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State-constrained optimal control of semilinear elliptic equations with nonlocal radiation interface conditions

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Abstract

We consider a control- and state-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. The nonlocal radiation interface condition and the pointwise state-constraints represent the particular features of this problem. To deal with the state-constraints, continuity of the state is shown which allows to derive first-order necessary conditions. Afterwards, we establish second-order sufficient conditions that account for strongly active sets and ensure local optimality in an L^2 -neighborhood.

1 Introduction

In this paper, an optimal control problem is investigated that arises from the sublimation growth of semiconductor single crystals such as silicon carbide (SiC) or aluminum nitrite (AlN). To be more precise, the physical vapor transport (PVT) method is considered, where 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 singlecrystalline seed located at the cooled top of the cavity, such that the desired single crystal grows into the reaction chamber (see [11, 16] for more details). Here, we focus on the control of the conductive-radiative heat transfer in the reaction chamber, which is denoted by Ω_g . More precisely, we aim at optimizing the temperature gradient in Ω_g by directly controlling the heat source u in $\Omega_s := \Omega \setminus \Omega_g$, where Ω denotes the domain of the entire crucible including the gas phase. Thus, the objective functional, considered here, reads as follows:

(P) minimize
$$J(u, y) := \frac{1}{2} \int_{\Omega_g} |\nabla y - z|^2 dx + \frac{\beta}{2} \int_{\Omega_s} u^2 dx$$
,

where y denotes the temperature, z is the desired temperature gradient, and β is a given positive real number. Because of the high temperatures, it is essential to account for radiation on the outer boundary $\Gamma_0 := \partial \Omega$ and on the interface $\Gamma_r := \overline{\Omega}_s \cap \overline{\Omega}_g$. Thus, y is given by the solution of the stationary heat equation with radiation interface and boundary conditions on Γ_r and Γ_0 , respectively:

(SL)
$$\begin{cases} -\operatorname{div}(\kappa_s \nabla y) = u & \text{in } \Omega_s \\ -\operatorname{div}(\kappa_g \nabla y) = 0 & \text{in } \Omega_g \end{cases}$$
$$\kappa_g \left(\frac{\partial y}{\partial n_r}\right)_g - \kappa_s \left(\frac{\partial y}{\partial n_r}\right)_s = q_r & \text{on } \Gamma_r \\ \kappa_s \frac{\partial y}{\partial n_0} + \varepsilon \sigma |y|^3 y = \varepsilon \sigma y_0^4 & \text{on } \Gamma_0, \end{cases}$$

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 . Furthermore, σ represents the Boltzmann radiation constant, ε is the emissivity, and κ_s , κ_g denote the thermal conductivities in Ω_s , Ω_g , respectively. Moreover, q_r denotes the additional radiative heat flux on Γ_r which is discussed in more details in Section 1.2. In addition to the stationary semilinear heat equation, the optimization is subject to the following pointwise state- and control-constraints:

(1.1)
$$\begin{array}{rcl} u_a(x) &\leq u(x) \leq u_b(x) & \text{a.e. in } \Omega_s, \\ y_a(x) &\leq y(x) \leq y_b(x) & \text{a.e. in } \Omega_g, \\ y(x) &\leq y_{\max}(x) & \text{a.e. in } \Omega_s. \end{array}$$

Here, u_a and u_b reflect the minimum and maximum heating power. Furthermore, $y|_{\Omega_s}$ has to be bounded by y_{max} to avoid melting of the solid components of crucible in Ω_s . Finally, the state-constraints in Ω_g are required to ensure sublimation of the polycrystalline powder and crystallization at the seed, respectively.

The pointwise inequality constraints on the state and nonlocal radiation on Γ_r represent the crucial points of the problem. First, pointwise state-constraints are known to be theoretically and numerically difficult to handle since the associated Lagrange multipliers are in general only regular Borel measures, see Casas [5, 6], Alibert and Raymond [2] and Bergounioux and Kunisch [4]. Moreover, due to nonpositivity of G, the nonlinearity in the state equation in (P) is in general not monotone (see for instance [17]) such that standard techniques cannot be applied. The analysis of the purely control-constrained counterpart to (P) is already comparatively comprehensive. Based on the results of Laitinen and Tiihonen [12] for the nonlinear state equation, first-order necessary conditions for this problem are derived by Meyer, Philip, and Tröltzsch in [15]. Moreover, in [14], second-order sufficient conditions are established incorporating a generalized two-norm-discrepancy. However, these results cannot immediately be transferred to problem (P) due to the presence of pointwise state-constraints. Therefore, the inclusion of state-constraints represent the genuine contribution of this paper and requires to significantly extend the analysis of the aforementioned references. First, one has to show the continuity of the solution to (SL) which is performed in Section 2 by means of results on maximum elliptic regularity by Gröger [10] and Elschner et al. [9]. Based on this, a duality argument allows to discuss the adjoint equation involving measures as inhomogeneity (cf. Section 4), which leads to the derivation of first-order conditions in a standard way (see Section 5). Finally, in Section 6, second-order sufficient conditions are established that account for strongly active sets and guarantee local optimality with L^2 -quadratic growth in an L^2 -neighborhood, i.e. the two-norm discrepancy can be avoided. The associated analysis follows the lines of a very recent contribution by Casas et al. [7].

1.1 General Assumptions and Notation

We start now by introducing the general assumptions of the problem statement including the notation used throughout this paper. If X is a linear normed function space, then we use the notation $\|\cdot\|_X$ for a standard norm used in X. Moreover, we set $X^2 := X \times X$. The dual space of X is denoted by X^* , and for the associated duality pairing, we write $\langle ., . \rangle_{X^*,X}$. If it is obvious in which spaces the respective duality pairing is considered, then the subscript is occasionally neglected. Now, given another linear normed space Y, the space of all bounded linear operators from X to Y is called $\mathcal{B}(X, Y)$. For an arbitrary $A \in \mathcal{B}(X, Y)$, the associated adjoint operator is denoted by $A^* \in \mathcal{B}(Y^*, X^*)$, and for its inverse, if it exists, we write $A^{-*} := (A^*)^{-1}$. If X is continuously embedded in Y, we write $X \hookrightarrow Y$. The trace operators on Γ_r and Γ_0 are denoted by τ_r and τ_0 , respectively. Throughout the paper, they are considered with different domains and ranges. For simplicity, the associated operators are always called τ_r and τ_0 and we will mention their respective domains and ranges, if it is important. Furthermore, to improve readability, we sometimes neglect the trace operators in arguments of boundary integrals. The function $\mathbf{1} \in L^{\infty}(\Gamma_0)$ satisfies $\mathbf{1}(x) = 1$ a.e. on Γ_0 , while \mathcal{U} denotes the set of admissible controls with respect to the control constraints, i.e. $\mathcal{U} = \{u \in L^2(\Omega_s) \mid u_a(x) \leq u(x) \leq u_b(x) \text{ a.e. in } \Omega_s\}$. Further, A function $u \in L^2(\Omega_s)$ is called feasible for (P) if it satisfies the inequality constraints in (1.1). Finally, by c we denote a generic positive constant which can take different values on different occasions. Now, concerning the data specified in (P), we impose the following assumptions:

- Assumption 1.1 (\mathcal{A}_1) The domain $\Omega \subset \mathbb{R}^N$, $N \in \{2,3\}$, is a bounded open domain with a Lipschitz boundary Γ_0 . Moreover, $\Omega_g \subset \Omega$ is an open subset of Ω with a boundary $\Gamma_r \subset \Omega$. In two dimensions, Γ_r is assumed to be a closed Lipschitz surface which is piecewise $\mathcal{C}^{1,\delta}$, whereas it is of class C^1 in the three dimensional case. The subdomain Ω_s is defined by $\Omega_s = \Omega \setminus \overline{\Omega}_q$. The distance of Γ_r to Γ_0 is supposed to be positive.
- (\mathcal{A}_2) The desired temperature gradient z is given in $L^2(\Omega_q)^N$ and $\beta > 0$ is a fixed constant.
- (\mathcal{A}_3) The fixed function $\kappa \in L^{\infty}(\Omega)$ in the semilinear equation (SL) is defined by

$$\kappa(x) = \begin{cases} \kappa_s(x) & \text{if } x \in \Omega_s, \\ \kappa_g(x) & \text{if } x \in \Omega_g, \end{cases}$$

where $\kappa_s \in L^{\infty}(\Omega_s)$ and $\kappa_g \in L^{\infty}(\Omega_g)$ representing the thermal conductivity of solid and gas, respectively. Moreover, κ satisfies $\kappa(x) \geq \kappa_{\min}$ a.e. in Ω , with a fixed $\kappa_{\min} \in \mathbb{R}^+ \setminus \{0\}$.

- (\mathcal{A}_4) By $\varepsilon \in L^{\infty}(\Gamma_0 \cup \Gamma_r)$, we denote the emissivity satisfying $0 < \varepsilon_{\min} \leq \varepsilon(x) \leq 1$ a.e. on $\Gamma_r \cup \Gamma_0$. The term σ represents the Boltzmann radiation and is assumed to be a positive real number. The inhomogeneity on the boundary Γ_0 is given by a fixed function $y_0 \in L^{\infty}(\Gamma_0)$ satisfying $y_0(x) \geq \theta > 0$ a.e. on Γ_0 .
- (\mathcal{A}_5) The bounds in the state constraints are $y_{\max}, y_a, y_b \in \mathcal{C}(\overline{\Omega})$ with $y_b(x) > y_a(x) \ge \theta$ for all $x \in \overline{\Omega}_g$, $y_{\max}(x) \ge \theta$ for all $x \in \overline{\Omega}_s$, and $y_{\max}(x) > y_a(x)$ for all $x \in \Gamma_r$. For the control-constraints, we assume $u_a, u_b \in L^2(\Omega)$ with $0 \le u_a(x) < u_b(x)$ a.e. in Ω_s .
- (\mathcal{A}_6) There is a feasible point $(y^0, u^0) \in \mathcal{C}(\overline{\Omega}) \times L^2(\Omega_s)$ satisfying the state equation and the inequality constraints in (1.1).

1.2 Some well-known results

In the following, we recall some significant results regarding the nonlocal radiation on Γ_r as well as the solvability of the state equation. The results have been discussed in details in [17], [12], and [15]. We start with the following definition.

Definition 1.1 The radiative heat flux q_r on Γ_r is defined by

$$q_r = (I - K)(I - (1 - \varepsilon)K))^{-1}\varepsilon\sigma|y^3|y := G\sigma|y^3|y,$$

where the integral operator K is defined by

$$(Ky)(x) = \int_{\Gamma_r} \omega(x, z) y(z) \, ds_z,$$

with a symmetric kernel ω . In the case of two-dimensional domain, the kernel ω is formally given by

$$\omega(x,z) = \Xi(x,z) \frac{[n_r(z) \cdot (x-z)][n_r(x) \cdot (z-x)]}{2|z-x|^3}, \quad \forall x,z \in \Gamma_r,$$

and in the case of a three-dimensional domain

$$\omega(x,z) = \Xi(x,z) \frac{[n_r(z) \cdot (x-z)][n_r(x) \cdot (z-x)]}{\pi |z-x|^4}, \quad \forall x,z \in \Gamma_r.$$

Notice that Ξ denotes the visibility factor which is defined by

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

For the properties of ω and K we refer the reader to Tiihonen and Laitinen, [17]. The following lemma (see [12, Lemma 8] for the proof) provides some significant properties of the operator G, which will be useful for our analysis.

Lemma 1.1 The operator $G := (I - K)(I - (1 - \varepsilon)K)^{-1}\varepsilon$ is linear and bounded form $L^p(\Gamma_r)$ to $L^p(\Gamma_r)$ for all $1 \le p \le \infty$.

In the following, we shortly discuss the existence of solutions of the semilinear equation (SL). To that end, let us introduce the space

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

Moreover, we define the operator associated to the left-hand side of (SL) that is formally obtained by integration of (SL) by parts over the boundaries Γ_r and Γ_0 .

Definition 1.2 The operator $A: V \to V^*$ is given by

$$\langle A(y),v\rangle := \int_{\Omega} \kappa \nabla y \cdot \nabla v \, dx + \int_{\Gamma_r} (G\sigma |y|^3 y) v \, ds + \int_{\Gamma_0} \varepsilon \sigma |y|^3 y v \, ds, \quad y,v \in V$$

with $G: L^{5/4}(\Gamma_r) \to L^{5/4}(\Gamma_r)$.

