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Regularization of state-constrained elliptic optimal control problems with nonlocal radiation interface conditions

Christian Meyer[1], Irwin Yousept[2]

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[1] Weierstraß-Institut für Angewandte Analysis und Stochastik
Mohrenstr. 39
10117 Berlin
Germany
E-Mail: meyer@wias-berlin.de

[2] Institut für Mathematik
Technische Universität Berlin
Straße des 17. Juni 136
10623 Berlin
Germany
E-Mail: yousept@math.tu-berlin.de

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Edited by
Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS)
Mohrenstraße 39
10117 Berlin
Germany

Fax: + 49 30 2044975
E-Mail: preprint@wias-berlin.de
World Wide Web: http://www.wias-berlin.de/

Abstract

A state-constrained optimal control problem with nonlocal radiation interface conditions arising from the modeling of crystal growth processes is considered. The problem is approximated by a Moreau-Yosida type regularization. Optimality conditions for the regularized problem are derived and the convergence of the regularized problems is shown. In the last part of the paper, some numerical results are presented.

1 Introduction

The seeded sublimation growth technique, which is also known as "physical vapor transport" (PVT), is nowadays widely used for producing semiconductor single crystal. The most common design of PVT systems is to place the polycrystalline powder source under a low-pressure inert gas atmosphere at the bottom of a cavity inside a graphite crucible. At high temperatures of 2000-3000 K and low pressure, the polycrystalline powder sublimates, and the resulting gas diffuses to the relatively cold seed at top of the cavity. Hereafter, crystallization takes place, see [18, 19] for further details. One of the main factors influencing the quality of the produced crystal is the temperature distribution in the growth system. In particular, the temperature gradient close to the surface of the growing crystal plays a significant role on the growth rate as well as on the quality of the resulting crystal, cf. [25].

In the recent years, some efforts were made in optimizing the growth process. We only refer to [21, 22], where the temperature gradient inside the cavity is optimized by directly controlling the heat sources in the crucible. In [23], the corresponding model is extended by including pointwise inequality constraints on the temperature to ensure sublimation of the source powder and crystallization at the seed. As these additional constraints represent pointwise state constraints, this extension significantly increases the complexity of the problem. The first- and second-order analysis for the associated control problem is performed in [23]. Based on these results, we here focus on the numerical treatment of the problem. To be more precise, a regularization in the spirit of [16] is under consideration. In our framework, we consider a fairly simplified geometry: The solid graphite crucible and the cavity inside the crucible are denoted by open bounded domains Ω_g and Ω_s, respectively. The outer and interface boundaries denoted by $\Gamma_0 := \partial\Omega$ and $\Gamma_r := \overline{\Omega}_s \cap \overline{\Omega}_g$, respectively. An exemplary two-dimensional domain is depicted in Figure 1.1.

As in [21, 22, 23], we optimize the gradient temperature in the gas phase Ω_g by controlling the heat source u in the solid phase Ω_s. The objective functional, considered here, reads as follows:

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

where y denotes the temperature and the desired temperature gradient $z \in L^2(\Omega_g)$ is assumed to be fixed. As it is essential to account for radiation due to the high temperature, y is given by the solution of the stationary heat equation with radiation interface and boundary conditions

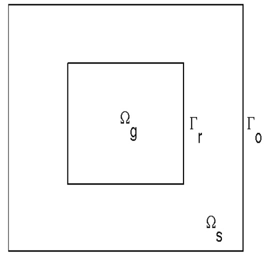

Figure 1.1: An exemplary two-dimensional domain.

on Γ_r and Γ_0, respectively:

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

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. For a detailled description of the model see [24]. In addition to the stationary semilinear heat equation, the optimization is subject to the following pointwise state- and control-constraints:

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

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, as mentioned above, the state-constraints in Ω_g are required to ensure sublimation of the polycrystalline powder and crystallization at the seed, respectively. The first- and second-order analysis for (P) has been carried out quite recently in [23]. In order to obtain the Karush-Kuhn-Tucker (KKT) type optimality conditions, the constraints, imposed on the state y in (1.1), have to be considered in the space of continuous functions, denoted by $\mathcal{C}(\overline{\Omega})$. In other words, we require the continuity of the solutions to (SL) for the optimality conditions for (P). In fact, based on maximum elliptic regularity results (see [12, 11]), the continuity of the state y is shown in [23]. Hereafter, first-order optimality conditions for (P) were derived. Furthermore, second-order sufficient optimality conditions for (P) are presented in [23]. The corresponding arguments basically follow a recent work of Casas et al. [8]. As demonstrated in [23], the Lagrange multipliers associated with the state-constraints of (P) are elements of the dual space $\mathcal{C}(\overline{\Omega})^*$. Consequently, they are in general nonregular and might have measure type components, cf. also [6, 7] or Alibert and Raymond [2] for general state-constrained problems. Therefore, direct application of semismooth Newton methods, or equivalently primal-dual active set strategies [13, 17] to the control problem (P) is not possible.

We overcome this obstacle by utilizing a "Moreau-Yosida" type regularization approach that removes the pointwise state inequality constraints of (P) by adding a penalty term to the objective functional of (P). Notice that the Moreau-Yosida type regularization for state-constratined control problems was originally introduced by Ito and Kunisch [16], see also [14, 15, 4, 5]. We investigate the regularized problem analytically. Essentially, we show the convergence of the regularized problems in the following sense:

If $\bar{u} \in L^2(\Omega_s)$ is a local solution of (P) satisfying the second-order sufficient optimality conditions for (P), then there exists a sequence of local solutions of regularized problems converging strongly in $L^2(\Omega_s)$ to $\bar{u}$, as the penalty parameter tends to infinity.

The paper is organized as follows: First, we introduce the general assumptions as well as the notation used throughout the paper. Then, in Section 2 and 3, we recall some important results concerning with the optimality conditions for (P). Afterwards, a Moreau-Yosida type regularization is introduced in Section 4. Section 5 is devoted the convergence analysis. Finally, in the last part of the paper, some numerical results are presented.

1.1 General Assumptions and Notation

We start by introducing the general assumptions of the problem statement including the notation used throughout this paper. If V is a linear normed function space, then we use the notation $\|\cdot\|_V$ for a standard norm used in V. The dual space of V is denoted by V^* and for the associated duality pairing, we write $< . , . >_{V^*,V}$. 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 V to Y is defined by $\mathcal{B}(V,Y)$. For an arbitrary $A \in \mathcal{B}(V,Y)$, the associated adjoint operator of A is denoted by $A^* \in \mathcal{B}(Y^*, V^*)$, and for its inverse, if it exists, we write $A^{-*} := (A^*)^{-1}$. By $\mathcal{C}(\overline{\Omega})$, we define all continuous function on $\overline{\Omega}$. We identify the dual space $\mathcal{C}(\overline{\Omega})^*$ with the space of real regular Borel measures on $\overline{\Omega}$, devoted $\mathcal{M}(\overline{\Omega})$. 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-dimensional case, Γ_r is assumed to be a closed Lipschitz surface and piecewise $\mathcal{C}^{1,\delta}$, whereas it is of class C^1 in the three-dimensional case. The subdomain Ω_s is defined by $\Omega_s = \Omega \setminus \overline{\Omega}_g$. The distance of Γ_r to Γ_0 is supposed to be positive.*

($\mathcal{A}_2$) The desired temperature gradient z is given in $L^2(\Omega_g)^N$ 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 positive real number $\kappa_{\min}$.

($\mathcal{A}_4$) 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 $y_0(x) \geq \theta$ a.e. on Γ_0 with $\theta \in \mathbb{R}^+ \setminus \{0\}$.

($\mathcal{A}_5$) *The bounds in the state constraints are $y_{\max} \in \mathcal{C}(\overline{\Omega}_s)$ and $y_a, y_b \in \mathcal{C}(\overline{\Omega}_g)$ with $y_{\max}(x) \geq \theta$ for all $x \in \overline{\Omega}_s$ and $y_b(x) > y_a(x) \geq \theta$ for all all $x \in \overline{\Omega}_g$. Further, $y_{\max}(x) > y_a(x)$ for all $x \in \Gamma_r$. For the control-constraints, we assume $u_a, u_b \in L^2(\Omega)$ with $0 \leq u_a(x) < u_b(x)$ a.e. in Ω_s.*

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.

2 Optimal control problem

Let us start by recalling some definitions regarding the nonlocal radiation on Γ_r.

Definition 2.1 *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 a two-dimensional domain, the kernel ω is given by

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

and in the case of a three-dimensional domain by

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

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, [26]. The following lemma provides some significant properties of the operator G, which will be useful for our analysis (see [20, Lemma 8] for the proof).

Lemma 2.1 *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 $1 \leq p \leq \infty$.*

In the following, we define the weak formulation of the state equation (SL) that is obtained by formal integration of (SL) by parts over the boundaries Γ_r and Γ_0.

Definition 2.2 *Let $q > N$ and $q' > 0$ such that $\frac{1}{q} + \frac{1}{q'} = 1$.*

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

$$< A_q(y), v >:= \int_\Omega \kappa \nabla y \cdot \nabla v \; dx + \int_{\Gamma_r} (G\sigma|y|^3 y)v \; ds + \int_{\Gamma_0} \varepsilon\sigma|y|^3 yv \; ds \;\forall v \in W^{1,q}(\Omega), \tag{2.1}$$

where we specify $G : L^s(\Gamma_r) \to L^s(\Gamma_r)$ with $s \in \mathbb{R}$ such that $\frac{1}{s} + \frac{1}{s'} = 1$. Here, $s' = \frac{(N-1)q'}{N-q'}$.

