{1}{2}\,j''(\bar{u})(u-\bar{u})^2 + r_j^{(2)} \tag{7.1}$$

with $u \in U_{ad}$.

(i) Estimation of the first derivative $j'(\bar{u})(u-\bar{u})$
A pointwise evaluation of the necessary conditions in (4.20) yields

$$j'(\bar{u})(x)\big(u(x)-\bar{u}(x)\big) = \big(p(x)+\nu\bar{u}(x)\big)\big(u(x)-\bar{u}(x)\big) \geq 0 \quad \textit{a.e.} \text{ in } \Omega_{\mathrm{s}}, \quad \forall\, u \in U_{ad}.$$

This implies $(p(x)+\nu\bar{u}(x))(u(x)-\bar{u}(x)) = |p(x)+\nu\bar{u}(x)|\,|u(x)-\bar{u}(x)|$. Hence, with Definition 5.2, we obtain for the first derivative of j

$$\begin{aligned} j'(\bar{u})(u-\bar{u}) &= \int_{A_\tau} \big|p(x)+\nu\bar{u}(x)\big|\big|u(x)-\bar{u}(x)\big|\,\mathrm{d}x + \int_{\Omega_{\mathrm{s}}\setminus A_\tau} \big|p(x)+\nu\bar{u}(x)\big|\big|u(x)-\bar{u}(x)\big|\,\mathrm{d}x \\ &\geq \int_{A_\tau} \tau|u(x)-\bar{u}(x)|\,\mathrm{d}x = \tau\,\|u-\bar{u}\|_{L^1(A_\tau)}. \end{aligned} \tag{7.2}$$

(ii) Estimation of the second derivative $j''(\bar{u})(u-\bar{u})^2$
Let $\tilde{u}$ be defined by

$$\tilde{u}(x) = \begin{cases} \bar{u}(x), & \text{for } x \in A_\tau \\ u(x), & \text{for } x \notin A_\tau, \end{cases}$$

and thus $(\tilde{u}-\bar{u}) \in C_\tau(\bar{u})$, thanks to Definition 5.4. We continue with

$$\begin{aligned} j''(\bar{u})(u-\bar{u})^2 &= j''(u-\tilde{u}+\tilde{u}-\bar{u}) \\ &= j''(\bar{u})(u-\tilde{u})^2 + 2\,j''(\bar{u})[u-\tilde{u},\tilde{u}-\bar{u}] + j''(\bar{u})(\tilde{u}-\bar{u})^2. \end{aligned} \tag{7.3}$$

In the following, we estimate the three addends on the right-hand side of (7.3) separately. To that end, define $y = S'(\bar{u})u$ and $\tilde{y} = S'(\bar{u})\tilde{u}$. Then, with (6.24) and Lemma 6.10, one obtains

$$\begin{aligned} j''(\bar{u})(u-\tilde{u})^2 &= \|\nabla(y-\tilde{y})\|_{L^2(\Omega_{\mathrm{g}})} + \nu\|u-\tilde{u}\|_{L^2(\Omega_{\mathrm{s}})} \\ &\quad - 12\int_{\Gamma_{\mathrm{r}}} G\big(\sigma\,|\bar{y}|\bar{y}\,(y-\tilde{y})^2\big)p\,\mathrm{d}s - 12\int_{\Gamma_0} \varepsilon\sigma\,|\bar{y}|\bar{y}\,(y-\tilde{y})^2\,p\,\mathrm{d}s \\ &\geq -12\Big|\int_{\Gamma_{\mathrm{r}}} G\big(\sigma\,|\bar{y}|\bar{y}\,(y-\tilde{y})^2\big)p\,\mathrm{d}s + \int_{\Gamma_0} \varepsilon\sigma\,|\bar{y}|\bar{y}\,(y-\tilde{y})^2\,p\,\mathrm{d}s)\Big| \\ &\geq -c_1\,\|u-\tilde{u}\|^2_{L^q(\Omega_{\mathrm{s}})}, \end{aligned} \tag{7.4}$$

where c_1 denotes a positive generic constant. Moreover, here and in the following, q is as before given by Definition 5.3 such that $q \in [4/3, 2]$. The second addend is transformed into