Notice that thanks to the definition of V, the operator A is well-defined and continuous. Furthermore, $E_s: L^2(\Omega_s) \to V^*$ and $E_0: L^{5/4}(\Gamma_0) \to V^*$ are defined by

(1.2)
$$\langle E_s u, v \rangle := \int_{\Omega_s} uv \, dx \quad \forall v \in V \quad \text{and} \quad \langle E_0 z \rangle := \int_{\Gamma_0} zv \, ds \quad \forall v \in V.$$

Clearly, E_s and E_0 are linear and bounded in their respective spaces.

Definition 1.3 A function $y \in V$ is said to be a (weak) solution of (SL) if y satisfies the following operator equation

(1.3)
$$A(y) = E_s u + E_0 \varepsilon \sigma y_0^4 \quad in \quad V^*.$$

To show the existence of solutions according to this definition, the theory of monotone operators is not applicable here, since the operator G is not positive, i.e. $v(x) \ge 0$ a.e. on Γ_r does in general not imply $(Gv)(x) \ge 0$ a.e. on Γ_r , see [13] for details. However, the existence of weak solutions can be verified by Brezis' Theorem for pseudomonotone operators, cf. [18]. In fact, Laitinen and Tiihonen showed in [12] that A is pseudomonotone giving in turn the existence of weak solutions of (1.3). The uniqueness then follows from a comparison principle (cf. [12]). Furthermore, Meyer et al. [15] showed the boundedness of the solution. We summarize these results in the following theorem:

Theorem 1.1 Let Assumption 1.1 be satisfied. Then for each $u \in L^2(\Omega_s)$, there exists a unique solution $y \in V$ to (SL) in the sense of Definition 1.3. Moreover, the solution is bounded, i.e. $y \in L^{\infty}(\Omega)$, and satisfies

(1.4)
$$\|y\|_{L^{\infty}(\Omega)} + \|y\|_{L^{\infty}(\Gamma_{r}\cup\Gamma_{0})} \le c(\Omega)(1+\|u\|_{L^{2}(\Omega_{s})} + \|y_{0}\|_{L^{16}(\Gamma_{0})}^{4})$$

with some constant $c(\Omega) > 0$.

2 Continuous solutions

Our goal in the upcoming sections consists of providing the first-order necessary optimality conditions for (P). To accomplish this task, we will utilize the Karush-Kuhn-Tucker theory (see Section 5 below). Mainly, we follow the lines of [6]. However, to apply this technique, one has to consider the state constraints in a space such that the convex set, defined by these constraints, admits a nonempty interior. Here, we choose the space of continuous functions, denoted by $\mathcal{C}(\overline{\Omega})$. Therefore, it is at first necessary to show the continuity of the solutions to (SL). The subsequent analysis follows a classical bootstrapping argument. Based on Theorem 1.1, one shows that, (SL) admits solutions in the space $W^{1,q}(\Omega)$ with q > N. Afterwards the continuous embedding $W^{1,q}(\Omega) \hookrightarrow \mathcal{C}(\overline{\Omega}), q > N$, implies the desired continuity. We start with a lemma that represents the key-point within the proof of continuity.

Lemma 2.1 There is a positive real number \hat{q} with $N < \hat{q} < 6$ such that the operator B(f): $W^{1,q}(\Omega) \to W^{1,q'}(\Omega)^*, 1/q + 1/q' = 1$, defined by

$$\langle B(f)y,v\rangle := \int_{\Omega} \kappa \nabla y \cdot \nabla v \, dx + \int_{\Gamma_0} fyv \, ds, \quad y \in W^{1,q}(\Omega), v \in W^{1,q'}(\Omega), v \in W^{1,q'}(\Omega$$

is continuously invertible for all $q \in [N, \hat{q}]$ and all nonnegative functions $f \in L^{\infty}(\Gamma_0)$ that are positive on a set of measure greater than zero.

Proof. In the two-dimensional case, N = 2, the assertion is an immediate consequence of a result of Gröger [10, Theorem 1]. In three dimensions, N = 3, we apply a result of Elschner

et al. [9]. First, the Lax-Milgram lemma implies that for every functional $g \in H^1(\Omega)^*$, there exists a unique solution $y \in H^1(\Omega)$ of

(2.1)
$$\int_{\Omega} \kappa \nabla y \cdot \nabla v \, dx + \int_{\Gamma_0} f y v \, ds = g(v) \quad \forall v \in H^1(\Omega).$$

Let $g \in W^{1,q'}(\Omega)^*$ be arbitrarily fixed. Since $q \ge 2$, the dual space $W^{1,q'}(\Omega)^*$ is continuously embedded in $H^1(\Omega)^*$. Consequently, there exists a unique solution $y \in H^1(\Omega)$ of (2.1) with $g \in W^{1,q'}(\Omega)^*$ in the right hand side of (2.1).

Now, consider the following equation

(2.2)
$$\int_{\Omega} \kappa \nabla \eta \cdot \nabla v \, dx + \int_{\Omega} \eta v \, dx = g(v) - \int_{\Gamma_0} fyv \, ds + \int_{\Omega} yv \, dx \quad \forall v \in W^{1,q'}(\Omega).$$

Due to $y \in H^1(\Omega)$ and N = 3, it holds that $y \in L^6(\Omega)$ and $\tau_0 y \in L^4(\Gamma_0)$. Hence, since $f \in L^{\infty}(\Gamma_0)$, we have $fy \in L^{4/3}(\Gamma_0)^*$. For this reason, since $q' \in [6/5, 3/2]$ and because of the continuity of the trace operator from $W^{1,6/5}(\Omega)$ to $L^{4/3}(\Gamma_0)$ for N = 3, the right hand side of (2.2) defines an element $\xi \in W^{1,q'}(\Omega)^*$ with

$$\langle \xi, v \rangle_{W^{1,q'}(\Omega)^*, W^{1,q'}(\Omega)} = g(v) - \int_{\Gamma_0} fyv \, ds + \int_{\Omega} yv \, dx \quad \forall v \in W^{1,q'}(\Omega).$$

Therefore, in view of our assumptions on Ω for N = 3 (cf. Assumption 1.1) and Remark 3.18 in [9], there exists a real number $\hat{q} > 3$ (independent of f, g) such that for all $q \in [3, \hat{q}]$, (2.2) admits a unique solution $\eta \in W^{1,q}(\Omega)$. Moreover, the solution can be estimated by

(2.3)
$$\|\eta\|_{W^{1,q}(\Omega)} \leq c \|\xi\|_{W^{1,q'}(\Omega)^*} \leq c \left(\|g\|_{W^{1,q'}(\Omega)^*} + (1 + \|f\|_{L^{\infty}(\Gamma_0)}) \|y\|_{H^1(\Omega)} \right) \\ \leq c \|g\|_{W^{1,q'}(\Omega)^*},$$

with a constant c > 0 independent of g. Clearly, due to $H^1(\Omega) \subset W^{1,q'}(\Omega)$, η also solves

$$\int_{\Omega} \kappa \nabla \eta \cdot \nabla v \, dx + \int_{\Omega} (\eta - y) v \, dx = g(v) - \int_{\Gamma_0} fyv \, ds, \quad \forall v \in H^1(\Omega).$$

Subtracting the equation (2.1) from the above equation and inserting $v = y - \eta$ in the resulting equation, we have

(2.4)
$$\min\{\kappa_{\min}, 1\} \|\eta - y\|_{H^1(\Omega)}^2 \le \int_{\Omega} \kappa |\nabla(\eta - y)|^2 dx + \int_{\Omega} (\eta - y)^2 dx = 0.$$

Notice that we have used (\mathcal{A}_3) in Assumption 1.1 for the latter inequality. Obviously, (2.4) implies that $\eta(x) = y(x)$ a.e. in Ω and a.e. on $\Gamma_r \cup \Gamma_0$. Therefore, possibly after a modification on a set of measure zero, we have $y = \eta$ in $W^{1,q}(\Omega)$.

Thus, for $q \in [3, \hat{q}]$, the operator equation

$$B(f)y = g \quad \text{in } W^{1,q'}(\Omega)^*$$

admits a unique solution in $W^{1,q}(\Omega)$ for every given $g \in W^{1,q'}(\Omega)^*$. Moreover, (2.3) yields the continuity of $B(f)^{-1}: W^{1,q'}(\Omega)^* \to W^{1,q}(\Omega)$.

For the rest of this paper, let us fix an arbitrary $q \in (N, \hat{q})$. Next, let us redefine the notion of weak solutions of (SL).

Definition 2.1 The operator $A_q: W^{1,q}(\Omega) \to W^{1,q'}(\Omega)^*$ is defined by

$$\langle A_q(y), v \rangle := \int_{\Omega} \kappa \nabla y \cdot \nabla v \, dx + \int_{\Gamma_r} (G\sigma |y|^3 y) v \, ds + \int_{\Gamma_0} \varepsilon \sigma |y|^3 y v \, ds$$

with $y \in W^{1,q}(\Omega)$, $v \in W^{1,q'}(\Omega)$, and $G : L^{\infty}(\Gamma_r) \to L^{\infty}(\Gamma_r)$. Moreover, similarly to (1.2), the operators $E_{q,s} : L^2(\Omega_s) \to W^{1,q'}(\Omega)^*$ and $E_{q,0} : L^{\infty}(\Gamma_0) \to W^{1,q'}(\Omega)^*$ are given by

$$\langle E_{q,s} \, u, v \rangle := \int_{\Omega_s} uv \, dx, \quad \forall v \in W^{1,q'}(\Omega) \quad and \quad \langle E_{q,0} \, z, v \rangle := \int_{\Gamma_0} zv \, ds, \quad \forall v \in W^{1,q'}(\Omega).$$

Then, analogously to Definition 1.3, a function $y \in W^{1,q}(\Omega)$ is said to be a (weak) solution of (SL), if it fulfills the operator equation

(2.5)
$$A_{q}(y) = E_{q,s} u + E_{q,0} \varepsilon \sigma y_{0}^{4} \quad in \quad W^{1,q'}(\Omega)^{*}.$$

Notice that A_q is well defined since $y \in W^{1,q}(\Omega), q > N$, implies $\tau_r y \in L^{\infty}(\Gamma_r)$ and $\tau_0 y \in L^{\infty}(\Gamma_0)$, respectively. Moreover, $E_{q,s} : L^2(\Omega_s) \to W^{1,q'}(\Omega)^*$ is continuous because of $W^{1,q'}(\Omega) \hookrightarrow L^{s'}(\Omega)$ with $s' = \frac{Nq'}{N-q'} = \frac{Nq}{(N-1)q-q} \ge 2$ for $q \le 6$.

Theorem 2.1 For every $u \in L^2(\Omega_s)$, there exists a unique weak solution $y \in W^{1,q}(\Omega)$ of (SL) in the sense of Definition 2.1. Moreover, the following estimate holds true

(2.6)
$$\|y\|_{W^{1,q}(\Omega)} \le c \left(1 + \|u\|_{L^2(\Omega_s)} + \|y_0\|_{L^{\infty}(\Gamma_0)}^4 + \|u\|_{L^2(\Omega_s)}^4 + \|y_0\|_{L^{\infty}(\Gamma_0)}^{16}\right)$$

with a constant c > 0 independent of u, y_0 .