(ii) 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 defined by

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

(iii) A function $y \in W^{1,q}(\Omega)$ is called a (weak) solution of (SL)*, if it satisfies*

$$A_q(y) = E_{q,s}\, u + E_{q,0}\, \varepsilon\sigma y_0^4 \quad in \quad W^{1,q'}(\Omega)^*. \tag{2.2}$$

Notice that for $q > N$, $W^{1,q}(\Omega)$ is continuously embedded to $\mathcal{C}(\overline{\Omega})$ and hence $y_{|\Gamma_r} \in L^\infty(\Gamma_r)$ and $y_{|\Gamma_0} \in L^\infty(\Gamma_0)$ hold true for every $y \in W^{1,q}(\Omega)$. Furthermore, it is well known that the trace operators τ_r is continuous from $W^{1,q'}(\Omega)$ to $L^{s'}(\Gamma_r)$ for $s' = \frac{(N-1)q'}{N-q'}$ ($s' > 1$ since $q > N$). For this reason, (2.1) is well-defined for all $y \in W^{1,q}(\Omega)$. Further, we point out that A_q is twice-continuously Fréchet-differentiable from $W^{1,q}(\Omega)$ to $W^{1,q'}(\Omega)^*$ (see [23]). Its first derivative at $\bar{y} \in W^{1,q}(\Omega)$ is given by

$$< A_q'(\bar{y})y, v >= \int_\Omega \kappa \nabla y \cdot \nabla v \; dx + 4\int_{\Gamma_r} (G\sigma|\bar{y}|^3 y)v \; ds + 4\int_{\Gamma_0} \varepsilon\sigma|\bar{y}|^3 yv \; ds \quad \forall v \in W^{1,q'}(\Omega). \tag{2.3}$$

The second derivative of A_q at $\bar{y} \in W^{1,q}(\Omega)$ in the directions $y_1, y_2 \in W^{1,q}(\Omega)$ is given by

$$< A_q''(\bar{y})[y_1, y_2], v >= 12\int_{\Gamma_r} (G\sigma|\bar{y}|\bar{y}\, y_1 y_2)v \, ds + 12\int_{\Gamma_0} \varepsilon\sigma|\bar{y}|\bar{y}\, y_1 y_2\, v \, ds \quad \forall v \in W^{1,q'}(\Omega). \tag{2.4}$$

The investigation of existence and uniqueness of solutions to (2.2) has been carried out in [23, Theorem 2.1], where it is shown there exists a $q = q_0 \in (N, 6)$ such that for every $u \in L^2(\Omega_s)$, the variational equation (2.2) admits a unique solution $y \in W^{1,q}(\Omega)$. For the rest of this paper, we fix therefore $q = q_0$ (and hence $q' = 1 + \frac{1}{1-q} = 1 + \frac{1}{1-q_0}$). Based on this result, we define the control-to-state-operator by $\mathcal{G} : L^2(\Omega_s) \to W^{1,q}(\Omega)$ that assigns to each $u \in L^2(\Omega_s)$ the weak solution $y \in W^{1,q}(\Omega)$ of (SL). With this setting at hand, the optimal control problem (P) can equivalently be stated as follows:

$$\begin{cases} \min\limits_{u \in \mathcal{U}} & f(u) := J(u, \mathcal{G}(u)) \\ \text{subject to} & y_a \leq \mathcal{G}(u) \leq y_b \quad \text{a.e. in } \Omega_g, \\ & \mathcal{G}(u) \leq y_{\max} \quad \text{a.e. in } \Omega_s, \end{cases} \tag{P}$$

where $\mathcal{U} := \{u \in L^2(\Omega_s) \mid u_a \leq u \leq u_b$ a.e. in $\Omega_s\}$. Furthermore, the differentiability of G was established in [23] by utilizing the Fredholm theorem. To demonstrate this, consider a fixed but arbitrary $u \in \mathcal{U}$ and set $\bar{y} = \mathcal{G}(\bar{u})$. Let us introduce a linear operator $F(\bar{y}) : L^\infty(\Gamma_r) \to W^{1,q'}(\Omega)^*$ by

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

Moreover, we define the operator $B(\bar{y}) : W^{1,q}(\Omega) \to W^{1,q'}(\Omega)^*$ by

$$< B(\bar{y})y, v >:= \int_\Omega \kappa \nabla y \cdot \nabla v \, dx + \int_{\Gamma_0} 4\varepsilon\sigma \, |\bar{y}^3| y v \, ds, \quad y \in W^{1,q}(\Omega), v \in W^{1,q'}(\Omega).$$

In [23, Lemma 2.1], it is shown that $B(\bar{y})$ is continuously invertible. Thus,

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

is well defined as an operator from $L^\infty(\Gamma_r)$ to $L^\infty(\Gamma_r)$. Notice that 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.

Definition 2.3 *We say that $\bar{u} \in L^2(\Omega_s)$ satisfies the "eigenvalue restriction" if $\lambda = -1$ is not an eigenvalue of $\mathcal{F}(\bar{y})$.*

In [23], it is shown that this assumption implies the Fréchet-differentiability of $\mathcal{G}$. We summarize the results in the following:

Theorem 2.1 *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 $\bar{y} = \mathcal{G}(\bar{u})$.*

(i) If $\bar{u}$ satisfies the eigenvalue restriction, then the operator $A_q'(\bar{y}) : W^{1,q}(\Omega) \to W^{1,q'}(\Omega)^*$ is continuously invertible, i.e., $A_q'(\bar{y})^{-1} \in \mathcal{B}(W^{1,q'}(\Omega)^*, W^{1,q}(\Omega))$.

(ii) If $A_q'(\bar{y}) : W^{1,q}(\Omega) \to W^{1,q'}(\Omega)^*$ is continuously invertible, then there exists an open neighborhood $B(\bar{u})$ of $\bar{u}$ in $L^2(\Omega_s)$ such that $\mathcal{G} : L^2(\Omega_s) \to W^{1,q}(\Omega)$ is on $B(\bar{u})$ twice continuously Fréchet-differentiable. The first derivative of $\mathcal{G}$ at $\bar{u}$ is given by $\mathcal{G}'(\bar{u})u = y$ where $y = A_q'(\bar{y})^{-1} E_{q,s} u$, i.e., $y \in W^{1,q}(\Omega)$ is the unique solution of

$$\int\limits_\Omega \kappa \nabla y \nabla v dx + 4 \int\limits_{\Gamma_r} (G\sigma|y_\gamma|^3 y) v ds + 4 \int\limits_{\Gamma_0} \varepsilon\sigma |y_\gamma|^3 y v ds = \int\limits_{\Omega_s} u v dx \quad \forall v \in W^{1,q'}(\Omega).$$

For the details, we refer the reader to [23], Theorem 3.1, Theorem 3.2. In view of the inverse function theorem, we infer from the above theorem the following result:

Corollary 2.1 *Let $\bar{u} \in L^2(\Omega_s)$ with $\bar{u}(x) \geq 0$ a.e. in Ω_s and let $\bar{y} = \mathcal{G}(\bar{u})$. Furthermore, suppose that $\bar{u}$ satisfies the eigenvalue restriction. Then, there exists an open Neighborhood $U_{\bar{y}}$ of $\bar{y}$ in $W^{1,q}(\Omega)$ such that for every $y \in U_{\bar{y}}$, $A_q'(y) : W^{1,q}(\Omega) \to W^{1,q'}(\Omega)^*$ is continuously invertible.*

We close this section by presenting an auxiliary result that is useful for our analysis.

Theorem 2.2 *Let $\bar{u} \in L^2(\Omega_s)$ with $\bar{u}(x) \geq 0$ a.e. in Ω_s. Further, suppose that $\bar{u}$ satisfies the eigenvalue restriction. Then, the solution operator $\mathcal{G} : L^2(\Omega_s) \to W^{1,q}(\Omega)$ is completely continuous at $\bar{u}$.*

Proof. First of all, let us demonstrate that $E_{q,s} : L^2(\Omega_s) \to W^{1,q'}(\Omega)^*$ is completely continuous. Let $\{\hat{u}_n\}_{n=1}^\infty \subset L^2(\Omega_s)$ be a sequence converging weakly to $\hat{u} \in L^2(\Omega_s)$. Further, set $E_{q,s}\hat{u}_n = \hat{\omega}_n$ and $E_{q,s}\hat{u} = \hat{\omega}$. We now show that $\{\hat{\omega}_n\}_{n=1}^\infty$ converging strongly to $\hat{\omega}$ in $W^{1,q'}(\Omega)^*$. By the definition of $E_{q,s}$, one has for all $n \in \mathbb{N}$:

$$0 \leq \|\hat{\omega}_n - \hat{\omega}\|_{W^{1,q'}(\Omega)^*} = \sup_{\|v\|_{W^{1,q'}} \leq 1} |\int_{\Omega_s} (\hat{u}_n - \hat{u})v \, dx|. \tag{2.5}$$

For each $n \in \mathbb{N}$, one can show by standard arguments the existence of $v_n \in W^{1,q'}(\Omega)$ with $\|v_n\|_{W^{1,q'}} \leq 1$ such that

$$\sup_{\|v\|_{W^{1,q'}} \leq 1} |\int_{\Omega_s} (\hat{u}_n - \hat{u})v \, dx| = |\int_{\Omega_s} (\hat{u}_n - \hat{u})v_n \, dx|.$$

Obviously, the resulting sequence $\{v_n\}_{n=1}^\infty$ is uniformly bounded in $W^{1,q'}(\Omega)$ and hence there exists a subsequence of $\{v_n\}_{n=1}^\infty$, w.l.o.g. again denoted by $\{v_n\}_{n=1}^\infty$, converging weakly to a $\hat{v} \in W^{1,q'}(\Omega)$. Thus, the compactness of the embedding $W^{1,q'}(\Omega) \subset L^2(\Omega)$ (notice that $q' = 1 + \frac{1}{q-1} > \frac{6}{5}$) implies that $\{v_n\}_{n=1}^\infty$ converges strongly in $L^2(\Omega)$ to $\hat{v}$. For this reason, we obtain due to the weak convergence of u_n to $\hat{u}$:

$$\lim_{n\to\infty} |\int_{\Omega_s} (\hat{u}_n - \hat{u})v_n \, dx| = 0.$$

Thus, (2.5) implies that

$$0 \leq \lim \|\hat{\omega}_n - \hat{\omega}\|_{W^{-1,q}(\Omega)^*} = \lim_{n\to\infty} |\int_{\Omega_s} (\hat{u}_n - \hat{u})v_n \, dx| = 0.$$

Hence, $E_{q,s} : L^2(\Omega_s) \to W^{1,q'}(\Omega)^*$ is completely continuous.