$$\begin{aligned} j''(\bar{u})[u-\tilde{u},\tilde{u}-\bar{u}] &= \big(\nabla(y-\tilde{y})\,,\,\nabla(\tilde{y}-\eta)\big)_{L^2(\Omega_{\mathrm{g}})} + \nu\big(u-\tilde{u}\,,\,\tilde{u}-\bar{u}\big)_{L^2(\Omega_{\mathrm{s}})} \\ &\quad -12\int_{\Gamma_{\mathrm{r}}} G\big(\sigma\,|\bar{y}|\bar{y}\,(y-\tilde{y})\,(\tilde{y}-\eta)\big)p\,\mathrm{d}s - 12\int_{\Gamma_0} \varepsilon\sigma\,|\bar{y}|\bar{y}\,(y-\tilde{y})\,(\tilde{y}-\eta)\,p\,\mathrm{d}s, \end{aligned}$$

where y and $\tilde{y}$ are defined as above and η is given by $\eta = S'(\bar{u})\bar{u}$. By the definition of $\tilde{u}$, we have $(\tilde{u}-\bar{u})(x) = 0$, if $x \in A_\tau$, and $(u-\tilde{u})(x) = 0$, if $x \in \Omega_s \backslash A_\tau$, and hence $(u-\tilde{u}\,,\,\tilde{u}-\bar{u})_{L^2(\Omega_s)} = 0$. Moreover, Lemma 6.6 implies

$$-\big|\big(\nabla(y-\tilde{y})\,,\,\nabla(\tilde{y}-\eta)\big)_{L^2(\Omega_g)}\big| \geq -\|y-\tilde{y}\|_{H^1(\Omega)}\,\|\tilde{y}-\eta\|_{H^1(\Omega)} \\ \geq -c\,\|u-\tilde{u}\|_{L^q(\Omega_s)}\,\|\tilde{u}-\bar{u}\|_{L^q(\Omega_s)}.$$

The boundary integrals are again estimated with Lemma 6.10, and hence it follows that

$$j''(\bar{u})[u-\tilde{u},\tilde{u}-\bar{u}] \geq -c_2\,\|u-\tilde{u}\|_{L^q(\Omega_s)}\,\|\tilde{u}-\bar{u}\|_{L^q(\Omega_s)}$$

with a positive generic constant c_2. Due to $(\tilde{u}-\bar{u}) \in C_\tau(\bar{u})$, condition (SSC) yields for the last addend in (7.3)

$$j''(\bar{u})(\tilde{u}-\bar{u})^2 \geq \delta\,\|\tilde{u}-\bar{u}\|^2_{L^q(\Omega_s)}. \tag{7.5}$$

In view of

$$\|u-\bar{u}\|^2_{L^q(\Omega_s)} = \|u-\tilde{u}+\tilde{u}-\bar{u}\|^2_{L^q(\Omega_s)} \\ \leq \|u-\tilde{u}\|^2_{L^q(\Omega_s)} + 2\,\|u-\tilde{u}\|_{L^q(\Omega_s)}\,\|\tilde{u}-\bar{u}\|_{L^q(\Omega_s)} + \|\tilde{u}-\bar{u}\|^2_{L^q(\Omega_s)},$$

this, together with (7.4) and (7.5), implies

$$j''(\bar{u})(u-\bar{u})^2 \geq \delta\,\|u-\bar{u}\|^2_{L^q(\Omega_s)} - (\delta+c_1)\,\|u-\tilde{u}\|^2_{L^q(\Omega_s)} \\ -(2\delta+c_2)\,\|u-\tilde{u}\|_{L^q(\Omega_s)}\,\|\tilde{u}-\bar{u}\|_{L^q(\Omega_s)}.$$

By applying Young's inequality, we obtain

$$j''(\bar{u})(u-\bar{u})^2 \geq \delta\,\|u-\bar{u}\|^2_{L^q(\Omega_s)} - \left(\delta + c_1 + \frac{2\delta+c_2}{\kappa}\right)\|u-\bar{u}\|^2_{L^q(A_\tau)} - (2\delta+c_2)\kappa\,\|u-\bar{u}\|^2_{L^q(\Omega_s)}, \tag{7.6}$$

with an arbitrary $\kappa > 0$. Here, we used that

$$\|u-\tilde{u}\|_{L^q(\Omega_s)} = \|u-\bar{u}\|_{L^q(A_\tau)}$$

and

$$\|\tilde{u}-\bar{u}\|_{L^q(\Omega_s)} = \|u-\bar{u}\|_{L^q(\Omega\backslash A_\tau)} \leq \|u-\bar{u}\|_{L^q(\Omega_s)}$$

hold true thanks to the definition of $\tilde{u}$.