Proof. As stated above, we apply Lemma 2.1 to the state equation (SL). First, we observe that the solution of (1.3) for an arbitrary $u \in L^2(\Omega_s)$, again denoted by y, solves

(2.7)
$$\int_{\Omega} \kappa \nabla y \cdot \nabla v \, dx + \int_{\Gamma_0} yv \, ds = \int_{\Omega_s} uv \, dx - \int_{\Gamma_r} \alpha_G(y)v \, ds + \int_{\Gamma_0} (\varepsilon \sigma y_0^4 + \alpha_0(y))v \, ds \quad \forall v \in V$$

with $\alpha_0(y) := y - \varepsilon \sigma |y|^3 y$ and $\alpha_G(y) := G \sigma |y|^3 y$. Due to Theorem 1.1, we have $\alpha_0(y) \in L^{\infty}(\Gamma_0)$ and $\alpha_G(y) \in L^{\infty}(\Gamma_r)$. Now, let us consider the following equality

(2.8)
$$\langle B(\mathbf{1})\eta, v \rangle = \int_{\Omega_s} uv \, dx - \int_{\Gamma_r} \alpha_G(y) v \, ds + \int_{\Gamma_0} (\varepsilon \sigma y_0^4 + \alpha_0(y)) v \, ds \quad \forall v \in W^{1,q'}(\Omega).$$

Lemma 2.1 implies that $B(\mathbf{1})^{-1} \in \mathcal{B}(W^{1,q'}(\Omega)^*, W^{1,q}(\Omega))$. Moreover, the right hand side in (2.8), denoted by ω_y , defines a functional in $W^{1,q'}(\Omega)^*$, which is demonstrated in the following. As mentioned above, embedding theorems imply $W^{1,q'}(\Omega) \hookrightarrow L^2(\Omega)$ if $q \leq 6$. Moreover, the trace operators τ_r and τ_0 are continuous from $W^{1,q'}(\Omega)$ to $L^{r'}(\Gamma_r)$ and $L^{r'}(\Gamma_0)$, respectively,

with $r' = \frac{(N-1)q'}{N-q'} = \frac{(N-1)q}{(N-1)q-N} > 1$. Hence, Hölder's inequality implies

(2.9)
$$\begin{aligned} \|\omega_{y}\|_{W^{1,q'}(\Omega)^{*}} &= \sup_{\|v\|_{W^{1,q'}=1}} \left| \int_{\Omega_{s}} uv \, dx - \int_{\Gamma_{r}} \alpha_{G}(y) v \, ds + \int_{\Gamma_{0}} (\varepsilon \sigma y_{0}^{4} + \alpha_{0}(y)) v \, dx \right| \\ &\leq \sup_{\|v\|_{W^{1,q'}=1}} \left(\left\| u \|_{L^{2}(\Omega_{s})} \|v\|_{L^{2}(\Omega)} + \|\alpha_{G}(y)\|_{L^{\infty}(\Gamma_{r})} \|v\|_{L^{1}(\Gamma_{r})} \right. \\ &+ \left(\|\varepsilon \sigma y_{0}^{4}\|_{L^{\infty}(\Gamma_{0})} + \|\alpha_{0}(y)\|_{L^{\infty}(\Gamma_{0})} \right) \|v\|_{L^{1}(\Gamma_{0})} \right) \\ &\leq c \Big(\|u\|_{L^{2}(\Omega_{s})} + \|G\|_{\mathcal{B}(L^{\infty}(\Gamma_{r}))} \|y\|_{L^{\infty}(\Gamma_{r})}^{4} \\ &+ \|y_{0}\|_{L^{\infty}(\Gamma_{0})}^{4} + \|y\|_{L^{\infty}(\Gamma_{0})} + \|y\|_{L^{\infty}(\Gamma_{0})}^{4} \Big), \end{aligned}$$

with a constant c > 0 independent of u, y_0 , and y. Together with (1.4), the latter inequality ensures $\|\omega_y\|_{W^{1,q}(\Omega)^*} < \infty$. Therefore, (2.8) admits a unique solution $\eta \in W^{1,q}(\Omega)$, satisfying

(2.10)
$$\|\eta\|_{W^{1,q}(\Omega)} \le \|B(\mathbf{1})^{-1}\|_{\mathcal{B}(W^{1,q'}(\Omega)^*,W^{1,q}(\Omega))} \|\omega_y\|_{W^{1,q'}(\Omega)^*}.$$

An argument analogously to the proof of Lemma 2.1 implies that

 $\eta = y$ in $W^{1,q}(\Omega)$.

For this reason $y \in W^{1,q}(\Omega)$ is the unique solution of

(2.11)
$$B(\mathbf{1})y = \omega_y \text{ in } W^{1,q'}(\Omega)^*.$$

Thanks to the definition of B(1), (2.11) is equivalent to

$$\int_{\Omega} \kappa \nabla y \cdot \nabla v \, dx + \int_{\Gamma_0} yv \, ds = \int_{\Omega_s} uv \, dx - \int_{\Gamma_r} \alpha_G(y)v \, ds + \int_{\Gamma_0} (\varepsilon \sigma y_0^4 + \alpha_0(y))v \, ds \quad \forall v \in W^{1,q'}(\Omega),$$

Thus, by the definition of $\alpha_0(y)$ and $\alpha_G(y)$, $y \in W^{1,q}(\Omega)$ is the unique solution of

$$\int_{\Omega} \kappa \nabla y \cdot \nabla v \, dx + \int_{\Gamma_r} (G\sigma |y|^3 y) v \, ds + \int_{\Gamma_0} \varepsilon \sigma |y|^3 y v \, ds = \int_{\Omega_s} uv \, dx + \int_{\Gamma_0} \varepsilon \sigma y_0^4 v \, ds \quad \forall v \in W^{1,q'}(\Omega).$$

Hence, for every $u \in L^2(\Omega_s)$, (2.5) admits a unique solution $y \in W^{1,q}(\Omega)$. Finally, (2.6) follows from (2.10) together with (2.9) and (1.4).

Remark 2.1 Thanks to $W^{1,q}(\Omega) \hookrightarrow \mathcal{C}(\overline{\Omega})$, the solution of (SL) is continuous.

Based on Theorem 2.1, we define the control-to-state-operator $\mathcal{G} : L^2(\Omega_s) \to W^{1,q}(\Omega)$ associated to (P), i.e. the solution operator for (SL), that assigns to each $u \in L^2(\Omega_s)$ the weak solution $y \in W^{1,q}(\Omega)$. With this setting at hand, the optimal control problem can equivalently be stated as follows:

(P)
$$\begin{cases} \min_{u \in \mathcal{U}} & f(u) := J(u, \mathcal{G}(u)) \\ \text{subject to} & y_a(x) \le (E_c \mathcal{G}(u))(x) \le y_b(x) \quad \forall x \in \overline{\Omega}_g, \\ & (E_c \mathcal{G}(u))(x) \le y_{\max}(x) \quad \forall x \in \overline{\Omega}_s, \end{cases}$$

where E_c denotes the embedding operator from $W^{1,q}(\Omega)$ to $\mathcal{C}(\overline{\Omega})$. Notice that f(u) is clearly well defined since $\mathcal{G}(u) \in W^{1,q}(\Omega) \subset H^1(\Omega)$.

3 Differentiability of the control-to-state-operator

Next, let us turn to the linearized version of (SL). First, recall a result of Meyer, Philip, Tröltzsch [15], that is the following maximum principle:

Lemma 3.1 Suppose that $u \in L^2(\Omega_s)$ satisfies $u(x) \ge 0$ a.e. in Ω_s , while $y_0 \in L^{\infty}(\Gamma_0)$ fulfills $y_0(x) \ge \theta > 0$ a.e. on Γ_0 according to Assumption 1.1. Then, the weak solution y of (SL) satisfies $y(x) \ge \theta > 0$ a.e. in Ω and a.e. on Γ_r and Γ_0 .

Now, let $\bar{u} \in L^2(\Omega_s)$ with associated state $\bar{y} \in W^{1,q}(\Omega)$. Moreover, we assume for the rest of this section that $\bar{u}(x) \geq 0$ a.e. in Ω_s such that Lemma 3.1 implies $\bar{y}(x) > 0$ a.e. on Γ_r and Γ_0 . Next, we turn to the derivative of the operator A_q , as given in Definition 2.1, at the point \bar{y} . We already mentioned that τ_r and τ_0 are continuous from $W^{1,q}(\Omega)$ to $L^{\infty}(\Gamma_r)$ and $L^{\infty}(\Gamma_0)$, respectively. Furthermore, the Nemyzki-operator $\Phi(y) := |y|^3 y$ is continuously Fréchet-differentiable from $L^{\infty}(\Gamma_r \cup \Gamma_0)$ to $L^{\infty}(\Gamma_r \cup \Gamma_0)$. Since all other parts of A_q are linear and continuous in their respective spaces, in particular $G : L^{\infty}(\Gamma_r) \to L^{\infty}(\Gamma_r)$, A_q is clearly Fréchet-differentiable from $W^{1,q}(\Omega)$ to $W^{1,q'}(\Omega)^*$, and its derivative at \bar{y} in an arbitrary direction $y \in W^{1,q}(\Omega)$ is given by

(3.1)
$$\langle A'_{q}(\bar{y})y,v\rangle = \int_{\Omega} \kappa \nabla y \cdot \nabla v \, dx + 4 \int_{\Gamma_{r}} (G\sigma |\bar{y}|^{3}y)v \, ds + 4 \int_{\Gamma_{0}} \varepsilon \sigma |\bar{y}|^{3}yv \, ds, \quad \forall v \in W^{1,q'}(\Omega).$$

By the same arguments, A_q is also twice continuously Fréchet-differentiable and the second derivative at \bar{y} in arbitrary directions $y_1, y_2 \in W^{1,q}(\Omega)$ is given by

(3.2)
$$\langle A_q''(\bar{y})[y_1, y_2], v \rangle = 12 \int_{\Gamma_r} (G\sigma |\bar{y}| \bar{y} y_1 y_2) v \, ds + 12 \int_{\Gamma_0} \varepsilon \sigma |\bar{y}| \bar{y} y_1 y_2 v \, ds, \quad \forall v \in W^{1,q'}(\Omega).$$

Notice that $A''_q(\bar{y})$ is clearly continuous from $W^{1,q}(\Omega) \times W^{1,q}(\Omega)$ to $W^{1,q'}(\Omega)^*$. Now, consider the operator equation

(3.3)
$$A'_{q}(\bar{y})y = w \quad \text{in} \quad W^{1,q'}(\Omega)^*$$

with a given $w \in W^{1,q'}(\Omega)^*$. Our aim is to show the existence of a unique solution to (3.3). In [13], an analogous equation in $H^1(\Omega)^*$ is investigated. By means of an numerical example, it is illustrated that the Lax-Milgram lemma cannot be applied to derive existence of solutions because of the non-positivity of G (see [13] for details). Instead of that, the Fredholm alternative is employed to prove existence and uniqueness. Here, we argue similarly which is demonstrated in the following. First, we introduce a linear operator $F(\bar{y}) : L^{\infty}(\Gamma_r) \to W^{1,q'}(\Omega)^*$, defined by

$$\langle F(\bar{y})y,v\rangle := 4 \int_{\Gamma_r} (G\sigma |\bar{y}|^3 y)v \ ds \quad \forall v \in W^{1,q'}(\Omega).$$

As already stated in Section 2, the trace operator is continuous from $W^{1,q'}(\Omega)$ to $L^{r'}(\Gamma_r)$, r' > 1. Hence, thanks to $\bar{y} \in L^{\infty}(\Gamma_r)$, $F(\bar{y})$ is linear and continuous. Then, together with the Definition of B in Lemma 2.1, (3.3) is equivalent to

$$\left(B(\bar{\alpha}_0) + F(\bar{y})\tau_r\right)y = w,$$

where $\bar{\alpha}_0$ is defined by $\bar{\alpha}_0 := 4\varepsilon \sigma |\bar{y}|^3$ such that $\bar{\alpha}_0 \in L^{\infty}(\Gamma_0)$. Moreover, here and in the following, τ_r is considered as an operator from $W^{1,q}(\Omega)$ to $L^{\infty}(\Gamma_r)$. Now, since $\bar{y}(x) \ge \theta > 0$ a.e. on Γ_r , Lemma 2.1 is applicable such that

(3.4)
$$y = B(\bar{\alpha}_0)^{-1}(w - F(\bar{y})\tau_r y) = B(\bar{\alpha}_0)^{-1}w - B(\bar{\alpha}_0)^{-1}F(\bar{y})\tau_r y.$$

Applying τ_r to (3.4), we infer further

(3.5)
$$(I + \tau_r B(\bar{\alpha}_0)^{-1} F(\bar{y})) \tau_r y = \tau_r B(\bar{\alpha}_0)^{-1} w.$$

Let us now define a linear and continuous operator $\mathcal{F}(\bar{y}): L^{\infty}(\Gamma_r) \to L^{\infty}(\Gamma_r)$ by

$$\mathcal{F}(\bar{y}) := \tau_r B(\bar{\alpha}_0)^{-1} F(\bar{y}),$$

and hence (3.5) is equivalent to

(3.6)
$$(I + \mathcal{F}(\bar{y}))\tau_r y = \tau_r B(\bar{\alpha}_0)^{-1} w \quad \text{in} \quad L^{\infty}(\Gamma_r).$$

We point out that, due to q > N, the trace operator τ_r is compact from $W^{1,q}(\Omega)$ to $L^{\infty}(\Gamma_r)$ (see [1]). Hence, $\mathcal{F}(\bar{y})$ is compact as well.