Let $\{u_n\}_{n=1}^\infty \subset L^2(\Omega_s)$ be given converging weakly to $\bar{u}$. Moreover, for each $n \in \mathbb{N}$, we set $y_n = \mathcal{G}(u_n)$. Our goal now to show that y_n converges strongly to $\bar{y} := \mathcal{G}(\bar{u})$ in $W^{1,q}(\Omega)$, as $n \to \infty$. To this purpose, let us introduce the operator $T : W^{1,q}(\Omega) \times W^{1,q'}(\Omega)^* \to W^{1,q'}(\Omega)^*$ by

$$T(y, \omega) = A_q(y) - \omega.$$

We define the element $\bar{\omega} \in W^{1,q'}(\Omega)^*$ by $\bar{\omega} = E_{q,s}\,\bar{u} + E_{q,0}\,\varepsilon\sigma y_0^4$. Furthermore, we set $\bar{y} = \mathcal{G}(\bar{u})$, i.e., $\bar{y} \in W^{1,q}(\Omega)$ is the unique solution of

$$A_q(\bar{y}) = E_{q,s}\,\bar{u} + E_{q,0}\,\varepsilon\sigma y_0^4.$$

Hence, we obtain $T(\bar{y}, \bar{\omega}) = 0$. Moreover, since $\bar{u}$ satisfies the eigenvalue restriction, Theorem 2.1 ensures that $\partial_y T(\bar{y}, \bar{\omega})^{-1} = A_q(\bar{y})^{-1} \in \mathcal{B}(W^{1,q'}(\Omega)^*, W^{1,q}(\Omega))$. Consequently, the implicit theorem implies the existence of an open neighborhood $U_{\bar{w}}$ of $\bar{w}$ in $W^{1,q'}(\Omega)^*$ and an open neighborhood $U_{\bar{y}}$ of $\bar{y}$ in $W^{1,q}(\Omega)$ such that the inverse operator

$$A_q^{-1} : W^{1,q'}(\Omega)^* \supset U_{\bar{w}} \to U_{\bar{y}} \subset W^{1,q}(\Omega)$$

is well-defined and continuous.

Since $E_{q,s} : L^2(\Omega_s) \to W^{1,q}(\Omega)$ is completely continuous and since u_n converging weakly in $L^2(\Omega_s)$ to $\bar{u}$, we have

$$\lim_{n\to\infty} (E_{q,s}\, u_n + E_{q,0}\, \varepsilon\sigma y_0^4) = E_{q,s}\, \bar{u} + E_{q,0}\, \varepsilon\sigma y_0^4 = \bar{w} \quad \text{in } W^{1,q'}(\Omega)^*.$$

In particular, there exists $\bar{n} \in \mathbb{N}$ such that

$$(E_{q,s}\, u_n + E_{q,0}\, \varepsilon\sigma y_0^4) \in U_{\bar{w}} \quad \forall n \geq \bar{n}. \tag{2.6}$$

On the other hand, based on the definition of $\mathcal{G}$, $y_n \in W^{1,q}(\Omega)$ is given by the unique solution of

$$A_q(y_n) = E_{q,s}\, u_n + E_{q,0}\, \varepsilon\sigma y_0^4.$$

Therefore, by (2.6)

$$y_n = A_q^{-1}(E_{q,s}\, u_n + E_{q,0}\, \varepsilon\sigma y_0^4), \quad \forall n \geq \bar{n}.$$

Therefore, utilizing the continuity of $A_q^{-1} : U_{\bar{w}} \to W^{1,q}(\Omega)$, the compactness of $E_{q,s}$ we obtain:

$$\lim_{n\to\infty} y_n = \lim_{n\to\infty} A_q^{-1}(E_{q,s}\, u_n + E_{q,0}\, \varepsilon\sigma y_0^4) = A_q^{-1}(E_{q,s}\, \bar{u} + E_{q,0}\, \varepsilon\sigma y_0^4) = \bar{y} \quad \text{in } W^{1,q}(\Omega).$$

Thus, the theorem is verified. □

3 Optimality conditions for (P)

In a standard way, one shows that (P) admits a solution provided that there exists a feasible control u of (P). However, due to the nonlinearity of the state equation (SL), we cannot expect the uniqueness of the solution to (P). Therefore, let us introduce the notion of local solutions for (P):

Definition 3.1 *A feasible control $\bar{u}$ of (P) is called local solution for* (P)*, if there exists a positive real number ε such that $f(\bar{u}) \leq f(u)$ holds for all feasible controls u of (P) with $\|u - \bar{u}\|_{L^2(\Omega_s)} \leq \varepsilon$.*

Thanks to the embedding $W^{1,q}(\Omega) \subset \mathcal{C}(\overline{\Omega})$, the following Slater assumption makes sense:

Definition 3.2 *Let $\bar{u} \in \mathcal{U}$ satisfying the eigenvalue restriction. Then, we say that $\bar{u}$ satisfies the* linearized Slater condition *for* (P)*, if there exists an interior point $u_0 \in \mathcal{U}$ such that*

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

with a fixed positive real number δ.

Let us now present the first-order necessary optimality system for (P), cf. [23, Theorem 5.2].

Theorem 3.1 (First-order necessary optimality conditions for (P)) *Let $\bar{u} \in L^2(\Omega_s)$ be an optimal solution of* (P) *with associated state $\bar{y} = \mathcal{G}(\bar{u}) \in W^{1,q}(\Omega)$, $q > N$. Suppose further that $\bar{u}$ satisfies the eigenvalue restriction (Definition 2.3) and the linearized Slater conditions (Definition 3.2). Then, there exist an adjoint state $p \in W^{1,q'}(\Omega)$, $q' < \frac{N}{N-1}$, and Lagrange multipliers $\mu_s \in \mathcal{M}(\overline{\Omega}_s)$, $\mu_g^a, \mu_g^b \in \mathcal{M}(\overline{\Omega}_g)$ satisfying*

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

$$(3.1) \qquad \begin{cases} -\mathit{div}(\kappa_g \nabla p) = -\Delta \bar{y} + \mathit{div}\, z + (\mu_g^b - \mu_g^a)_{|\Omega_g} & \text{in } \Omega_g, \\ -\mathit{div}(\kappa_s \nabla p) = \mu_{s|\Omega_s} & \text{in } \Omega_s, \\ \kappa_g \left(\dfrac{\partial p}{\partial_{n_r}}\right)_g - \kappa_s \left(\dfrac{\partial p}{\partial_{n_r}}\right)_s - 4\sigma|\bar{y}|^3 G^\star p = -\dfrac{\partial \bar{y}}{\partial n_r} + z \cdot n_r & \text{on } \Gamma_r, \\ \qquad\qquad + (\mu_g^b - \mu_g^a + \mu_s)_{|\Gamma_r} & \\ \kappa_s \dfrac{\partial p}{\partial n_0} + 4\varepsilon\sigma |\bar{y}|^3 p = \mu_{s|\Gamma_0} & \text{on } \Gamma_0, \end{cases}$$

$$(3.2) \qquad \mu_s \geq 0, \quad \mu_g^a \geq 0, \quad \mu_g^b \geq 0,$$

$$(3.3) \qquad \int_{\Omega_s} \mathcal{G}(\bar{u}) - y_{\max}\, d\mu_s = \int_{\Omega_g} y_a - \mathcal{G}(\bar{u})\, d\mu_g^a = \int_{\Omega_g} \mathcal{G}(\bar{u}) - y_b\, d\mu_g^b = 0,$$

$$(3.4) \qquad \bar{u} = \mathcal{P}_{ad}\big\{ -\frac{1}{\beta}\, p(x) \big\},$$

where $\mathcal{P}_{ad} : L^2(\Omega_s) \to L^2(\Omega_s)$ denotes the pointwise projection operator on the admissible set $\mathcal{U}$.

Here, the PDEs (SL) and (3.1) are considered in a variational sense, cf. Definition 2.2 and [23]. Next, we continue with second-oder sufficient optimality conditions for (P) that was derived in [23].

Definition 3.3 *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* (3.1)-(3.4).

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

$$\mathcal{H}_{\bar{u}} := \big\{ h \in L^2(\Omega_s) \mid h(x) = \begin{cases} \geq 0 & \text{if} \quad \bar{u}(x) = u_a(x) \\ \leq 0 & \text{if} \quad \bar{u}(x) = u_b(x) \end{cases} \big\}.$$

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

$$\mathcal{C}_{\bar u} = \{h \in \mathcal{H}_{\bar u} \mid h \text{ satisfies } (3.5), (3.6) \text{ and } (3.7)\}$$

$$h(x) = 0 \quad \text{if} \quad p(x) + \beta \bar u(x) \neq 0 \tag{3.5}$$

$$y_h(x) = \begin{cases} \geq 0 & \text{if } \bar y(x) = y_a(x),\ x \in \overline{\Omega}_g \\ \leq 0 & \text{if } \bar y(x) = y_b(x),\ x \in \overline{\Omega}_g \\ \leq 0 & \text{if } \bar y(x) = y_{\max}(x),\ x \in \overline{\Omega}_s \end{cases} \tag{3.6}$$

$$\int_{\bar\Omega_g} y_h \, d\mu_g^a = \int_{\bar\Omega_g} y_h \, d\mu_g^b = \int_{\bar\Omega_s} y_h \, d\mu_s = 0, \tag{3.7}$$

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

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

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

holds true for every $h \in \mathcal{C}_{\bar u} \setminus \{0\}$.

Theorem 3.2 (Second-order sufficient optimality conditions for (P)**)** *Let* $\bar u \in \mathcal{U}$ *be a feasible control of* (P) *satisfying the eigenvalue restriction (Definition 2.3). Furthermore, suppose 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* (3.1)-(3.4)*. If* $\bar u$ *additionally satisfies* (SSC)*, then there exist positive real numbers* ε *and* δ *such that*

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

holds true for every feasible control u *of* (P) *with* $\|u - \bar u\|_{L^2(\Omega_s)} < \varepsilon$.

We underline that the above result does not exhibit any two-norm discrepancy and thus Theorem 3.2 guarantees local optimality in "L^2-neighborhood", cf. also [8].

4 Moreau-Yosida type regularization

As pointed out in the Introduction, the basic concept of the Moreau-Yosida type regularization is to remove the pointwise state constraints (1.1) and to add a corresponding Lagrangian-type penalty to the objective functional of (P), cf. [16]. More precisely, we regularize (P) in the following way:

$$(P_\gamma) \qquad \begin{cases} \min\limits_{u \in L^2(\Omega_s)} & f_\gamma(u) \\ \text{over} & u \in L^2(\Omega_s) \\ \text{subject to} & u_a \leq u \leq u_b \quad \text{a.e. in } \Omega_s. \end{cases}$$

The objective functional in (P_γ) is defined as follows:

$$
\begin{aligned}
f_\gamma(u) &:= f(u) + \frac{1}{2\gamma_1}\int_{\Omega_g} \max\big(0, \gamma_1(\mathcal{G}(u) - y_b)\big)^2 dx \\
&+ \frac{1}{2\gamma_2}\int_{\Omega_g} \max\big(0, \gamma_2(y_a - \mathcal{G}(u))\big)^2 dx + \frac{1}{2\gamma_3}\int_{\Omega_s} \max\big(0, \gamma_3(\mathcal{G}(u) - y_{\max})\big)^2 dx,
\end{aligned} \tag{4.1}
$$

where $\gamma = (\gamma_1, \gamma_2, \gamma_3)$ with $\gamma_i > 0$ for $i = 1, 2, 3$. Notice that we write $\gamma > 0$ if and only if $\gamma_i > 0$ for all $i = 1, 2, 3$. Moreover, the notation $\gamma \to \infty$ means that $(\gamma_1, \gamma_2, \gamma_3) \to (\infty, \infty, \infty)$.