(iii) The quadratic growth condition

Next, we insert (7.2) and (7.6) in the Taylor expansion (7.1) and obtain

$$j(u) \geq j(\bar{u}) + \tau\,\|u-\bar{u}\|_{L^1(A_\tau)} - \frac{1}{2}\left(\delta + c_1 + \frac{2\delta+c_2}{\kappa}\right)\|u-\bar{u}\|^2_{L^q(A_\tau)} \\ + \frac{1}{2}\left(\delta - (2\delta+c_2)\kappa - 2\,\frac{|r_j^{(2)}|}{\|u-\bar{u}\|^2_{L^q(\Omega_s)}}\right)\|u-\bar{u}\|^2_{L^q(\Omega_s)}. \tag{7.7}$$

The well-known interpolation inequality (*cf.* Brezis [2]) implies

$$\|u-\bar{u}\|^2_{L^q(A_\tau)} \leq \|u-\bar{u}\|_{L^1(A_\tau)}\|u-\bar{u}\|_{L^s(A_\tau)} \\ \leq \|u-\bar{u}\|_{L^1(A_\tau)}\|u-\bar{u}\|_{L^s(\Omega_s)}, \tag{7.8}$$

with s and q according to Definition 5.3. Then (7.7) results in

$$j(u) \geq j(\bar{u}) + a_1 \, \|u - \bar{u}\|_{L^1(A_\tau)} + \frac{1}{2} \, a_2 \, \|u - \bar{u}\|^2_{L^q(\Omega_s)}, \tag{7.9}$$

with

$$a_1 = \tau - \frac{1}{2} \left(\delta + c_1 + \frac{2\delta + c_2}{\kappa} \right) \|u - \bar{u}\|_{L^s(\Omega_s)}$$

and

$$a_2 = \delta - (2\delta + c_2)\kappa - 2 \, \frac{|r_j^{(2)}|}{\|u - \bar{u}\|^2_{L^q(\Omega_s)}} \cdot$$

To derive the quadratic growth condition (5.9), we show that a_1 and a_2 are non negative, if $\|u - \bar{u}\|_{L^s(\Omega_s)}$ is sufficiently small. We start with a_2 and define $\varepsilon_r := |r_j^{(2)}| / \|u - \bar{u}\|^2_{L^q(\Omega_s)}$. Due to Lemma 6.11, *i.e.* the property of the second-order remainder term, ε_r tends to zero if $\varepsilon_1 := \|u - \bar{u}\|_{L^2(\Omega_s)}$ is chosen sufficiently small. Therefore, if we also set κ sufficiently small, there exists a constant $\bar{\sigma}$ such that

$$a_2 = \delta - (2\delta + c_2)\kappa - 2 \, \varepsilon_r \geq 2 \, \bar{\sigma} > 0. \tag{7.10}$$

Furthermore, a_1 is non negative, if $\varepsilon_2 := \|u - \bar{u}\|_{L^s(\Omega_s)}$ is sufficiently small, *i.e.*

$$\varepsilon_2 \leq \frac{2 \, \tau}{\delta + c_1 + (2\delta + c_2)/\kappa} \cdot$$

By assumption, we have $s \geq 2$ and therefore,

$$\|u - \bar{u}\|_{L^2(\Omega_s)} \leq c_s \, \|u - \bar{u}\|_{L^s(\Omega_s)} \leq c_s \, \varepsilon_2$$

follows. Thus, if we set $\bar{\varepsilon} = \min\{\varepsilon_2 \, ; \, \varepsilon_1 / c_s\}$, then (7.10) is satisfied and a_1 is non negative. Therefore, for every $u \in U_{ad}$ with $\|u - \bar{u}\|_{L^s(\Omega_s)} \leq \bar{\varepsilon}$,