Assumption 3.1 The operator $\mathcal{F}(\bar{y}) : L^{\infty}(\Gamma_r) \to L^{\infty}(\Gamma_r)$ does not admit the eigenvalue $\lambda = -1$.

Theorem 3.1 Let $\bar{u} \in L^2(\Omega_s)$ with $\bar{u}(x) \geq 0$ a.e. in Ω_s and denote the associated state by $\bar{y} = \mathcal{G}(\bar{u})$. Moreover, suppose that Assumption 3.1 holds true. Then, for every $w \in W^{1,q'}(\Omega)^*$, there exists a unique solution $y \in W^{1,q}(\Omega)$ to (3.3) that satisfies the following estimate

(3.7)
$$\|y\|_{W^{1,q}(\Omega)} \le c \|w\|_{W^{1,q'}(\Omega)^*}$$

with a constant c > 0 independent of w. Hence, $A'_q(\bar{y})^{-1} \in \mathcal{B}(W^{1,q'}(\Omega)^*, W^{1,q}(\Omega))$ holds true.

Proof. Thanks to the compactness of $\mathcal{F}(\bar{y})$, the theory of Fredholm operators implies that, either $\lambda = -1$ is one of countable many eigenvalues of $\mathcal{F}(\bar{y})$, or $I + \mathcal{F}(\bar{y})$ is continuously invertible. Hence, Assumption 3.1 ensures that $(I + \mathcal{F}(\bar{y}))^{-1} \in \mathcal{B}(L^{\infty}(\Gamma_r))$ such that

$$\tau_r y = (I + \mathcal{F}(\bar{y}))^{-1} \tau_r B(\bar{\alpha}_0)^{-1} w.$$

Inserting this in (3.4), we have

(3.8)
$$y = B(\bar{\alpha}_0)^{-1} (I - F(\bar{y})(I + \mathcal{F}(\bar{y}))^{-1} \tau_r B(\bar{\alpha}_0)^{-1}) w.$$

Since Assumption 3.1 ensures that

$$\|(I+\mathcal{F}(\bar{y}))^{-1}\|_{\mathcal{B}(L^{\infty}(\Gamma_{r}))} < \infty,$$

(3.8) immediately implies (3.7).

Theorem 3.2 Let $\bar{u} \in L^2(\Omega_s)$ with $\bar{u}(x) \geq 0$ a.e. in Ω_s . Furthermore, suppose that Assumption 3.1 is fulfilled. Then, there exists an open neighborhood $U(\bar{u})$ of \bar{u} in $L^2(\Omega_s)$ such that $\mathcal{G} : L^2(\Omega_s) \to W^{1,q}(\Omega)$ is on $U(\bar{u})$ twice continuously Fréchet-differentiable. Moreover, the first derivative of \mathcal{G} at \bar{u} in an arbitrary direction $u \in L^2(\Omega_s)$ is given by

(3.9)
$$\mathcal{G}'(\bar{u})u = A'_a(\bar{y})^{-1}E_{q,s}u.$$

with $\bar{y} = \mathcal{G}(\bar{u})$. The second derivative of \mathcal{G} at \bar{u} in arbitrary directions $u_1, u_2 \in L^2(\Omega_s)$ is given by

$$\mathcal{G}''(\bar{u})[u_1, u_2] = A'_q(\bar{y})^{-1}(-A''_q(\tilde{y})[y_1, y_2]),$$

where $A''_q(\bar{y})$ is defined as in (3.2) and $y_i = \mathcal{G}'(\bar{u})u_i$, i = 1, 2.

Proof. First of all, Let us introduce the operator $T: W^{1,q}(\Omega) \times L^2(\Omega_s) \to W^{1,q'}(\Omega)^*$ given by

(3.10)
$$T(y,u) := A_q(y) - E_{q,s} u - E_{q,0} \varepsilon \sigma y_0^4$$

Further, we set $\bar{y} = \mathcal{G}(u)$ and hence, by the definition of the solution operator $\mathcal{G}, \bar{y} \in W^{1,q}(\Omega)$ is the unique solution of

$$A_q(\bar{y}) = E_{q,s} \,\bar{u} + E_{q,0} \,\varepsilon \sigma y_0^4 \text{ in } W^{1,q'}(\Omega)^*.$$

Thus, it holds that $T(\bar{y}, \bar{u}) = 0$. Moreover, Since $A_q : W^{1,q}(\Omega) \to W^{1,q'}(\Omega)$ is twice continuously Fréchet-differentiable, $T : W^{1,q}(\Omega) \times L^2(\Omega_s) \to W^{1,q'}(\Omega)^*$ is twice continuously Fréchet-differentiable. By (3.10), $\partial_y T(\bar{y}, \bar{u}) : W^{1,q}(\Omega) \to W^{1,q'}(\Omega)^*$ is given by

$$\partial_y T(\bar{y}, \bar{u}) = A'(\bar{y}).$$

Therefore, Theorem 3.1 implies that $\partial_y T(\bar{y}, \bar{u})^{-1} \in \mathcal{B}(W^{1,q'}(\Omega)^*, W^{1,q}(\Omega))$. Thus, taking account of the implicit function theorem, there exists an open neighborhood $U(\bar{u})$ of \bar{u} in $L^2(\Omega_s)$ such that the control-to-state operator $\mathcal{G} : L^2(\Omega_s) \to W^{1,q}(\Omega)$ is on $U(\bar{u})$ twice continuously Fréchet-differentiable. The first derivative of \mathcal{G} at \bar{u} in an arbitrarily direction $u \in L^2(\Omega_s)$ is given by

(3.11)
$$\mathcal{G}'(\bar{u})u = -\partial_y T(\bar{y}, \bar{u})^{-1} \partial_u T(\bar{y}, \bar{u})u = A'_q(\bar{y})^{-1} E_{q,s} u.$$

Moreover, the second derivative of \mathcal{G} at \bar{u} in arbitrary directions $u_1, u_2 \in L^2(\Omega_s)$ is given by

$$\mathcal{G}''(\bar{u})[u_1, u_2] = -\partial_y T(\bar{y}, \bar{u})^{-1} \partial_{yy}^2 T(\bar{y}, \bar{u})[y_1, y_2] = A'_q(\bar{y})^{-1} (-A''_q(\bar{y})[y_1, y_2]),$$

where $y_i = \mathcal{G}'(\tilde{u})u_i$, i = 1, 2. Notice that $\partial_{yu}^2 T = \partial_{uu}^2 T = 0$ and $\partial_{uy}^2 T = 0$ was used for the computation of \mathcal{G}'' .

Remark 3.1 Notice that the additional assumption $\bar{u}(x) \ge 0$ a.e. in Ω_s is automatically fulfilled for all $u \in \mathcal{U}$, since $u_a(x) \ge 0$ a.e. in Ω_s .

In view of the definition of $A'_q(\bar{y})$ in (3.1) and formal integration by parts, the equation $A'_q(\bar{y})y = E_{q,s}u$ in (3.11) can be considered as the variational formulation of the following linear PDE:

(3.12)
$$\begin{cases} -\operatorname{div}(\kappa_s \nabla y) = u & \text{in } \Omega_s \\ -\operatorname{div}(\kappa_g \nabla y) = 0 & \text{in } \Omega_g \\ \kappa_g \left(\partial_{n_r} y\right)_g - \kappa_s \left(\partial_{n_r} y\right)_s - 4 \, G \sigma |\bar{y}|^3 y = 0 & \text{on } \Gamma_r \\ \kappa_s \partial_{n_0} y + 4 \, \varepsilon \sigma |\bar{y}|^3 y = 0 & \text{on } \Gamma_0, \end{cases}$$

Similarly, $A'_q(\bar{y})\eta = -A''_q(\bar{y})[y_1, y_2]$ is interpreted as variational formulation of

(3.13)
$$\begin{cases} -\operatorname{div}(\kappa_s \nabla y) = 0 & \text{in } \Omega_s \\ -\operatorname{div}(\kappa_g \nabla y) = 0 & \text{in } \Omega_g \\ \kappa_g \left(\partial_{n_r} y\right)_g - \kappa_s \left(\partial_{n_r} y\right)_s - 4 \, G \sigma |\bar{y}|^3 y = -12 \, G \sigma |\bar{y}| \bar{y} \, y_1 y_2 & \text{on } \Gamma_r \\ \kappa_s \partial_{n_0} y + 4 \, \varepsilon \sigma |\bar{y}|^3 y = -12 \, \varepsilon \sigma |\bar{y}| \bar{y} \, y_1 y_2 & \text{on } \Gamma_0, \end{cases}$$

Definition 3.1 Let $\bar{u} \in L^2(\Omega_s)$, $\bar{u}(x) \geq 0$ a.e. in Ω_s , and $\bar{y} = \mathcal{G}(\bar{u})$ be given. Then, a function $y \in W^{1,q}(\Omega)$ is said to be a (weak) solution of (3.12) for $u \in L^2(\Omega_s)$ if it satisfies the following operator equation:

$$A'_{q}(\bar{y})y = E_{q,s} u \quad in \quad W^{1,q'}(\Omega)^*,$$

where $A'_q(\bar{y})$ is as defined in (3.1). Moreover, $\eta \in W^{1,q}(\Omega)$ is the (weak) solution of (3.13) for given $y_1, y_2 \in W^{1,q}(\Omega)$ if it fulfills

$$A'_{q}(\bar{y})\eta = -A''_{q}(\bar{y})[y_{1}, y_{2}]$$
 in $W^{1,q'}(\Omega)^{*}$.

4 Adjoint equation involving measures

In this section, we discuss the adjoint equation to (3.3), given by

(4.1)
$$A'_q(\bar{y})^* p = g \text{ in } W^{1,q}(\Omega)^*,$$

where $A'_q(\bar{y})^* : W^{1,q'}(\Omega) \to W^{1,q}(\Omega)^*$ denotes the adjoint of $A'_q(\bar{y})$ and g is a given element of $W^{1,q}(\Omega)^*$. We already know from Theorem 3.1 that, under Assumption 3.1, $A'_q(\bar{y})$ is an isomorphism from $W^{1,q}(\Omega)$ to $W^{1,q'}(\Omega)^*$. Thus, the adjoint operator $A'_q(\bar{y})^* : W^{1,q'}(\Omega) \to W^{1,q}(\Omega)^*$ is in turn continuously invertible and consequently, (4.1) admits a unique solution $p \in W^{1,q'}(\Omega), q' = \frac{q}{q-1} < \frac{N}{N-1}$, due to q > N.

Lemma 4.1 Let $\bar{u} \in L^2(\Omega_s)$ with associated state $\bar{y} = \mathcal{G}(\bar{u})$ satisfy $\bar{u}(x) \ge 0$ a.e. in Ω_s . Furthermore, suppose that Assumption 3.1 is satisfied. Then, $A'_q(\bar{y})^{-*} \in \mathcal{B}(W^{1,q}(\Omega)^*, W^{1,q'}(\Omega))$ holds true.