Hereafter, one obtains an optimal control problem (P_γ) with pure control-constraints. Since $\mathcal{U}$ is not empty, it can be shown by standard arguments that (P_γ) is solvable for all $\gamma > 0$. Similarly to (P), the solution to (P_γ) is not necessarily unique. Therefore, in our study we concentrate on investigating local solutions to (P_γ).

Definition 4.1 *Let $\gamma > 0$. A function $u_\gamma \in \mathcal{U}$ is called a local solution to (P_γ) if*

$$f_\gamma(u_\gamma) \le f_\gamma(u)$$

holds true for all $u \in \mathcal{U}$ satisfying $\|u - u_\gamma\|_{L^2(\Omega_s)} \le \epsilon$, for some $\epsilon > 0$.

Theorem 4.1 (First-order necessary optimality conditions for (P_γ)) *Let $\gamma > 0$ and let $u_\gamma \in L^2(\Omega_s)$ be a local solution of (P_γ) with the associated state $y_\gamma = \mathcal{G}(u_\gamma)$. Moreover, suppose that u_γ satisfies the eigenvalue restriction (Definition 2.3). Then, there exist an adjoint state $p_\gamma \in W^{1,q'}(\Omega)$, Lagrange multipliers $\mu^a_{g,\gamma}, \mu^b_{g,\gamma} \in L^2(\Omega_g)$ and $\mu_{s,\gamma} \in L^2(\Omega_s)$ such that*

$$
\left\{
\begin{aligned}
-div(\kappa_g \nabla y_\gamma) &= 0 && \text{in } \Omega_g,\\
-div(\kappa_s \nabla y_\gamma) &= u_\gamma && \text{in } \Omega_s,\\
\kappa_g(\frac{\partial y_\gamma}{\partial n_r})_g - \kappa_s(\frac{\partial y_\gamma}{\partial n_r})_s &= G\sigma|y_\gamma|^3 y_\gamma && \text{on } \Gamma_r,\\
\kappa_s \frac{\partial y_\gamma}{\partial n_0} + \varepsilon\sigma|y_\gamma|^3 y_\gamma &= \varepsilon\sigma y_0^4 && \text{on } \Gamma_0,
\end{aligned}
\right. \tag{4.2}
$$

$$
\left\{
\begin{aligned}
-div(\kappa_g \nabla p_\gamma) &= -\Delta y_\gamma + div\, z + \mu^b_{g,\gamma} - \mu^a_{g,\gamma} && \text{in } \Omega_g,\\
-div(\kappa_s \nabla p_\gamma) &= \mu_{s,\gamma} && \text{in } \Omega_s,\\
\kappa_g(\frac{\partial p_\gamma}{\partial n_r})_g - \kappa_s(\frac{\partial p_\gamma}{\partial n_r})_s - 4(\sigma|y_\gamma|^3)G^* p_\gamma &= -\frac{\partial y_\gamma}{\partial n_r} + z \cdot n_r && \text{on } \Gamma_r,\\
\kappa_s \frac{\partial p_\gamma}{\partial n_0} + 4\varepsilon\sigma|y_\gamma|^3 p_\gamma &= 0 && \text{on } \Gamma_0,
\end{aligned}
\right. \tag{4.3}
$$

$$
\begin{gathered}
\mu^b_{g,\gamma} = \max\big(0, \gamma_1(y_{\gamma|\Omega_g} - y_b)\big),\ \mu^a_{g,\gamma} = \max\big(0, \gamma_2(y_a - y_{\gamma|\Omega_g})\big),\\
\mu_{s,\gamma} = \max\big(0, \gamma_3(y_{\gamma|\Omega_s} - y_{\max})\big),
\end{gathered}
$$

$$u_\gamma = \mathcal{P}_{[u_a,u_b]}\{ -\frac{1}{\beta} p_\gamma(x)\} \tag{4.4}$$

hold in variational sense.

Proof. Let $\gamma > 0$ and let $u_\gamma \in L^2(\Omega_s)$ be an optimal solution to (P_γ) satisfying the eigenvalue restriction. The associated state of u_γ is denoted by $y_\gamma = \mathcal{G}(u_\gamma) \in W^{1,q}(\Omega)$ and we define:

$$\mu_{g,\gamma}^b = \max\big(0, \gamma_1(y_{\gamma|\Omega_g} - y_b)\big), \quad \mu_{g,\gamma}^a = \max\big(0, \gamma_2(y_a - y_{\gamma|\Omega_g})\big), \quad \mu_{s,\gamma} = \max\big(0, \gamma_3(y_{\gamma|\Omega_s} - y_{\max})\big).$$

By integrating formally by parts over the boundaries Γ_r and Γ_0, we obtain the weak formulation of (4.3), given by

$$\begin{aligned}\int_\Omega \kappa \nabla p_\gamma \nabla v dx + 4\int_{\Gamma_r} (\sigma|y_\gamma|^3) G^* p_\gamma v ds + 4\int_{\Gamma_0} \varepsilon\sigma|y_\gamma|^3 p_\gamma v ds = \int_{\Omega_g} (\nabla y_\gamma - z)\cdot\nabla v dx \\ + \int_{\Omega_g} (\mu_{g,\gamma}^b - \mu_{g,\gamma}^a) v dx + \int_{\Omega_s} \mu_{s,\gamma} v dx \quad \forall v \in W^{1,q}(\Omega).\end{aligned} \tag{4.5}$$

We point out that since $y_\gamma \in W^{1,q}(\Omega)$, $\mu_{g,\gamma}^b, \mu_{g,\gamma}^a, z \in L^2(\Omega_g)$ and $\mu_{s,\gamma} \in L^2(\Omega_s)$, the right hand side of (4.5) defines an element $\xi \in W^{1,q}(\Omega)^*$ with

$$< \xi, v > := \int_{\Omega_g} (\nabla y_\gamma - z)\cdot\nabla v dx + \int_{\Omega_g} (\mu_{g,\gamma}^b - \mu_{g,\gamma}^a) v dx + \int_{\Omega_s} \mu_{s,\gamma} v dx \quad \forall v \in W^{1,q}(\Omega).$$

Therefore, the weak formulation (4.5) can equivalently be written as follows (see the representation of A_q' in (2.3))

$$A_q'(y_\gamma)^* p_\gamma = \xi \quad \text{in } W^{1,q}(\Omega)^*. \tag{4.6}$$

Since u_γ satisfies the eigenvalue restriction, Theorem 2.1 implies that $A_q'(y_\gamma)$ is continuously invertible from $W^{1,q}(\Omega)$ to $W^{1,q'}(\Omega)^*$ and hence $A_q'(y_\gamma)^*$ is continuously invertible from $W^{1,q'}(\Omega)$ to $W^{1,q}(\Omega)^*$. Therefore, (4.5) admits a unique solution $p_\gamma \in W^{1,q'}(\Omega)$. It remains to show that the solution p_γ of (4.5) satisfies the projection formula in (4.4).

According to Theorem 2.1, f_γ is continuously differentiable at u_γ and the derivative of f_γ at u_γ in the direction $(u - u_\gamma)$ with an arbitrary $u \in \mathcal{U}$ is given by

$$\begin{aligned}f'(u_\gamma)(u - u_\gamma) = (\nabla y_\gamma - z, \nabla y)_{L^2(\Omega_g)} + \beta(u_\gamma, u - u_\gamma)_{L^2(\Omega_s)} \\ + (\mu_{g,\gamma}^b - \mu_{g,\gamma}^a, y)_{L^2(\Omega_g)} + (\mu_{s,\gamma}, y)_{L^2(\Omega_s)},\end{aligned} \tag{4.7}$$

with $y = \mathcal{G}'(u_\gamma)(u - u_\gamma)$. Hence by the definition of $\mathcal{G}'(u_\gamma)$ in Theorem 2.1, $y \in W^{1,q}(\Omega)$ is the unique solution of

$$\int_\Omega \kappa \nabla y \nabla v dx + 4\int_{\Gamma_r} (G\sigma|y_\gamma|^3 y) v ds + 4\int_{\Gamma_0} \varepsilon\sigma|y_\gamma|^3 y v ds = \int_{\Omega_s} (u - u_\gamma) v dx \quad \forall v \in W^{1,q'}(\Omega). \tag{4.8}$$

Inserting $v = p_\gamma$ in (4.8), $v = y$ in (4.5) and then subtracting the arising equations, we find that

$$\int_{\Omega_s} (u - u_\gamma) p_\gamma dx = \int_{\Omega_g} (\nabla y_\gamma - z)\cdot\nabla y dx + \int_{\Omega_g} (\mu_{g,\gamma}^b - \mu_{g,\gamma}^a) y dx + \int_{\Omega_s} \mu_{s,\gamma} y dx.$$

Inserting this in (4.7), we infer hence that

$$f'(u_\gamma)(u-u_\gamma) = (p_\gamma + \beta u_\gamma, u-u_\gamma)_{L^2(\Omega_s)}. \tag{4.9}$$

On the other hand, since the admissible set $\mathcal{U} = \{u \in L^2(\Omega_s) \mid u_a \le u \le u_b \text{ a.e. in } \Omega_s \}$ is convex, it is well-known that the necessary optimality condition to the optimal solution u_γ is given by the following variational inequality:

$$f'(u_\gamma)(u-u_\gamma) \ge 0 \quad \forall u \in \mathcal{U}. \tag{4.10}$$

Therefore, since (4.9) holds true for all $u \in \mathcal{U}$, we finally arrive at

$$(p_\gamma + \beta u_\gamma, u-u_\gamma)_{L^2(\Omega_s)} \ge 0 \quad \forall u \in \mathcal{U},$$

which implies by standard arguments the projection formula (4.4). □

Remark 4.1 *We point out that if $A'(y_\gamma)$ is invertible, then Theorem 4.1 remains true without the eigenvalue restriction on the optimal control u_γ.*

5 Convergence analysis

The goal of this section is to study the convergence behavior of the regularized solutions of (P_γ) in the case of $\gamma \to \infty$. The convergence of the Moreau-Yosida type approach was originally proven by Ito and Kunisch in [16]. However, since we consider nonlinear control problem (P) with a nonstandard objective functional f, the convergence result from [16] is not directly applicable to (P).