$$j(u) \geq j(\bar{u}) + \frac{1}{2} \, (\delta - (2\delta + c)\kappa - 2 \, \varepsilon_r) \, \|u - \bar{u}\|^2_{L^q(\Omega_s)} \geq j(\bar{u}) + \bar{\sigma} \, \|u - \bar{u}\|^2_{L^q(\Omega_s)}$$

holds true. □

Remark 7.1. The analysis, presented above, is mainly based on the fact that the control only appears linearly in the state equation and quadratically in the objective functional. According to this, it is easy to see that the presented theory also holds for a general class of semilinear elliptic control problems, namely

$$(\mathrm{P}) \quad \begin{cases} \text{minimize} & J(y,u) = \displaystyle\int_\Omega f_\Omega(y, \nabla y) \, \mathrm{d}x + \int_\Gamma f_\Gamma(y) \, \mathrm{d}s + \frac{\nu}{2} \int_\Omega u^2 \, \mathrm{d}x \\ \text{subject to} & A \, y(x) + d(x, y(x)) = u(x) + g_\Omega(x) \quad \text{in } \Omega \\ & \dfrac{\partial y}{\partial n} + b(x, y(x)) = g_\Gamma(x) \qquad \text{on } \Gamma \\ \text{and} & u_a \leq u(x) \leq u_b \quad \textit{a.e.} \text{ in } \Omega, \end{cases}$$

with functions f_Ω and f_Γ of class $C^{2,1}$. Furthermore, it has to be verified that the state equation admits a solution in $H^1(\Omega) \cap L^\infty(\Omega)$ and that the corresponding linearized equation admits solutions in $H^1(\Omega)$ for inhomogeneities in $H^1(\Omega)^*$. This is for instance the case if A is a second order elliptic operator with coefficients in $L^\infty(\Omega)$, d and b are of class $C^{2,1}$ with respect to both arguments and monotone increasing with respect to the second variable, and g_Ω and g_Γ are given functions in $L^2(\Omega)$ and $L^4(\Gamma)$, respectively. Finally, for u_a and u_b, one has to assume $u_a, u_b \in L^t(\Omega)$ as required in Assumption 2.

References

[1] J. Bonnans, Second order analysis for control constrained optimal control problems of semilinear elliptic systems. *Appl. Math. Optim.* **38** (1998) 303–325.

[2] H. Brezis, *Analyse fonctionelle.* Masson, Paris (1983).

[3] E. Casas and M. Mateos, Second order sufficient optimality conditions for semilinear elliptic control problems with finitely many state constraints. *SIAM J. Control Optim.* **40** (2002) 1431–1454.

[4] E. Casas, F. Tröltzsch and A. Unger, Second order sufficient optimality conditions for a nonlinear elliptic control problem. *J. Anal. Appl.* **15** (1996) 687–707.

[5] A.L. Dontchev, W.W. Hager, A.B. Poore and B. Yang, Optimality, stability, and convergence in optimal control. *Appl. Math. Optim.* **31** (1995) 297–326.

[6] O. Klein, P. Philip and J. Sprekels, Modeling and simulation of sublimation growth of SiC bulk single crystals. *Interfaces Free Boundaries* **6** (2004) 295–314.

[7] M. Laitinen and T. Tiihonen, Conductive-radiative heat transfer in grey materials. *Quart. Appl. Math.* **59** (2001) 737–768.

[8] C. Meyer, P. Philip, and F. Tröltzsch, Optimal control of a semilinear PDE with nonlocal radiation interface conditions. *SIAM J. Control Optim.* **45** (2006) 699–721.

[9] H.-J. Rost, D. Siche, J. Dolle, W. Eiserbeck, T. Müller, D. Schulz, G. Wagner and J. Wollweber, Influence of different growth parameters and related conditions on 6H-SiC crystals grown by the modified Lely method. *Mater. Sci. Eng. B* **61-62** (1999) 68–72.

[10] T. Tiihonen, A nonlocal problem arising from heat radiation on non-convex surfaces. *Eur. J. App. Math.* **8** (1997) 403–416.

[11] T. Tiihonen, Stefan-Boltzmann radiation on non-convex surfaces. *Math. Meth. Appl. Sci.* **20** (1997) 47–57.

[12] F. Tröltzsch and D. Wachsmuth, Second-order sufficient optimality conditions for the optimal control of Navier-Stokes equations. *ESAIM: COCV* **12** (2006) 93–119.