The concrete form of $A'_q(\bar{y})^*$ follows from

$$\begin{split} \langle A'_q(\bar{y})^*p, v \rangle_{(W^{1,q})^*, W^{1,q}} &= \langle p, A'_q(\bar{y})v \rangle_{W^{1,q'}, (W^{1,q'})^*} = \langle A'_q(\bar{y})v, p \rangle_{(W^{1,q'})^*, W^{1,q'}} \\ &= \int_{\Omega} \kappa \nabla p \cdot \nabla v \, dx + 4 \int_{\Gamma_r} (G\sigma |\bar{y}|^3 v) p \, ds \\ &+ 4 \int_{\Gamma_0} \varepsilon \sigma |\bar{y}|^3 p v \, ds \quad \forall v \in W^{1,q}(\Omega). \end{split}$$

Since the embedding $W^{1,q}(\Omega) \hookrightarrow \mathcal{C}(\overline{\Omega})$ is continuous and dense, one has the embedding $\mathcal{C}(\overline{\Omega})^* \hookrightarrow W^{1,q}(\Omega)^*$ with the associated embedding operator E_c^* . Further, we define by $\mathcal{M}(\overline{\Omega})$ the space of all regular Borel measures on the compact set $\overline{\Omega}$. By the Riesz-Radon theorem, cf. [3], it is well known that the dual space $\mathcal{C}(\overline{\Omega})^*$ can be isometrically identified with $\mathcal{M}(\overline{\Omega})$ with respect to the duality pairing

$$\langle \mu, \varphi \rangle_{\mathcal{C}(\overline{\Omega})^*, \mathcal{C}(\overline{\Omega})} := \int_{\overline{\Omega}} \varphi \, d\mu, \quad \phi \in \mathcal{C}(\overline{\Omega}), \ \mu \in \mathcal{M}(\overline{\Omega}).$$

According to this, we are allowed to insert regular Borel measures as inhomogeneity in (4.1). Moreover, given a $\mu \in \mathcal{M}(\overline{\Omega})$, the operator equation

(4.2)
$$A'_{q}(\bar{y})^{*}p = E^{*}_{c}\mu \quad \text{in} \quad W^{1,q}(\Omega)^{*},$$

is equivalent to

(4.3)

$$\int_{\Omega} \kappa \nabla p \cdot \nabla v \, dx + 4 \int_{\Gamma_r} (G\sigma |\bar{y}|^3 v) p \, ds + 4 \int_{\Gamma_0} \varepsilon \sigma |\bar{y}|^3 p v \, ds$$

$$= \langle E_c^* \mu, v \rangle_{W^{1,q}(\Omega)^*, W^{1,q}(\Omega)}$$

$$= \langle \mu, E_c v \rangle_{\mathcal{C}(\overline{\Omega})^*, \mathcal{C}(\overline{\Omega})} = \int_{\overline{\Omega}} E_c v \, d\mu \quad \forall v \in W^{1,q}(\Omega).$$

As mentioned in Section 2, the trace operator is continuous from $W^{1,q'}(\Omega)$ to $L^{r'}(\Gamma_r)$, $r' = \frac{(N-1)q}{(N-1)q-N} > 1$. Moreover, $v \in W^{1,q}(\Omega)$ clearly implies $v \in L^r(\Gamma_r)$ due to the continuous embedding $W^{1,q}(\Omega) \hookrightarrow C(\overline{\Omega})$. Hence, if we consider G as an operator from $L^r(\Gamma_r)$ to $L^r(\Gamma_r)$, one obtains

$$\int_{\Gamma_r} (G\sigma |\bar{y}|^3 v) p \, ds = \int_{\Gamma_r} \sigma |\bar{y}|^3 (G^* p) v \, ds,$$

where $G^* : L^{r'}(\Gamma_r) \to L^{r'}(\Gamma_r)$ is the adjoint of G, i.e. $G^* = \varepsilon(I - (1 - \varepsilon)K^*))^{-1}(I - K^*)$ (cf. Definition 1.1). Notice in this context that K is formally self-adjoint due to the symmetry of its kernel. In view of this and formal integration by parts, (4.2) and (4.3), respectively, can be considered as a variational formulation of the following linear PDE with measure data on the right hand side:

(4.4)
$$\begin{cases} -\operatorname{div}(\kappa_s \nabla p) = \mu_{|\Omega_g|} & \text{in } \Omega_s \\ -\operatorname{div}(\kappa_g \nabla p) = \mu_{|\Omega_s|} & \text{in } \Omega_g \end{cases} \\ \kappa_g \left(\frac{\partial p}{\partial_{n_r}}\right)_g - \kappa_s \left(\frac{\partial p}{\partial_{n_r}}\right)_s - 4 \,\sigma |\bar{y}|^3 G^* p = \mu_{|\Gamma_r|} & \text{on } \Gamma_r \\ \kappa_s \partial_{n_0} p + 4 \,\varepsilon \sigma |\bar{y}|^3 p = \mu_{|\Gamma_0|} & \text{on } \Gamma_0, \end{cases}$$

where $\mu_{|\Omega_g}$, $\mu_{|\Omega_s}$, $\mu_{|\Gamma_r}$, and $\mu_{|\Gamma_0}$ denote the restrictions of μ on Ω_g , Ω_s , Γ_r , and Γ_0 , respectively. In other words, $\mu \in \mathcal{M}(\overline{\Omega})$ is decomposed into $\mu = \mu_{|\Omega_g} + \mu_{|\Omega_s} + \mu_{|\Gamma_r} + \mu_{|\Gamma_0}$, where $\mu_{|\Omega_g}$, $\mu_{|\Omega_s}$, $\mu_{|\Gamma_r}$, and $\mu_{|\Gamma_0}$ are Borel measures concentrated on Ω_g , Ω_s , Γ_r , and Γ_0 .

Definition 4.1 Let $\bar{y} \in W^{1,q}(\Omega)$ be given. Then, a function $p \in W^{1,q'}(\Omega)$, $q' < \frac{N}{N-1}$, is said to be a (weak) solution of (4.4) if it satisfies the operator equation (4.2).

Clearly, Lemma 4.1 implies that there is a solution of (4.4) in the sense of Definition 4.1. Furthermore, the right-hand side in (4.2) can be estimated by

$$\begin{split} \|E_c^*\mu\|_{W^{1,q}(\Omega)^*} &= \sup_{y \neq 0} \frac{\langle E_c^*\mu, y \rangle_{W^{1,q}(\Omega)^*, W^{1,q}(\Omega)}}{\|y\|_{W^{1,q}(\Omega)}} \\ &\leq c \sup_{y \neq 0} \frac{\langle \mu, E_c y \rangle_{\mathcal{C}(\overline{\Omega})^*, \mathcal{C}(\overline{\Omega})}}{\|y\|_{\mathcal{C}(\overline{\Omega})}} = c \sup_{y \neq 0} \frac{\int_{\overline{\Omega}} y \, d\mu}{\|y\|_{\mathcal{C}(\overline{\Omega})}} = c \|\mu\|_{\mathcal{M}(\overline{\Omega})} \end{split}$$

such that one obtains the following result:

Theorem 4.1 Let $\bar{u} \in L^2(\Omega_s)$ with $\bar{u}(x) \geq 0$ a.e. in Ω_s and the associated state is denoted by $\bar{y} = \mathcal{G}(\bar{u}) \in W^{1,q}(\Omega)$. Furthermore, suppose that Assumption 3.1 is satisfied. Then, $A_q(\bar{y})^{-*} \in \mathcal{B}(W^{1,q}(\Omega)^*, W^{1,q'}(\Omega))$ and consequently, for every $\mu \in \mathcal{M}(\overline{\Omega})$, there exists a unique solution $p \in W^{1,q'}(\Omega)$ of (4.4) in the sense of Definition 4.1 that satisfies

 $\|p\|_{W^{1,q'}(\Omega)} \le c \, \|\mu\|_{\mathcal{M}(\overline{\Omega})}$

with a constant c > 0 independent of μ .

5 First-order necessary optimality conditions for (P)

Before we establish Karush-Kuhn-Tucker (KKT) type optimal conditions for (P), let us shortly address the existence of an optimal solution. Clearly, thanks to (\mathcal{A}_6) in Assumption 1.1, standard arguments imply the existence of at least one (global) optimum (cf. also [15, Theorem 5.2]). Due to the nonlinearities in the state equation, uniqueness of the optimal solution can certainly not be expected. Let us now introduce the notion of local optima:

Definition 5.1 A feasible control \bar{u} of (P) is called a local solution for (P), if there exists a positive real number ε such that $f(\bar{u}) \leq f(u)$ holds for all feasible $u \in L^2(\Omega_s)$ with $||u - \bar{u}||_{L^2(\Omega_s)} \leq \varepsilon$.

Throughout this section, let $\bar{u} \in \mathcal{U}$ be a local solution of (P), and assume that Assumption 3.1 is fulfilled at \bar{u} . Notice that everything what follows also holds for a global optimum of (P). To apply the KKT theory, the existence of an interior (Slater) point with respect to the state constraints in (1.1) has to be assumed. This assumption is referred to as the so-called "linearized Slater condition": **Definition 5.2** Let $\bar{u} \in \mathcal{U}$ be a local solution of (P), and assume that Assumption 3.1 is fulfilled at \bar{u} . We say that $\bar{u} \in \mathcal{U}$ satisfies the linearized Slater condition for (P), if there exists an interior point $u_0 \in \mathcal{U}$ such that

$$y_a(x) + \delta \le E_c \mathcal{G}(\bar{u})(x) + E_c \mathcal{G}'(\bar{u})(u_0 - \bar{u})(x) \le y_b(x) - \delta \qquad \forall x \in \overline{\Omega}_g,$$
$$E_c \mathcal{G}(\bar{u})(x) + E_c \mathcal{G}'(\bar{u})(u_0 - \bar{u})(x) \le y_{\max}(x) - \delta \qquad \forall x \in \overline{\Omega}_s,$$

with a fixed $\delta > 0$.

Notice that $\bar{u} \in \mathcal{U}$ automatically satisfies $\bar{u}(x) \geq 0$ a.e. in Ω_s (cf. Remark 3.1) such that Assumption 3.1 implies that $\mathcal{G}'(\bar{u}) : L^2(\Omega_s) \to W^{1,q}(\Omega)$ is well defined.

Definition 5.3 The Lagrange functional $\mathcal{L} : \mathcal{U} \times \mathcal{M}(\overline{\Omega}_s) \times \mathcal{M}(\overline{\Omega}_g) \to \mathbb{R}$ for (P) is given by

$$\mathcal{L}(u,\mu) = f(u) + \langle \mu_s, E_c \mathcal{G}(u) - y_{\max} \rangle_s + \langle \mu_g^a, y_a - E_c \mathcal{G}(u) \rangle_g + \langle \mu_g^b, E_c \mathcal{G}(u) - y_b \rangle_g,$$

with $\langle \cdot, \cdot \rangle_g := \langle \cdot, \cdot \rangle_{\mathcal{C}(\overline{\Omega}_g)^*, \mathcal{C}(\overline{\Omega}_g)}, \langle \cdot, \cdot \rangle_s := \langle \cdot, \cdot \rangle_{\mathcal{C}(\overline{\Omega}_s)^*, \mathcal{C}(\overline{\Omega}_s)}, and \mu = (\mu_s, \mu_g^a, \mu_g^b).$

Since \mathcal{G} is twice continuously Fréchet-differentiable at \bar{u} (see Corollary 3.2), it is straight forward to see that f is twice continuously Fréchet-differentiable at \bar{u} , and its derivative at $\bar{u} \in L^2(\Omega_s)$ in an arbitrary direction $u \in L^2(\Omega_s)$ is given by

$$f'(\bar{u})u = \int_{\Omega_g} (\nabla \mathcal{G}(\bar{u}) - z) \cdot \nabla \mathcal{G}'(\bar{u})u \, dx + \beta \int_{\Omega_s} \bar{u} \, u \, dx.$$

Due to $\mathcal{G}(\bar{u}) \in W^{1,q}(\Omega)$ and $z \in L^2(\Omega_g)^N$, the first addend defines an element of $W^{1,q}(\Omega)^*$ such that linear and continuous operator $L: W^{1,q}(\Omega) \to W^{1,q}(\Omega)^*$ exists with

$$\langle L\bar{y},v\rangle := \int_{\Omega_g} (\nabla\bar{y}-z)\cdot\nabla v\,dx, \quad v\in W^{1,q}(\Omega)$$

where $\bar{y} = \mathcal{G}(\bar{u}) \in W^{1,q}(\Omega)$. With this setting, $f'(\bar{u})u = \langle L\bar{y}, \mathcal{G}'(\bar{u})u \rangle + \beta(\bar{u}, u)$. Notice that since f and \mathcal{G} are continuously Fréchet-differentiable at \bar{u} , \mathcal{L} is continuously Fréchetdifferentiable at \bar{u} such that the following definition makes sense:

Definition 5.4 let $\bar{u} \in \mathcal{U}$ be a local solution of (P), and suppose that Assumption 3.1 is fulfilled. Then, $\mu_s \in \mathcal{M}(\overline{\Omega}_s)$, $\mu_g^a \in \mathcal{M}(\overline{\Omega}_g)$, and $\mu_g^b \in \mathcal{M}(\overline{\Omega}_g)$ are said to be Lagrange multipliers associated to the state constraints in (P), if it holds that

(5.1)
$$\partial_u \mathcal{L}(\bar{u},\mu)(u-\bar{u}) \ge 0 \quad \forall u \in \mathcal{U},$$

(5.2) $\mu_s \ge 0, \quad \mu_g^a \ge 0, \quad \mu_g^b \ge 0,$

(5.3)
$$\int_{\overline{\Omega}_s} (E_c \mathcal{G}(\bar{u}) - y_{\max}) d\mu_s = \int_{\overline{\Omega}_g} (y_a - E_c \mathcal{G}(\bar{u})) d\mu_g^a = \int_{\overline{\Omega}_g} (E_c \mathcal{G}(\bar{u}) - y_b) d\mu_g^b = 0,$$

where we set $\mu = (\mu_s, \mu_q^a, \mu_q^b)$.