It is well known that the unregularized problem (P) does not admit a unique global solution. Moreover, optimization algorithms compute in general only local solutions. For this reason, we focus mainly on the convergence of the regularized solutions to local solutions of unregularized problem. Suppose that a local solution $\bar{u}$ of (P) is given. We aim at finding a sequence $(u_\gamma)_\gamma$ of local solutions to (P_γ) converging strongly to $\bar{u}$ as $\gamma \to \infty$. In fact, if $\bar{u}$ satisfies the second order optimality conditions (SSC), then the desired sequence can be found.

Assumption 5.1 *Let $\bar{u} \in \mathcal{U}$ be a local solution to (P) in $L^2(\Omega_s)$ satisfying the eigenvalue restriction (Definition 2.3), the linearized Slater condition (Definition 3.2) and the second order sufficient condition (SSC) (Definition 3.3).*

Based on Assumption 5.1, Theorem 3.2 implies the existence of positive real numbers ε and δ such that

$$f(\bar{u}) + \frac{\delta}{2}\|u-\bar{u}\|^2_{L^2(\Omega_s)} \le f(u) \tag{5.1}$$

holds true for every feasible control u of (P) with $\|u-\bar{u}\|_{L^2(\Omega_s)} < \varepsilon$.

Let us introduce now the following auxiliary problem:

$$(P^r_\gamma) \qquad \begin{cases} \min & f_\gamma(u) \\ \text{subject to} & u \in \mathcal{U}^r, \end{cases}$$

with $r = \frac{\varepsilon}{2}$ and $\mathcal{U}^r = \{u \in \mathcal{U} \mid \|u - \bar{u}\|_{L^2(\Omega_s)} \le r\}$. By the construction, $\bar{u}$ is a feasible control of (P^r_γ), for all $\gamma > 0$. Thus, (P^r_γ) admits at least one global solution and by $u^r_\gamma \in \mathcal{U}^r$, we denote an arbitrary one of them. Our goal now is to show that u^r_γ converges strongly to $\bar{u}$, as $\gamma \to \infty$. It should be underlined that the idea of considering an auxiliary problem of the form (P^r_γ) is based on Casas and Tröltzsch [9].

Since $u^r_\gamma \in \mathcal{U}$ for all $\gamma > 0$, the sequence $(u^r_\gamma)_{\gamma>0}$ is uniformly bounded in $L^2(\Omega_s)$. For this reason, there exists a subsequence of $(u^r_\gamma)_{\gamma>0}$, w.l.o.g also denoted by $(u^r_\gamma)_{\gamma>0}$, converging weakly to $\tilde{u}$ in $L^2(\Omega)$. Since $\mathcal{U}^r$ is weakly closed, the weak limit $\tilde{u}$ belongs to the admissible set $\mathcal{U}^r$. Our goal now is to show that $\tilde{u}$ is a feasible control of (P).

Lemma 5.1 *The weak limit $\tilde{u} \in \mathcal{U}^r$ defined above is feasible for (P), i.e., the associate state of $\tilde{u}$, denoted by $\tilde{y} = \mathcal{G}(\tilde{u})$, satisfies:*

$$y_a \le \tilde{y} \le y_b \text{ a.e. in } \Omega_g \quad \text{and} \quad \tilde{y} \le y_{\max} \text{ a.e. in } \Omega_s.$$

Proof. Since $\bar{u}$ is not only feasible for all (P^r_γ) but also feasible for (P), we have

$$f_\gamma(u^r_\gamma) \le f_\gamma(\bar{u}) = f(\bar{u}) \quad \forall \gamma > 0.$$

Hence, by the definition of f_γ, we find a constant $c > 0$ independent of γ_i, $i = 1, 2, 3$, such that

$$\begin{aligned} \frac{\gamma_1}{2} \int_{\Omega_g} \max(0, \mathcal{G}(u^r_\gamma) - y_b)^2 dx &\le c, \\ \frac{\gamma_2}{2} \int_{\Omega_g} \max(0, y_a - \mathcal{G}(u^r_\gamma))^2 dx &\le c, \\ \frac{\gamma_3}{2} \int_{\Omega_s} \max(0, \mathcal{G}(u^r_\gamma) - y_{\max})^2 dx &\le c. \end{aligned}$$

Consequently, we obtain:

$$\begin{aligned} \lim_{\gamma_1 \to \infty} \int_{\Omega_g} \max(0, \mathcal{G}(u^r_\gamma) - y_b)^2 dx &= 0, \\ \lim_{\gamma_2 \to \infty} \int_{\Omega_g} \max(0, y_a - \mathcal{G}(u^r_\gamma))^2 dx &= 0, \\ \lim_{\gamma_3 \to \infty} \int_{\Omega_s} \max(0, \mathcal{G}(u^r_\gamma) - y_{\max})^2 dx &= 0. \end{aligned}$$

For this reason, Fatou's Lemma implies

$$\begin{aligned} \lim_{\gamma_1 \to \infty} \max(0, \mathcal{G}(u^r_\gamma)_{|\Omega_g} - y_b) = \lim_{\gamma_2 \to \infty} \max(0, y_a - \mathcal{G}(u^r_\gamma)_{|\Omega_g}) &= 0, \\ \lim_{\gamma_3 \to \infty} \max(0, \mathcal{G}(u^r_\gamma)_{|\Omega_s} - y_{\max}) &= 0. \end{aligned} \tag{5.2}$$

The compactness of the embedding from $W^{1,q}(\Omega)$ to $\mathcal{C}(\overline{\Omega})$ yields

$$\lim_{\gamma \to \infty} \mathcal{G}(u^r_\gamma) = \mathcal{G}(\tilde{u}) = \tilde{y} \text{ in } \mathcal{C}(\overline{\Omega}) \tag{5.3}$$

Finally, due (5.2), (5.3) and the continuity of $\mathbb{M} : \mathcal{C}(\overline{\Omega}) \to \mathcal{C}(\overline{\Omega})$, $\mathbb{M}(z) = \max(0, z)$, we find

$$\begin{aligned} \max(0, \tilde{y}_{|\Omega_g} - y_b) = \max(0, y_a - \tilde{y}_{|\Omega_g}) &= 0, \\ \max(0, \tilde{y}_{|\Omega_s} - y_{\max}) &= 0, \end{aligned}$$

which implies:

$$y_a \leq \tilde{y} \leq y_b \text{ a.e. in } \Omega_g \quad \text{and} \quad \tilde{y} \leq y_{\max} \text{ a.e. in } \Omega_s$$

and hence the lemma is verified. □

Theorem 5.1 *The sequence $(u_\gamma^r)_{\gamma>0}$ converges strongly in $L^2(\Omega)$ to $\bar{u}$ as $\gamma \to \infty$.*

Proof. First, since $\bar{u}$ is feasible for all (P_γ^r) and also feasible for (P),

$$f(u_\gamma^r) \leq f_\gamma(u_\gamma^r) \leq f_\gamma(\bar{u}) = f(\bar{u}) \tag{5.4}$$

holds true for all $\gamma > 0$. Therefore, owing to the lower semi-continuity of f, we have by passing to the limit $\gamma \to \infty$:

$$f(\tilde{u}) \leq \liminf_{\gamma\to\infty} f(u_\gamma^r) \leq \limsup_{\gamma\to\infty} f(u_\gamma^r) \leq f(\bar{u}). \tag{5.5}$$

On the one hand, due to Assumption 5.1 Theorem 3.2 implies that

$$f(\bar{u}) + \frac{\delta}{2}\|u - \bar{u}\|^2_{L^2(\Omega_s)} \leq f(u) \tag{5.6}$$

holds true for every feasible control u of (P) with $\|u - \bar{u}\|_{L^2(\Omega_s)} < \varepsilon$. Moreover, by Lemma 5.1, the weak limit $\tilde{u}$ is a feasible control of (P) and it satisfies

$$\|\tilde{u} - \bar{u}\|_{L^2(\Omega_s)} \leq r = \frac{\varepsilon}{2}.$$

For this reason, (5.6) is particularly satisfied for the choice $u = \tilde{u}$ and thus (5.5) implies

$$f(\tilde{u}) + \frac{\delta}{2}\|\tilde{u} - \bar{u}\|^2_{L^2(\Omega_s)} \leq f(\bar{u}) + \frac{\delta}{2}\|\tilde{u} - \bar{u}\|^2_{L^2(\Omega_s)} \leq f(\tilde{u}).$$

Consequently, $\tilde{u} = \bar{u}$.

Now, let us show that $(u_\gamma^r)_{\gamma>0}$ converges strongly to $\bar{u}$ as $\gamma \to \infty$. From (5.5) and (5.6), we infer

$$\|\nabla\bar{y}-z\|^2_{L^2(\Omega_g)}+\|\bar{u}\|^2_{L^2(\Omega_s)} = f(\bar{u}) = \lim_{\gamma\to\infty} f(u_\gamma^r) = \lim_{\gamma\to\infty} (\|\nabla\mathcal{G}(u_\gamma^r)-z\|^2_{L^2(\Omega_g)}+\|u_\gamma^r\|^2_{L^2(\Omega_s)}). \tag{5.7}$$

Since u_γ^r converges weakly to $\bar{u}$ and since $\bar{u}$ satisfies the eigenvalue restriction, Theorem 2.2 implies that $\mathcal{G}(u_\gamma^r)$ converges strongly to $\bar{y}$ in $W^{1,q}(\Omega)$ and consequently

$$\lim_{\gamma\to\infty} \|\nabla\mathcal{G}(u_\gamma^r) - z\|^2_{L^2(\Omega_g)} = \|\nabla\bar{y} - z\|^2_{L^2(\Omega_g)}$$

Thus, (5.7) implies

$$\lim_{\gamma\to\infty} \|u_\gamma^r\|^2_{L^2(\Omega_s)} = \|\bar{u}\|^2_{L^2(\Omega_s)}$$

and hence due to the weak convergence of $(u_\gamma^r)_{\gamma>0}$ to $\bar{u}$ as $\gamma \to \infty$, the theorem is verified. □

We have shown the existence of a sequence $(u_\gamma^r)_{\gamma>0}$ of global solutions to (P_γ^r) converging strongly to $\bar{u}$ in $L^2(\Omega_s)$. In the following, we show that for all sufficiently large $\gamma > 0$, u_γ^r is a local solution of (P_γ).

Lemma 5.2 *For all sufficient large $\gamma > 0$, u_γ^r is a local solution of (P_γ).*

Proof. Let $u \in \mathcal{U}$ with $\|u - u_\gamma^r\|_{L^2(\Omega_s)} \leq \frac{r}{2}$. Then, for sufficient large $\gamma > 0$, we obtain due to the strong convergence of u_γ^r to $\bar{u}$, as $\gamma \to \infty$:

$$\|u - \bar{u}\|_{L^2(\Omega_s)} \leq \|u - u_\gamma^r\|_{L^2(\Omega_s)} + \|u_\gamma^r - \bar{u}\|_{L^2(\Omega_s)} \leq \frac{r}{2} + \frac{r}{2} = r. \tag{5.8}$$

Consequently, we have $u \in \mathcal{U}^r$ and hence since u_γ^r is a global solution to (P_γ^r), we infer:

$$f_\gamma(u_\gamma^r) \leq f_\gamma(u).$$

Alltogether, we have just shown for all sufficiently large $\gamma > 0$:

$$f_\gamma(u_\gamma^r) \leq f_\gamma(u)$$

holds true for all $u \in \mathcal{U} \cap B_{\frac{r}{2}}(u_\gamma^r)$ with $B_{\frac{r}{2}}(u_\gamma^r) = \{u \in L^2(\Omega_s) \mid \|u - u_\gamma^r\|_{L^2(\Omega_s)} \leq \frac{r}{2}\}$. Thus, u_γ^r is a local solution of (P_γ). □

Collecting the results above, we finally arrive at the following theorem:

Theorem 5.2 *Let $\bar{u}$ be a local solution of (P) satisfying Assumption 5.1. Then there exists a sequence $(u_\gamma)_{\gamma>0}$ of local solutions to (P_γ) converging strongly to $\bar{u}$ as $\gamma \to \infty$. Moreover, for all sufficiently large γ, the first-order necessary optimality conditions for (P_γ) are satisfied for u_γ.*

Proof. Let $\bar{u}$ be a local solution of (P) satisfying Assumption 5.1. By Theorem 5.1 and Lemma 5.2, we have shown the existence of a sequence $(u_\gamma)_{\gamma>0}$ of local solutions to (P_γ) converging strongly to $\bar{u}$ as $\gamma \to \infty$. Further, we define $y_\gamma = \mathcal{G}(u_\gamma)$. Hence, y_γ converges strongly to $\bar{y}$ in $W^{1,q}(\Omega)$, as $\gamma \to \infty$. Consequently, since $\bar{u}$ satisfies the eigenvalue restriction, Corollary 2.1 implies the existence of a positive real number $\bar{\gamma}$ such that $A_q'(y_\gamma)$ is continuously invertible for every $\gamma > \bar{\gamma}$. This particularly implies that for every $\gamma > \bar{\gamma}$, the first-order necessary optimality conditions for (P_γ) are satisfied for u_γ, cf. Remark 4.1. □

6 Numerical verification

Mainly due to the lack of sufficient regularity of the Lagrange multipliers associated to (P), the semismooth Newton method cannot directly be used to solve the model problem (P). This difficulty was already overcome by the regularization. Thanks to the L^2-regularity of the Lagrange multipliers associated to (P_γ), semismooth Newton methods are applicable to (P_γ), for all $\gamma \in \mathbb{R}^+$. We point out that semismooth Newton methods for nonlinear control-constrained control problems are basically equivalent to the primal-dual active-set strategy, where the linearization of the optimality system is solved only one time in the inner iteration, see Ito Kunisch [17] or [10]. In our present paper, we do not intend to study Algorithm 6.1, below, in details, since it would go beyond the scope of our framework. We basically follow [17]. Let us present the complete algorithm for (P_γ) in the following:

Algorithm 6.1 (1) *Initialization: Choose $y^0, p^0 \in L^2(\Omega)$ and set $n = 1$*

(2) *Set*

$$\begin{aligned}
\mathcal{U}_a^n &= \{x \in \Omega_s \mid u_a(x) + \tfrac{1}{\beta} p_{n-1}(x) > 0\} & \mathcal{U}_b^n &= \{x \in \Omega_s \mid -\tfrac{1}{\beta} p_{n-1}(x) - u_b(x) > 0\} \\
\mathcal{A}_{g,n}^a &= \{x \in \Omega_g \mid \ y_a(x) - y_{n-1}(x) > 0\} & \mathcal{A}_{g,n}^b &= \{x \in \Omega_g \mid \ y_{n-1}(x) - y_b(x) > 0\} \\
\mathcal{A}_{s,n} &= \{x \in \Omega_s \mid \ y_{n-1}(x) - y_{\max}(x) > 0\}
\end{aligned}$$

(3) *Find the solution* (y_n, u_n, p_n) *of the following linearized problem*

$$\begin{aligned}
-\operatorname{div}(\kappa_g \nabla y_n) &= 0 && \text{in } \Omega_g, \\
-\operatorname{div}(\kappa_s \nabla y_n) &= u_n && \text{in } \Omega_s, \\
\kappa_g(\frac{\partial y_n}{\partial n_r})_g - \kappa_s(\frac{\partial y_n}{\partial n_r})_s - 4G\sigma|y_{n-1}|^3 y_n &= -3G\sigma|y_{n-1}|^3 y_{n-1} && \text{on } \Gamma_r, \\
\kappa_s \frac{\partial y_n}{\partial n_0} + 4\varepsilon\sigma|y_{n-1}|^3 y_n &= 3\varepsilon\sigma|y_{n-1}|^3 y_{n-1} + \varepsilon\sigma y_0^4 && \text{on } \Gamma_0,
\end{aligned}$$

$$\begin{aligned}
-\operatorname{div}(\kappa_g \nabla p_n) &= -\Delta y_n + \operatorname{div} z + \mu_{g,n}^b - \mu_{g,n}^a && \text{in } \Omega_g, \\
-\operatorname{div}(\kappa_s \nabla p_n) &= \mu_{s,n} && \text{in } \Omega_s, \\
\kappa_g(\frac{\partial p_n}{\partial n_r})_g - \kappa_s(\frac{\partial p_n}{\partial n_r})_s - 4(\sigma|\bar{y}_{n-1}|^3)G^* p_n &= -\frac{\partial y_n}{\partial n_r} + z \cdot n_r \\
&\quad - 12(\sigma|y_{n-1}|y_{n-1})G^* p_{n-1}(y_n - y_{n-1}) && \text{on } \Gamma_r, \\
\kappa_s \frac{\partial p}{\partial n_0} + 4\varepsilon\sigma|\bar{y}_{n-1}|^3 p_n &= -12\varepsilon\sigma|y_{n-1}|y_{n-1} p_{n-1}(y_n - y_{n-1}) && \text{on } \Gamma_0.
\end{aligned}$$

$$u_{n+1} = \begin{cases} u_a & \text{in } \ \mathcal{U}_a^n \\ u_b & \text{in } \ \mathcal{U}_b^n, \\ -\frac{1}{\beta}\, p_n & \text{in } \ \Omega_s \setminus \{\mathcal{U}_a^n \cup \mathcal{U}_b^n\}, \end{cases}$$

$$\mu_{g,n}^b = \begin{cases} y_{n|\Omega_g} - y_b & \text{in } \ \mathcal{A}_b^n \\ 0 & \text{in } \ \Omega_g \setminus \mathcal{A}_b^n \end{cases} \qquad \mu_{g,n}^a = \begin{cases} y_a - y_{n|\Omega_g} & \text{in } \ \mathcal{A}_a^n \\ 0 & \text{in } \ \Omega_g \setminus \mathcal{A}_a^n \end{cases}$$

$$\mu_{s,n} = \begin{cases} y_{n|\Omega_s} - y_{\max} & \text{in } \ \mathcal{A}_s^n \\ 0 & \text{in } \ \Omega_s \setminus \mathcal{A}_s^n \end{cases}$$

(4) *Stop or set* $n = n + 1$ *and go to step* (2).

The efficiency of Algorithm 6.1 for the numerical solution of problem (P_γ) is tested by two different examples which is depicted in the following. Before we specify test settings in detail, let us shortly describe the discretization of the PDEs in step (3) of Algorithm 6.1. Here, all quantities are discretized by standard linear finite elements, in particular also μ_g^a, μ_g^b, and μ_s which is feasible since they are not measures but proper functions due to the regularization (cf. Theorem 4.1). Concerning the discretization of the integral operators K and G, we follow the lines of [3] and apply a summarized midpoint rule in combination with an exact integration of the kernel ω (cf. Definition 2.1). A detailed description of this method can be found in [21]. Furthermore, the algebraic equations in Step (3) of Algorithm 6.1 are evaluated in the nodes of the triangulation. The arising overall linear system of equations is then solved by a direct sparse solver. For the computational domain, we choose a square of side length 2 for Ω and a square of side length 1 for Ω_g located in the middle of Ω. This domain is divided into a mesh consisting of 25061 nodes that is refined five times around the interface Γ_r. In

Table 6.1: Matrial parameters for the numerical tests.

κ_g $\left(\frac{\mathrm{W}}{\mathrm{m\,K}}\right)$	κ_s $\left(\frac{\mathrm{W}}{\mathrm{m\,K}}\right)$	ε	σ $\left(\frac{\mathrm{W}}{\mathrm{m^2K^4}}\right)$
0.08	24.0	0.65	$5.6696 \cdot 10^{-8}$

contrast to the rather academic geometry, the material parameters are close to approximate the realistic distributions given in [24]. The respective values are given in Table 6.1.