Notice that if $\nu \in \mathcal{M}(\overline{\Omega})$, then we write

$$\nu \ge 0 \quad \Leftrightarrow \quad \int_{\overline{\Omega}} y \, d\nu \ge 0 \quad \forall \, y \in \{ y \in \mathcal{C}(\overline{\Omega}) \, | \, y(x) \ge 0 \, \forall \, x \in \overline{\Omega} \}.$$

The following theorem states the first-order necessary optimality conditions for (P), i.e. the existence of Lagrange multipliers in the sense of Definition 5.4. The proof can be found for instance in [6]

Theorem 5.1 Let \bar{u} be a locally optimal solution of (P) satisfying the linearized Slater condition. Furthermore, let Assumption 3.1 be satisfied. Then, there exist corresponding Lagrange multipliers $(\mu_s, \mu_g^a, \mu_g^b) \in \mathcal{M}(\overline{\Omega}_s) \times \mathcal{M}(\overline{\Omega}_g) \times \mathcal{M}(\overline{\Omega}_g)$ according to Definition 5.4 such that (5.1)-(5.3) are satisfied.

Next, let us transform (5.1)–(5.3) into the optimality system of (P) by introducing the adjoint equation. First, by the definition of \mathcal{L} and (3.11), (5.1) is equivalent to

(5.4)
$$\langle A'_{q}(\bar{u})^{-*} (L\bar{y} + E^{*}_{c}\mu_{s} - E^{*}_{c}\mu^{a}_{g} + E^{*}_{c}\mu^{b}_{g}), E_{q,s}(u - \bar{u}) \rangle + (\beta \,\bar{u}, \, u - \bar{u})_{L^{2}(\Omega_{s})} \geq 0 \quad \forall \, u \in \mathcal{U}.$$

Consider now the following operator equation

(5.5)
$$A'_{q}(\bar{y})^{*}p = L\bar{y} + E^{*}_{c}\mu_{s} - E^{*}_{c}\mu^{a}_{g} + E^{*}_{c}\mu^{b}_{g} \quad \text{in} \quad W^{1,q}(\Omega)^{*}$$

which is equivalent to

(5.6)

$$\int_{\Omega} \kappa \nabla p \cdot \nabla v \, dx + 4 \int_{\Gamma_r} (G\sigma |\bar{y}|^3 v) p \, ds + 4 \int_{\Gamma_0} \varepsilon \sigma |\bar{y}|^3 p v \, ds$$

$$= \int_{\Omega_g} (\nabla \bar{y} - z) \cdot \nabla v \, dx + \int_{\overline{\Omega}_s} E_c v \, d\mu_s - \int_{\overline{\Omega}_g} E_c v \, d\mu_g^a$$

$$+ \int_{\overline{\Omega}_g} E_c v \, d\mu_g^b \quad \forall v \in W^{1,q}(\Omega)$$

(cf. (4.2) and (4.3)). As in case of (4.4), (5.6) can be considered as the variational formulation of

(5.7)
$$\begin{cases} -\operatorname{div}(\kappa_g \nabla p) = -\Delta \bar{y} + \operatorname{div} z + (\mu_g^b - \mu_g^a)_{|\Omega_g|} & \text{in } \Omega_g, \\ -\operatorname{div}(\kappa_s \nabla p) = \mu_{s|\Omega_s} & \text{in } \Omega_s, \end{cases}$$
$$\kappa_g \left(\frac{\partial p}{\partial_{n_r}}\right)_g - \kappa_s \left(\frac{\partial p}{\partial_{n_r}}\right)_s - 4\sigma |\bar{y}|^3 G^* p = -\frac{\partial \bar{y}}{\partial n_r} + z \cdot n_r & \text{on } \Gamma_r, \end{cases}$$

$$\kappa_s \frac{\partial p}{\partial n_0} + 4\varepsilon \sigma |\bar{y}|^3 p = \mu_{s|\Gamma_0} \qquad \text{on } \Gamma_0.$$

Again, the multipliers are decomposed into their restrictions on Ω_s , Ω_g , Γ_r , and Γ_0 , respectively. Analogously to Definition 4.1, we define solutions to (5.7):

Definition 5.5 A function $p \in W^{1,q'}(\Omega)$ is said to be the weak solution of (5.7) if it satisfies (5.5).

Clearly, thanks to Lemma 4.1, there exists a unique solution of (5.7) in the sense of Definition 5.5 (cf. Theorem 4.1). Using the definition of p and (5.4), (5.1) can be transformed into

(5.8)
$$\frac{\partial \mathcal{L}}{\partial u}(\bar{u},\mu)(u-\bar{u}) = \int_{\Omega_s} (p+\beta\bar{u})(u-\bar{u}) \, dx \ge 0 \quad \forall u \in \mathcal{U}.$$

By standard arguments, a pointwise evaluation of this equation implies

(5.9)
$$\bar{u} = \mathcal{P}_{ad} \Big\{ -\frac{1}{\beta} p(x) \Big\},$$

where $\mathcal{P}_{ad}: L^2(\Omega_s) \to L^2(\Omega_s)$ denotes the pointwise projection operator on the admissible set \mathcal{U} . In this way, we find the following theorem that states the first-order necessary optimality conditions for (P):

Theorem 5.2 (First-order necessary optimality conditions for (P)) Let $\bar{u} \in L^2(\Omega_s)$ be an optimal solution of (P) with the associated state $\bar{y} = \mathcal{G}(\bar{u}) \in W^{1,q}(\Omega)$, q > N. Suppose further that \bar{u} satisfies Assumption 3.1 and the linearized Slater conditions. Then, there exist an adjoint state $p \in W^{1,q'}(\Omega)$, $q' < \frac{N}{N-1}$, and Lagrange multipliers $\mu_s \in \mathcal{M}(\overline{\Omega}_s)$, $\mu_g^a \in \mathcal{M}(\overline{\Omega}_g)$, and $\mu_g^b \in \mathcal{M}(\overline{\Omega}_g)$ such that the following relations are satisfied:

- the state equation (SL) in the sense of Definition 2.1
- the adjoint equation (5.7) in the sense of Definition 5.5
- the projection formula (5.9)
- the nonnegativity of the Lagrange multipliers (5.2)
- the complimentary slackness conditions (5.3).

It is straight forward to see that, if $u_a, u_b \in W^{1,q'}(\Omega_s)$, then \mathcal{P}_{ad} is continuous from $W^{1,q'}(\Omega_s)$ to $W^{1,q'}(\Omega_s)$ such that the following regularity result for the optimal control is obtained:

Remark 5.1 If $u_a, u_b \in W^{1,q'}(\Omega_s)$, then the optimal control \bar{u} is a function in $W^{1,q'}(\Omega_s)$, $q' < \frac{N}{N-1}$.

6 Second-order sufficient optimality conditions for (P)

In the following, we present second-order sufficient optimality conditions for (P) that guarantee local optimality in an L^2 -neighborhood. The investigation of second-order sufficient optimality conditions for semilinear control problems with pointwise state constraints was originally undertaken by Casas et al. in [8]. They suggested second-order optimality conditions that deal with strongly active sets. However, owing to the presence of the two-norm discrepancy, the result only provides sufficient optimality conditions for local solutions in $L^{\infty}(\Omega)$. Later on, Casas et al. [7] modified this result and arrived at sufficient conditions that are in some sense less restrictive than the original one. In particular, under certain assumptions, these conditions ensure the existence of local solutions in $L^2(\Omega)$. The result is, however, not directly applicable for (P) since we here deal with a nonmonotone operator Gand the objective functional in (P) is different from that considered in [7]. However, thanks to Theorem 3.2, we obtain analogous second-order sufficient conditions for the existence of local solutions to (P) in $L^2(\Omega_s)$. At this point, let us underline that the proof of Theorem 6.1 below basically follows the lines of a similar technique proposed in [7]. First of all, let us define the operator $S: L^2(\Omega_s) \to C(\overline{\Omega})$ by $S = E_c \mathcal{G}$. Since the embedding $W^{1,q}(\Omega) \hookrightarrow C(\overline{\Omega})$ is compact (note that q > N) and by the continuity of \mathcal{G} , the operator $S = E_c \mathcal{G} : L^2(\Omega_s) \to C(\overline{\Omega})$ is as well compact.

Definition 6.1 Let $\bar{u} \in \mathcal{U}$ be a feasible control of (P) with the associated state $\mathcal{G}(\bar{u}) = \bar{y}$. We assume that there exist $\mu_g^a, \mu_g^b \in \mathcal{M}(\overline{\Omega}_g), \mu_s \in \mathcal{M}(\overline{\Omega}_s)$ and $p \in W^{1,q'}(\Omega), 1 \leq q' \leq N/(N-1)$, satisfying (5.1)-(5.3) and (5.7).

(i) The convex, closed subset $\mathcal{H}_{\bar{u}} \subset L^2(\Omega_s)$ is given by:

$$\mathcal{H}_{\bar{u}} := \left\{ h \in L^2(\Omega_s) \mid h(x) = \left\{ \begin{array}{ccc} \geq & 0 & if & \bar{u}(x) = u_a(x) \\ \leq & 0 & if & \bar{u}(x) = u_b(x) \end{array} \right\}.$$

(ii) The subset $C_{\bar{u}} \subset \mathcal{H}_{\bar{u}}$ is defined as follows:

 $\mathcal{C}_{\bar{u}} = \{h \in \mathcal{H}_{\bar{u}} \mid h \text{ satisfies } (6.1), (6.2) \text{ and } (6.3)\}$

(6.1)
$$h(x) = 0 \quad if \quad p(x) + \beta \bar{u}(x) \neq 0$$

(6.2)
$$y_h(x) = \begin{cases} \geq 0 & \text{if } \bar{y}(x) = y_a(x), \ x \in \overline{\Omega}_g \\ \leq 0 & \text{if } \bar{y}(x) = y_b(x), \ x \in \overline{\Omega}_g \\ \leq 0 & \text{if } \bar{y}(x) = y_{\max}(x), \ x \in \overline{\Omega}_s \end{cases}$$

(6.3)
$$\int_{\bar{\Omega}_g} y_h \ d\mu_g^a = \int_{\bar{\Omega}_g} y_h \ d\mu_g^b = \int_{\bar{\Omega}_s} y_h \ d\mu_s = 0,$$

where $y_h = \S'(\bar{u})h$.

(iii) We say that \bar{u} satisfies the second order sufficient condition (SSC) if

(SSC)
$$\frac{\partial^2 \mathcal{L}}{\partial u^2} (\bar{u}, \mu) h^2 > 0$$

holds true for every $h \in C_{\bar{u}} \setminus \{0\}$.

Theorem 6.1 (Second-order sufficient optimality conditions for (P)) Let $\bar{u} \in \mathcal{U}$ be a feasible control of (P) and let Assumption 3.1 be fulfilled. Furthermore, assume that there exist $\mu_g^a, \mu_g^b \in \mathcal{M}(\overline{\Omega}_g), \ \mu_s \in \mathcal{M}(\overline{\Omega}_s)$ and $p \in W^{1,q'}(\Omega), \ 1 \leq q' \leq N/(N-1)$, satisfying (5.1)-(5.3) and (5.7). If \bar{u} additionally satisfies (SSC), then there exist positive real numbers ε and δ such that

$$f(\bar{u}) + \frac{\delta}{2} \|u - \bar{u}\|_{L^2(\Omega_s)}^2 \le f(u),$$

holds true for every feasible control u of (P) with $||u - \bar{u}||_{L^2(\Omega_s)} < \varepsilon$. Hence, \bar{u} is a local solution of (P) according to Definition 5.1.