Furthermore, the external temperature y_0 is assumed to be constant and equal to 293.0 K. Throughout the following numerical tests, the desired temperature gradient (in $\frac{\mathrm{K}}{\mathrm{m}}$) is given by $z \equiv (0, -20)^T$, and we took $u_a \equiv 0$, and $u_b \equiv 400000$ for the control constraints (in $\frac{\mathrm{W}}{\mathrm{m}^3}$). Due to the comparatively large values of the control, one has to deal with rather small Tikhonov regularization parameters to control the influence of the cost term within the objective functional. Hence, we choose $\beta = 10^{-8}$. Moreover, in both test examples, the lower bound in the state constraints is set to $y_a \equiv 2000$ K and we neglect the state constraints in Ω_s since, in all computations, the temperature stays by far below the melting temperature of graphite. The two test cases differ in the value for the upper bound in the state constraints. In the first test case we choose $y_b \equiv 2010$ K, whereas y_b is set to 2050 K in the second example. Moreover, the penalty parameters γ_i, $i = 1, 2$, are all fixed at $\gamma = 10^4$. To illustrate the influence of the regularization parameters, the second test case is later on also performed with modified values of β and γ (see below). In the first example, the desired temperature gradient of -20 in x_2-direction is not achievable with the values for y_a and y_b. Note in this context that Ω_g has the side length 1 such that the difference between y_a and y_b must be greater or equal 20 to allow for a temperature derivative of -20 a.e. in Ω_g. Therefore, we expect the state constraints to be active in the first test case. Figures 6.1–6.6 show the computed solution for this example. We observe that the optimal control exhibits

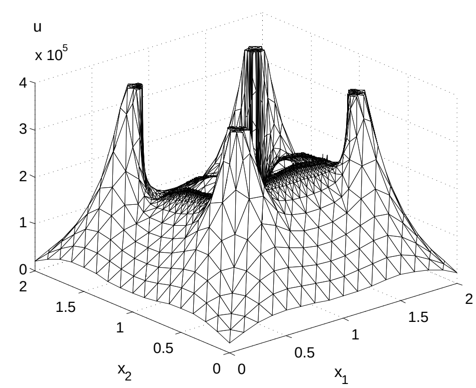

Figure 6.1: Control u in the first example.

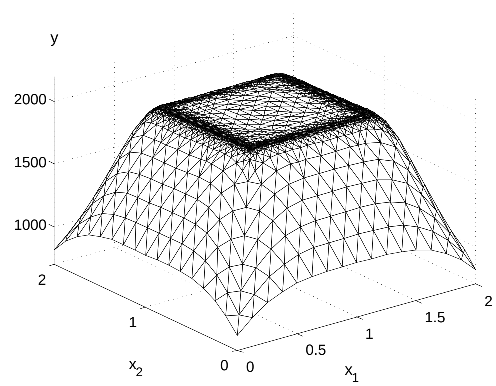

Figure 6.2: State y in the first example.

characteristic peaks in the corners of Ω_g. This finding agrees with the results of [22] where the purely control constrained counterpart of (P) is investigated. A possible explanation of this observation could be the strong cooling effect of the external temperature in combination with the comparatively high thermal conductivity in Ω_s which leads to a large heat flow away from the gas phase, in particular in the corners of Ω_g where more graphite is concentrated than in the other points on Γ_r. As the desired temperature gradient is fairly small, the optimal control tries to compensate for this effect by means of the observed peaks. Since our aim is to

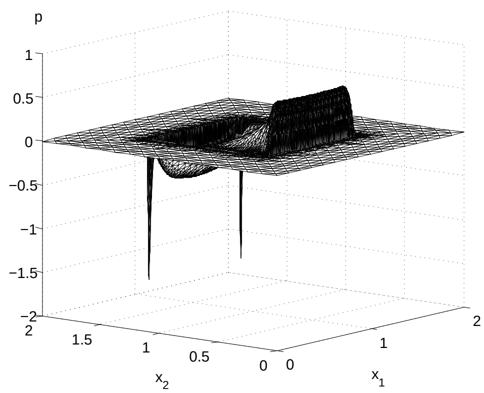

Figure 6.3: Adjoint state p in the first example.

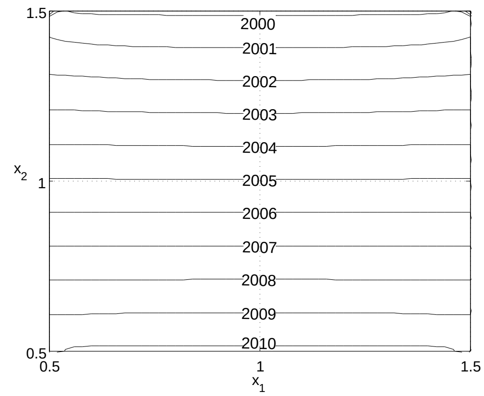

Figure 6.4: Isothermes in Ω_g in the first example.

control the temperature gradient in the gas phase, we are naturally in particular interested in the isothermes in Ω_g which are depicted in Figure 6.4. First one observes that the isothermes are nearly horizontal as required. In contrast to that, the desired temperature difference of 20 K between the lower and upper edge of Γ_r is naturally not achieved due to the bounds on the state. Nevertheless, the state attains the largest possible temperature difference of 10 K. Figures 6.5 and 6.6 show μ_g^a and μ_g^b as approximations of the Lagrange multipliers associated

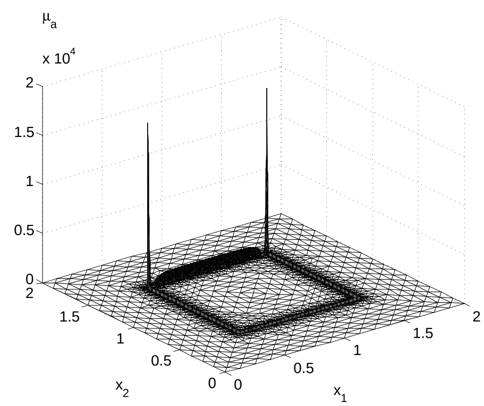

Figure 6.5: μ_g^a in the first example.

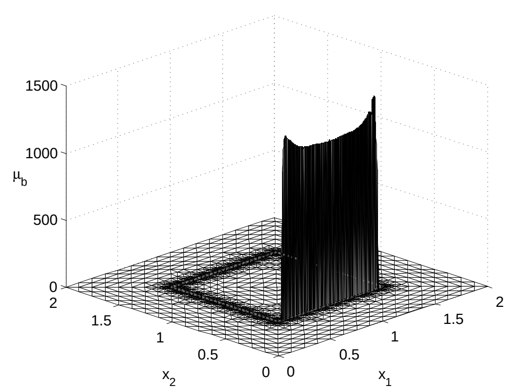

Figure 6.6: μ_g^b in the first example.

to the state constraints. It seems that μ_g^b tends to a line measure on $\{x \in \Gamma_r \,|\, x_2 = 0.5\}$, while μ_g^a tends to point measures in the upper corners of Ω_g. This observation corresponds to the weak regularity of Lagrange multipliers associated to pointwise state constraints. To illustrate the convergence behavior of Algorithm 6.1 Table 6.2 presents the different contributions to the regularized objective functional f_γ, as defined in (4.1), during the iteration. To be more precise, we define

$$f_\gamma^{(y)} := \frac{1}{2}\int_{\Omega_g} |\nabla y - z|^2 dx\,, \quad f_\gamma^{(u)} := \frac{\beta}{2}\int_{\Omega_s} u^2 dx$$
$$f_\gamma^{(b)} := \frac{\gamma}{2}\int_{\Omega_g} \max(0, y - y_b)^2 dx\,, \quad f_\gamma^{(a)} := \frac{\gamma}{2}\int_{\Omega_g} \max(0, y_a - y)^2 dx.$$

In addition, Table 6.2 shows the relative difference between two iterates of Algorithm 6.1 given by

$$\delta := \frac{1}{3}\Big(\frac{\|u_{n+1} - u_n\|_{L^2(\Omega_s)}}{\|u_n\|_{L^2(\Omega_s)}} + \frac{\|y_{n+1} - y_n\|_{L^2(\Omega)}}{\|y_n\|_{L^2(\Omega)}} + \frac{\|p_{n+1} - p_n\|_{L^2(\Omega)}}{\|p_n\|_{L^2(\Omega)}}\Big),$$

which was used for the termination criterion of Algorithm 6.1.

Table 6.2: Convergence of the objective functional in the first example.

it	$f_\gamma^{(y)}$	$f_\gamma^{(u)}$	$f_\gamma^{(b)}$	$f_\gamma^{(a)}$	δ
1	1.99e+02	1.15e+02	0.0	3.38e-01	5.38e+03
2	1.83e+02	2.98e+02	0.0	2.01e+01	1.78e+00
3	1.66e+02	4.10e+02	0.0	6.23e+00	2.95e-01
4	1.43e+02	4.34e+02	0.0	3.63e+00	2.69e-01
5	1.23e+02	4.39e+02	0.0	1.73e+00	2.98e-01
6	9.22e+01	4.43e+02	0.0	1.42e+00	2.96e-01
7	5.34e+01	4.49e+02	1.95e+03	1.53e+00	2.60e-01
8	7.38e+01	4.43e+02	5.69e+01	1.21e+00	5.19e-01
9	6.94e+01	4.42e+02	4.92e+00	7.26e-01	2.58e-01
10	6.49e+01	4.42e+02	1.09e+00	7.81e-01	3.03e-01
11	6.06e+01	4.42e+02	6.07e-01	8.36e-01	3.24e-01
12	5.42e+01	4.42e+02	5.30e-01	9.25e-01	2.18e-01
13	5.14e+01	4.42e+02	4.44e-01	9.46e-01	1.94e-01
14	5.16e+01	4.42e+02	3.39e-01	9.46e-01	1.18e-01
15	5.16e+01	4.42e+02	3.23e-01	9.46e-01	1.33e-02
16	5.16e+01	4.42e+02	3.23e-01	9.46e-01	1.19e-04
17	5.16e+01	4.42e+02	3.23e-01	9.46e-01	1.67e-09

As a semismooth Newton method, Algorithm 6.1 is clearly just locally convergent, which is confirmed by the fact that a significant speed up of convergence is observed after the 14th iteration (see Table 6.2). Moreover, in accordance with Figures 6.5 and 6.6, $f_\gamma^{(b)}$ and $f_\gamma^{(a)}$ do not vanish in the optimum indicating that the state constraints are indeed active. An interesting aspect of the convergence behavior is illustrated by the seventh iteration step where $f_\gamma^{(y)}$ is fairly small but $f_\gamma^{(b)} = 1950$. Hence, distance between the gradient of the actual state and the desired gradient is indeed comparatively small at this stage, but the solution is still non-feasible.