Proof. Let us assume the contrary: There exists a sequence $\{u_k\}_{k=1}^{\infty} \subset L^2(\Omega_s)$ of feasible controls of (P) such that:

(6.4)
$$f(\bar{u}) + \frac{1}{k} \|u_k - \bar{u}\|_{L^2(\Omega_s)}^2 > f(u_k) \ \forall k \in \mathbb{N} \text{ and } \lim_{k \to \infty} \|u_k - \bar{u}\|_{L^2(\Omega_s)} = 0.$$

We define $h_k := \frac{1}{a_k}(u_k - \bar{u})$ with $a_k := ||u_k - \bar{u}||_{L^2(\Omega_s)}$. Thus, $||h_k||_{L^2(\Omega_s)} = 1$ holds for all $k \in \mathbb{N}$. For this reason, there exists a subsequence denoted w.l.o.g. again by $\{h_k\}_{k=1}^{\infty}$, which converges weakly in $L^2(\Omega_s)$ to some $\bar{h} \in L^2(\Omega_s)$, i.e., $h_k \rightharpoonup \bar{h}$ as $k \to \infty$.

First, we show that $\frac{\partial \mathcal{L}}{\partial u}(\bar{u},\mu)\bar{h} = 0$. Since u_k is feasible for all $k \in \mathbb{N}$, the first order necessary conditions, see (5.1), imply

$$0 \leq \frac{1}{a_k} \frac{\partial \mathcal{L}}{\partial u} (\bar{u}, \mu) (u_k - \bar{u}) = \frac{\partial \mathcal{L}}{\partial u} (\bar{u}, \mu) h_k \quad \forall k \in \mathbb{N}.$$

Thus, since $h_k \rightarrow \bar{h}$ as $k \rightarrow \infty$, we find

(6.5)
$$0 \le \lim_{k \to \infty} \frac{\partial \mathcal{L}}{\partial u} (\bar{u}, \mu) h_k = \frac{\partial \mathcal{L}}{\partial u} (\bar{u}, \mu) \bar{h}.$$

On the other hand, the feasibility of u_k for (P) implies that $\mathcal{L}(u_k, \mu) \leq f(u_k)$ and hence from (6.4) we infer that

(6.6)
$$\mathcal{L}(u_k,\mu) \le f(u_k) < f(\bar{u}) + \frac{1}{k} \|u_k - \bar{u}\|_{L^2(\Omega_s)}^2 = \mathcal{L}(\bar{u},\mu) + \frac{1}{k} \|u_k - \bar{u}\|_{L^2(\Omega_s)}^2 \quad \forall k \in \mathbb{N},$$

where we used the complementary slackness conditions (5.3). Furthermore, Theorem 3.2 implies the existence of an open Ball $B_r(\bar{u})$, with radius r > 0, around \bar{u} in $L^2(\Omega_s)$ such that \mathcal{G} is twice continuously differentiable on $B_r(\bar{u})$. Since $\{u_k\}_{k=1}^{\infty}$ converges strongly to \bar{u} as $k \to \infty$, there exists in particular an index number $k_0 \in \mathbb{N}$ such that

(6.7)
$$u_k \in B_r(\bar{u}), \quad \forall k \ge k_0.$$

Notice that we define $\overline{u_k \overline{u}} := \{u_k + t(\overline{u} - u_k) \mid t \in [0, 1]\}$ and hence for all $k \ge k_0$, $\overline{u_k \overline{u}} \subset B_r(\overline{u})$. Consequently, for every $k \ge k_0$, there exists a point w_k between u_k and \overline{u} (i.e. $w_k \in \overline{u_k \overline{u}}$) such that

(6.8)
$$\mathcal{L}(u_k,\mu) - \mathcal{L}(\bar{u},\mu) = \frac{\partial \mathcal{L}}{\partial u}(w_k,\mu)(u_k - \bar{u}) = a_k \frac{\partial \mathcal{L}}{\partial u}(w_k,\mu)h_k \quad \forall \ k \ge k_0.$$

Therefore, from (6.6)-(6.8), we obtain:

(6.9)
$$\frac{\partial \mathcal{L}}{\partial u}(w_k,\mu)h_k < \frac{1}{k} \|u_k - \bar{u}\|_{L^2(\Omega_s)} \quad \forall \ k \ge k_0$$

Due to the strong convergence of u_k to \bar{u} in $L^2(\Omega_s)$, it holds that $\lim_{k\to\infty} w_k = \bar{u}$ in $L^2(\Omega_s)$ and consequently $\frac{\partial \mathcal{L}}{\partial u}(w_k,\mu) \to \frac{\partial \mathcal{L}}{\partial u}(\bar{u},\mu)$ strongly in $L^2(\Omega_s)^*$, as $k\to\infty$. For this reason, the weak convergence of h_k to \bar{h} in $L^2(\Omega_s)$ implies:

$$\lim_{k \to \infty} \frac{\partial \mathcal{L}}{\partial u} (w_k, \mu) h_k = \frac{\partial \mathcal{L}}{\partial u} (\bar{u}, \mu) \bar{h}.$$

From the above equality and by (6.4) as well as (6.9), we infer further

$$\frac{\partial \mathcal{L}}{\partial u}(\bar{u},\mu)\bar{h} \le 0,$$

which implies together with (6.5)

(6.10)
$$\frac{\partial \mathcal{L}}{\partial u}(\bar{u},\mu)\bar{h} = 0.$$

Next, we show that \overline{h} belongs to $\mathcal{H}_{\overline{u}}$, cf. Definition 6.1. Since u_k is feasible for (P) for every $k \in \mathbb{N}$, one finds that

$$h_k(x) = a_k(u_k - \bar{u}) = \begin{cases} \ge & 0 & \text{if } \bar{u}(x) = u_a(x) \\ \le & 0 & \text{if } \bar{u}(x) = u_b(x). \end{cases}$$

Consequently, $\{h_k\}_{k=1}^{\infty} \subset \mathcal{H}_{\bar{u}}$. Since $\mathcal{H}_{\bar{u}}$ is convex and closed, the weak limit \bar{h} belongs to $\mathcal{H}_{\bar{u}}$. Now let us prove that $\bar{h} \in \mathcal{C}_{\bar{u}}$. This is shown in three steps:

(i) The weak limit $\bar{h} \in \mathcal{H}_{\bar{u}}$ satisfies the condition (6.1):

From the projection formel (5.9), we infer that

(6.11)
$$p(x) + \beta \bar{u}(x) = \begin{cases} \geq 0 & \text{if } \bar{u}(x) = u_a(x), \\ = 0 & \text{if } u_a(x) < \bar{u}(x) < u_a(x), \\ \leq 0 & \text{if } \bar{u}(x) = u_b(x). \end{cases}$$

Moreover, since $\bar{h} \in \mathcal{H}_{\bar{u}}$,

(6.12)
$$(p+\beta\bar{u})\bar{h} \ge 0$$
 a.e. in Ω_s

On the other hand, (6.10) implies that

$$0 = \frac{\partial \mathcal{L}}{\partial u} (\bar{u}, \mu) \bar{h} = \int_{\Omega_s} (p + \beta \bar{u}) \bar{h} \, dx$$

(cf. (5.8)). Consequently, by (6.12), $\bar{h}(x) = 0$ if $p(x) + \beta \bar{u}(x) \neq 0$ such that \bar{h} satisfies (6.1).

(ii) The weak limit $\bar{h} \in \mathcal{H}_{\bar{u}}$ satisfies the condition (6.2):

Let us set $\bar{y} = S(\bar{u})$ and define the sets \mathcal{A}_a , \mathcal{A}_b and \mathcal{A}_{\max} by:

$$\begin{aligned} \mathcal{A}_a &:= \{ x \in \overline{\Omega}_g \mid \bar{y}(x) = y_a(x) \}, \\ \mathcal{A}_b &:= \{ x \in \overline{\Omega}_g \mid \bar{y}(x) = y_b(x) \}, \\ \mathcal{A}_{\max} &:= \{ x \in \overline{\Omega}_s \mid \bar{y}(x) = y_{\max}(x) \} \end{aligned}$$

Since u_k , for every $k \in \mathbb{N}$, is feasible for (P), we obtain for all $k \in \mathbb{N}$:

$$\frac{S(u_k)(x) - \bar{y}(x)}{\|u_k - \bar{u}\|_{L^2(\Omega_s)}} \ge 0 \quad \forall x \in \mathcal{A}_a.$$

Additionally, by passing to the limit $k \to \infty$, we obtain due to the continuous Fréchet differentiability of \mathcal{G} : $L^2(\Omega_s) \to W^{1,q}(\Omega)$ at \bar{u} and the compactness of the embedding $W^{1,q}(\Omega) \hookrightarrow \mathcal{C}(\overline{\Omega})$:

$$S'(\bar{u})\bar{h} = \lim_{k \to \infty} S'(\bar{u})h_k = \lim_{k \to \infty} \frac{S'(\bar{u})(u_k - \bar{u})}{\|u_k - \bar{u}\|_{L^2(\Omega_s)}} = \lim_{k \to \infty} \frac{S(u_k) - S(\bar{u})}{\|u_k - \bar{u}\|_{L^2(\Omega_s)}} \quad \text{in } \mathcal{C}(\overline{\Omega}).$$

Thus, $S'(\bar{u})\bar{h} =: y_{\bar{h}}$ satisfies: $y_{\bar{h}}(x) \ge 0$ for all $x \in \mathcal{A}_a$. In a similar way, we show $y_{\bar{h}}(x) \le 0$ for all $x \in \mathcal{A}_b$ and $y_{\bar{h}}(x) \le 0$ for all $x \in \mathcal{A}_{\max}$.

(iii) The weak limit $\bar{h} \in \mathcal{H}_{\bar{u}}$ satisfies the condition (6.3):

The complementarity slackness conditions (5.3) imply that $\mu_g^a = 0$ on $\overline{\Omega}_g \setminus \mathcal{A}_a$, $\mu_g^b = 0$ on $\overline{\Omega}_g \setminus \mathcal{A}_b$ and $\mu_s = 0$ on $\overline{\Omega}_s \setminus \mathcal{A}_{\text{max}}$. In view of (6.10), we hence obtain

(6.13)
$$0 = \frac{\partial \mathcal{L}}{\partial u}(\bar{u},\mu)\bar{h} = f'(\bar{u})\bar{h} + \int_{\mathcal{A}_{\max}} y_{\bar{h}}d\mu_s + \int_{\mathcal{A}_b} y_{\bar{h}}d\mu_g^b - \int_{\mathcal{A}_a} y_{\bar{h}}d\mu_g^a$$

On the one hand, we have due to the non-negativity of μ_s, μ_g^a, μ_g^b and (ii)

(6.14)
$$\int_{\mathcal{A}_b} y_{\bar{h}} d\mu_g^b \le 0, \quad \int_{\mathcal{A}_{\max}} y_{\bar{h}} d\mu_s \le 0 \quad \text{and} \quad -\int_{\mathcal{A}_a} y_{\bar{h}} d\mu_g^a \le 0.$$

On the other hand, by the assumption (6.4)

(6.15)
$$f'(\bar{u})\bar{h} = \lim_{k \to \infty} f'(\bar{u})h_k = \lim_{k \to \infty} \frac{f'(\bar{u})(u_k - \bar{u})}{\|u_k - \bar{u}\|_{L^2(\Omega_s)}} \\ = \lim_{k \to \infty} \frac{f(u_k) - f(\bar{u})}{\|u_k - \bar{u}\|_{L^2(\Omega_s)}} \le \lim_{k \to \infty} \frac{1}{k} \|u_k - \bar{u}\|_{L^2(\Omega_s)} = 0.$$

From (6.13), (6.14), and (6.15), we infer that

$$\int_{\mathcal{A}_{\max}} y_{\bar{h}} d\mu_s = \int_{\mathcal{A}_b} y_{\bar{h}} d\mu_g^b = \int_{\mathcal{A}_a} y_{\bar{h}} d\mu_g^a = 0.$$

Therefore, since $\mu_s = 0$ on $\overline{\Omega}_s \setminus \mathcal{A}_{\max}$, $\mu_g^a = 0$ on $\overline{\Omega}_g \setminus \mathcal{A}_a$ and $\mu_g^b = 0$ on $\overline{\Omega}_g \setminus \mathcal{A}_b$, (iii) is verified. Thus, we have just shown that $\overline{h} \in \mathcal{C}_{\overline{u}}$. Let us now demonstrate that $\overline{h} = 0$. From this, we obtain the desired contradiction. Again, since \mathcal{G} is twice continuously differentiable on $B_r(\overline{u})$, for each $k \ge k_0$ there exists a point $z_k \in L^2(\Omega_s)$ between u_k and \overline{u} (i.e. $z_k \in \overline{u_k \overline{u}}$) such that

$$\mathcal{L}(u_k,\mu) = \mathcal{L}(\bar{u},\mu) + a_k \frac{\partial \mathcal{L}}{\partial u}(\bar{u},\mu)h_k + \frac{a_k^2}{2} \frac{\partial^2 \mathcal{L}}{\partial u^2}(z_k,\mu)h_k^2 \quad \forall \ k \ge k_0$$

where k_0 is as defined before in (6.7). By rearranging and dividing by $a_k^2/2$, the above equation is equivalent to

$$2\frac{\partial \mathcal{L}}{\partial u}(\bar{u},\mu)(u_k-\bar{u}) + \frac{\partial^2 \mathcal{L}}{\partial u^2}(\bar{u},\mu)h_k^2 = \frac{2}{a_k^2} \{\mathcal{L}(u_k,\mu) - \mathcal{L}(\bar{u},\mu)\} + \left[\frac{\partial^2 \mathcal{L}}{\partial u^2}(\bar{u},\mu) - \frac{\partial^2 \mathcal{L}}{\partial u^2}(z_k,\mu)\right]h_k^2 \quad \forall \ k \ge k_0.$$

Hence, since u_k is feasible for (P) and $||h_k||_{L^2(\Omega_s)} = 1$ for all $k \in \mathbb{N}$, the latter equality together with (5.1) and (6.6) imply that

(6.16)
$$\frac{\partial^2 \mathcal{L}}{\partial u^2}(\bar{u},\mu)h_k^2 < \frac{1}{k} + \|\frac{\partial^2 \mathcal{L}}{\partial u^2}(\bar{u},\mu) - \frac{\partial^2 \mathcal{L}}{\partial u^2}(z_k,\mu)\|_{\mathcal{B}^2(L^2(\Omega_s))} \quad \forall \ k \ge k_0$$

where $\mathcal{B}^2(L^2(\Omega_s))$ denotes the space of bounded bilinear forms from $L^2(\Omega_s) \times L^2(\Omega_s)$ to \mathbb{R} . Notice that $\frac{\partial^2 \mathcal{L}}{\partial u^2}(\cdot, \mu)$ is continuous from $L^2(\Omega_s)$ to $\mathcal{B}^2(L^2(\Omega_s))$, and hence since $\lim_{k\to\infty} z_k = \bar{u}$ in $L^2(\Omega_s)$, the right hand side of (6.16) converges to zero as $k \to \infty$. We consider now the left hand side of (6.16). For each $k \in \mathbb{N}$, we set $y_k := \mathcal{G}'(\bar{u})h_k$ and $w_k := \mathcal{G}''(\bar{u})h_k^2$ and hence

(6.17)
$$\frac{\partial^{2} \mathcal{L}}{\partial u^{2}}(\bar{u},\mu)h_{k}^{2} = \|\nabla y_{k}\|_{L^{2}(\Omega_{g})}^{2} + (\nabla \bar{y} - z, \nabla w_{k})_{L^{2}(\Omega_{g})} + \beta \|h_{k}\|_{L^{2}(\Omega_{s})}^{2} + \int_{\bar{\Omega}_{s}} w_{k} \ d\mu_{s} + \int_{\bar{\Omega}_{g}} w_{k} \ d\mu_{g}^{b} - \int_{\bar{\Omega}_{g}} w_{k} \ d\mu_{g}^{a}.$$

Obviously, since $\mathcal{G}'(\bar{u})$ is continuous and linear from $L^2(\Omega_s)$ to $W^{1,q}(\Omega)$ and $h_k \rightharpoonup \bar{h}$ in $L^2(\Omega_s)$, one finds

(6.18)
$$\nabla y_k \rightharpoonup \nabla y_{\bar{h}} \text{ in } L^2(\Omega) \text{ as } k \rightarrow \infty,$$

with $y_{\bar{h}} = \mathcal{G}'(\bar{u})\bar{h}$. Moreover, the second term of the right hand side of the equality (6.17) can be written as follows, cf. [13] p. 79,

(6.19)
$$(\nabla \bar{y} - z, \nabla w_k)_{L^2(\Omega_g)} = -12 \int_{\Gamma_r} (G\sigma |\bar{y}| \bar{y} y_k^2) q \ ds - 12 \int_{\Gamma_0} \varepsilon \sigma |\bar{y}| \bar{y} y_k^2 q \ ds.$$

Here, q is the solution of the following PDE

$$-\operatorname{div}(\kappa_g \nabla q) = -\Delta \bar{y} + \operatorname{div} z \quad \text{in } \Omega_g,$$

$$-\operatorname{div}(\kappa_s \nabla q) = 0 \quad \text{in } \Omega_s,$$

$$\kappa_g \left(\frac{\partial p}{\partial_{n_r}}\right)_g - \kappa_s \left(\frac{\partial p}{\partial_{n_r}}\right)_s - 4\sigma |\bar{y}|^3 G^* q = -\frac{\partial \bar{y}}{\partial n_r} + z \cdot n_r \quad \text{on } \Gamma_r,$$

$$\kappa_s \frac{\partial q}{\partial n_0} + 4\varepsilon \sigma |\bar{y}|^3 q = 0 \quad \text{on } \Gamma_0,$$

i.e. (5.7) without the multipliers on the right-hand side. It is straight-forward to show that Assumption 3.1 implies the existence of a unique solution $q \in H^1(\Omega)$, cf. [13]. Now, since h_k converges weakly to \bar{h} as $k \to \infty$, and due to the compactness of the embedding $W^{1,q}(\Omega) \hookrightarrow C(\overline{\Omega})$, we obtain $\lim_{k\to\infty} y_k = y_{\bar{h}}$ in $C(\overline{\Omega})$ with $y_{\bar{h}}$ as defined above. Hence, from (6.19), one finds:

$$\lim_{k \to \infty} (\nabla \bar{y} - z, \nabla w_k)_{L^2(\Omega_g)} = \lim_{k \to \infty} \left\{ -12 \int_{\Gamma_r} (G\sigma |\bar{y}| \bar{y} y_k^2) q \ ds - 12 \int_{\Gamma_0} \varepsilon \sigma |\bar{y}| \bar{y} y_k^2 q \ ds \right\}$$

$$= -12 \int_{\Gamma_r} (G\sigma |\bar{y}| \bar{y} y_{\bar{h}}^2) q \ ds - 12 \int_{\Gamma_0} \varepsilon \sigma |\bar{y}| \bar{y} y_{\bar{h}}^2 q \ ds$$

$$= (\nabla \bar{y} - z, \nabla w_{\bar{h}})_{L^2(\Omega_g)}$$

where $w_{\bar{h}} = \mathcal{G}''(\bar{u})\bar{h}^2$ or equivalently $w_{\bar{h}} = -(A'_q(\bar{y}))^{-1}A''_q(\bar{y})[y_{\bar{h}}, y_{\bar{h}}]$ (see Theorem 3.2). In view of (3.2), $A''_q(\bar{y})$ is obviously continuous from $\mathcal{C}(\overline{\Omega}) \times \mathcal{C}(\overline{\Omega})$ to $W^{1,q'}(\Omega)^*$. Thus, together with the compactness of the embedding $W^{1,q}(\Omega) \hookrightarrow \mathcal{C}(\overline{\Omega})$, Theorem 3.1 implies that $\lim_{k \to \infty} w_k = w_{\bar{h}}$ in $\mathcal{C}(\overline{\Omega})$ (recall that $w_k = \mathcal{G}''(\bar{u})h_k^2$ or equivalently $w_k = -(A'_q(\bar{y}))^{-1}A''_q(\bar{y})[y_k, y_k]$). Therefore, one obtains as $k \to \infty$:

(6.21)
$$\int_{\bar{\Omega}_g} w_k d\mu_g^a \to \int_{\bar{\Omega}_g} w_{\bar{h}} d\mu_g^a, \ \int_{\bar{\Omega}_g} w_k d\mu_g^b \to \int_{\bar{\Omega}_g} w_{\bar{h}} d\mu_g^b, \ \int_{\bar{\Omega}_s} w_k d\mu_s \to \int_{\bar{\Omega}_s} w_{\bar{h}} d\mu_s.$$

Applying (6.16)-(6.21) and together with the weak convergence of h_k to \bar{h} in $L^2(\Omega_s)$, we continue with

$$\begin{aligned} \frac{\partial^{2} \mathcal{L}}{\partial u^{2}}(\bar{u},\mu)\bar{h}^{2} = & \|\nabla y_{\bar{h}}\|_{L^{2}(\Omega_{g})}^{2} + (\nabla \bar{y} - z, \nabla w_{\bar{h}})_{L^{2}(\Omega_{g})} + \beta \|\bar{h}\|_{L^{2}(\Omega_{s})}^{2} \\ & + \int_{\bar{\Omega}_{s}} w_{\bar{h}} d\mu_{s} - \int_{\bar{\Omega}_{g}} w_{\bar{h}} d\mu_{g}^{a} + \int_{\bar{\Omega}_{g}} w_{\bar{h}} d\mu_{g}^{b} \\ & \leq \liminf_{k \to \infty} \frac{\partial^{2} \mathcal{L}}{\partial u^{2}}(\bar{u},\mu)h_{k}^{2} \\ & \leq \lim_{k \to \infty} \left\{\frac{1}{k} + \|\frac{\partial^{2} \mathcal{L}}{\partial u^{2}}(\bar{u},\mu) - \frac{\partial^{2} \mathcal{L}}{\partial u^{2}}(z_{k},\mu)\|_{\mathcal{B}^{2}(L^{2}(\Omega_{s}))}\right\} = 0 \end{aligned}$$

For this reason and since $\bar{h} \in C_{\bar{u}}$, (SSC) implies that $\bar{h} = 0$. Thus, we have $y_{\bar{h}} = 0$ and $w_{\bar{h}} = 0$ and consequently, $\lim_{k \to \infty} (\nabla \bar{y} - z, \nabla w_k)_{L^2(\Omega_g)} = 0$. In view of (6.16), (6.17), and since $\|h_k\|_{L^2(\Omega_s)} = 1$ for all $k \in \mathbb{N}$, we therefore arrive at

$$\begin{split} 1 &= \|h_k\|_{L^2(\Omega_s)}^2 \leq \frac{1}{\beta} \Big[\frac{\partial^2 \mathcal{L}}{\partial u^2} (\bar{u}, \mu) h_k^2 - (\nabla \bar{y} - z, \nabla w_k)_{L^2(\Omega_g)} + \int_{\bar{\Omega}_g} w_k d\mu_g^a - \int_{\bar{\Omega}_g} w_k d\mu_g^b - \int_{\bar{\Omega}_s} w_k d\mu_s \Big] \\ &< \frac{1}{\beta} \Big[\frac{1}{k} + \| \frac{\partial^2 \mathcal{L}}{\partial u^2} (\bar{u}, \mu) - \frac{\partial^2 \mathcal{L}}{\partial u^2} (z_k, \mu) \|_{\mathcal{B}^2(L^2(\Omega_s))} \\ &- (\nabla \bar{y} - z, \nabla w_k)_{L^2(\Omega_g)} + \int_{\bar{\Omega}_g} w_k d\mu_g^a - \int_{\bar{\Omega}_g} w_k d\mu_g^b - \int_{\bar{\Omega}_s} w_k d\mu_s \Big], \quad \forall \ k \geq k_0. \end{split}$$

Finally, by passing to the limit $k \to \infty$, the theorem is verified.

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