Next, let us turn to the second example. As mentioned above, it nearly coincides with the first one, except the upper bound which is now given by $y_b \equiv 2050$ K such that a temperature difference of 20 K between lower and upper edge of Γ_r is possible. The numerical solution is shown in Figures 6.7–6.12. Again, the optimal control possesses the characteristic peaks

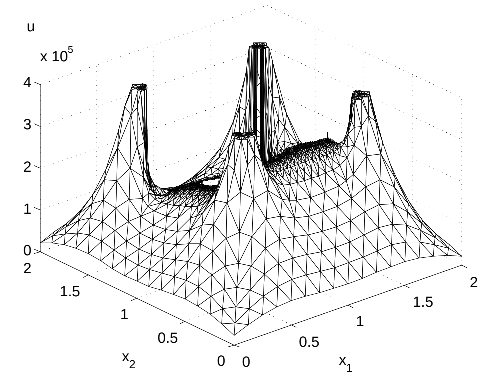

Figure 6.7: Control u in the second example.

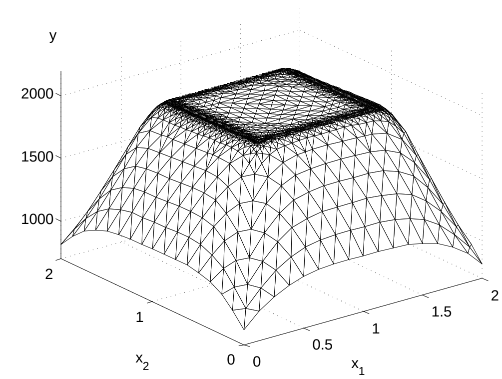

Figure 6.8: State y in the second example.

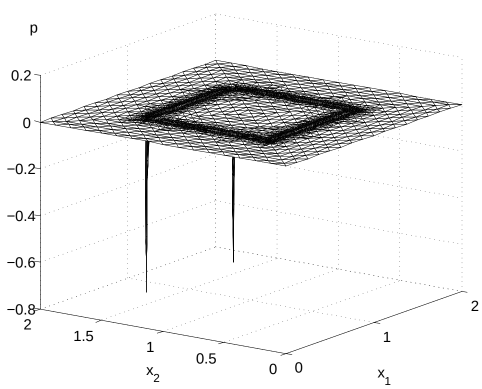

Figure 6.9: Adjoint state p in the second example.

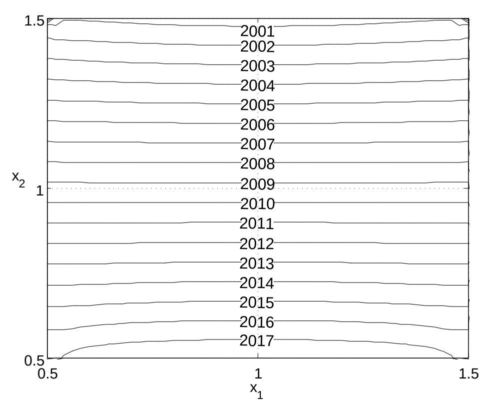

Figure 6.10: Isothermes in Ω_g in the second example.

in the corners of Ω_g. In comparison to the first example, the x_2-derivative of the state now agrees more with the desired one as Figure 6.10 demonstrates. However, especially in the corners of Ω_g, the temperature profile still differs noticeably from the desired one and a temperature difference of 20 K is not reached completely yet. Moreover, the lower state constraint is violated in the upper corner points of Ω_g (see also Figure 6.11). As described below, a modification of β and γ can prevent these irregularities. Similarly to Table 6.2, Table 6.3 shows the convergence history for this example. We observe that, in principle, the algorithm provides the same convergence behavior as in the first case such that number of iteration remains at the same level. Furthermore, since the bounds y_a and y_b do now not contradict the desired temperature gradient as in the first example, the values of $f_\gamma^{(y)}$, $f_\gamma^{(a)}$, and $f_\gamma^{(b)}$ are significantly reduced compared to the first case. According to Figure 6.12, $f_\gamma^{(b)}$ is zero throughout the whole iteration.

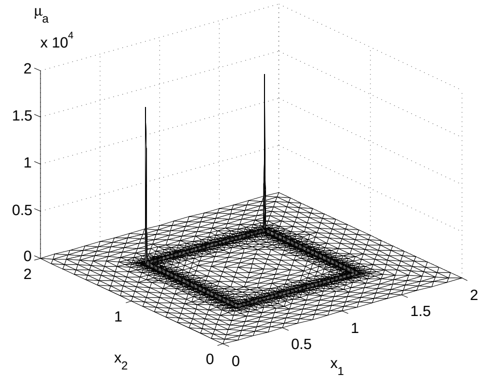

Figure 6.11: μ_g^a in the second example.

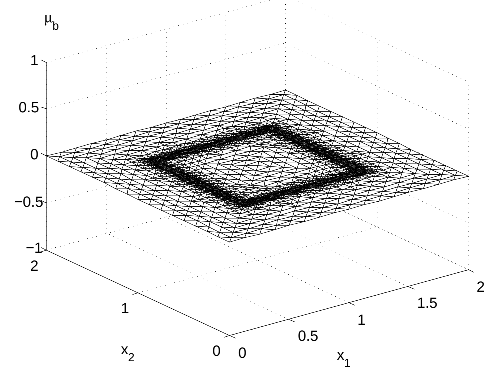

Figure 6.12: μ_g^b in the second example.

Table 6.3: Convergence history in the second example.

it	$f_\gamma^{(y)}$	$f_\gamma^{(u)}$	$f_\gamma^{(b)}$	$f_\gamma^{(a)}$	δ
1	1.99e+02	1.15e+02	0.0	3.38e-01	5.38e+03
2	1.83e+02	2.98e+02	0.0	2.00e+01	1.78e+00
3	1.66e+02	4.10e+02	0.0	6.23e+00	2.95e-01
4	1.43e+02	4.34e+02	0.0	3.63e+00	2.69e-01
5	1.23e+02	4.39e+02	0.0	1.73e+00	2.99e-01
6	9.22e+01	4.43e+02	0.0	1.42e+00	2.96e-01
7	5.34e+01	4.49e+02	0.0	1.53e+00	2.60e-01
8	1.08e+01	4.55e+02	0.0	1.50e+00	7.27e-01
9	1.10e+01	4.55e+02	0.0	8.35e-01	2.91e-01
10	1.11e+01	4.55e+02	0.0	6.14e-01	2.72e-01
11	1.13e+01	4.55e+02	0.0	4.99e-01	1.98e-01
12	1.14e+01	4.55e+02	0.0	4.42e-01	1.11e-01
13	1.16e+01	4.55e+02	0.0	3.62e-01	1.03e-01
14	1.17e+01	4.55e+02	0.0	3.02e-01	9.37e-02
15	1.17e+01	4.55e+02	0.0	2.97e-01	2.82e-03
16	1.17e+01	4.55e+02	0.0	2.97e-01	3.89e-10

However, the objective functional is dominated by the Tikhonov regularization part $f_\gamma^{(u)}$. The situation changes if β is reduced to $\beta = 10^{-10}$ as the Table 6.4 illustrates. Here, we just present values of the last iteration, as the other values contain only little information.

The results of Table 6.4 are also confirmed by Figures 6.13 and 6.14 showing the control and the isothermes for this setting.

Table 6.4: Convergence history in the second example with $\beta = 10^{-10}$ and $\gamma = 10^4$.

it	$f_\gamma^{(y)}$	$f_\gamma^{(u)}$	$f_\gamma^{(b)}$	$f_\gamma^{(a)}$	δ
18	2.12e+00	5.18e+00	0.0	9.30e-04	1.13e-08

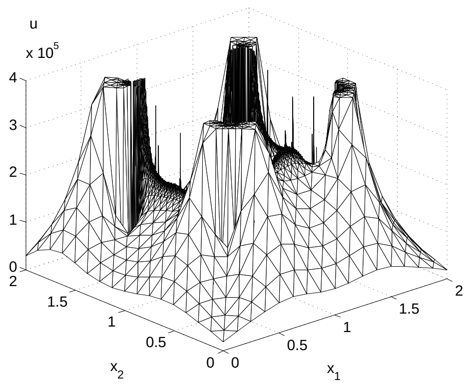

Figure 6.13: Control u in the second example with $\beta = 10^{-10}$ and $\gamma = 10^4$.

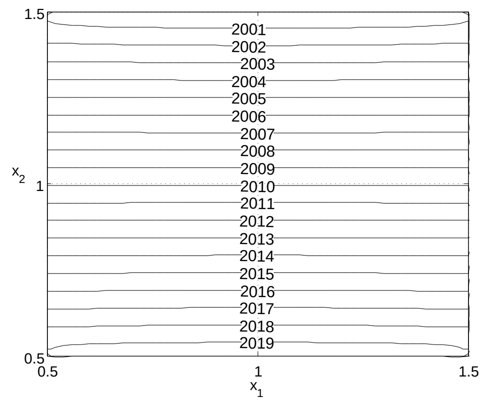

Figure 6.14: Isothermes in Ω_g in the second example with $\beta = 10^{-10}$ and $\gamma = 10^4$.

As one can see in Figure 6.14, the difference between the desired temperature gradient and the optimal one is significantly reduced. However, the reduction of the Tikhonov regularization parameter β clearly causes irregularities in the control, in particular on Γ_r and in the corners of Ω_g (cf. Figure 6.13). Moreover, the value for $f_\gamma^{(a)}$ in the fifth column of Table 6.4 indicates that the lower state constraint is still active in a few points. In this example, this can be prevented by increasing γ. To see this, we now set $\gamma = 10^6$. The corresponding results are shown in Table 6.5. Again, we just show the values of the last iteration. Furthermore, the plots of the solution are omitted since they contain only little additional information.

Table 6.5: Convergence history in the second example with $\beta = 10^{-10}$ and $\gamma = 10^6$.

it	$f_\gamma^{(y)}$	$f_\gamma^{(u)}$	$f_\gamma^{(b)}$	$f_\gamma^{(a)}$	δ
23	2.29e+00	5.60e+00	0.0	0.0	9.92e-09

We observe that, with this setting, also $f_\gamma^{(a)}$ equals zero such that the optimal state is indeed feasible. Notice however that the impact of the penalty terms $f_\gamma^{(a)}$ and $f_\gamma^{(b)}$ is increased by the magnification of γ and consequently, the results for $f_\gamma^{(y)}$ and $f_\gamma^{(u)}$ are slightly worsened in comparison to Table 6.4. Furthermore, the number of iterations is increased which indicates that the condition of the problem is worsened if γ is increased. Therefore, to avoid strong irregularities of the control and in view of a reasonable condition of the problem, the regularization parameters β and γ should not be chosen too small and large, respectively.

References

[1] R. A. Adams. *Sobolev Spaces.* Academic Press, Boston, 1978.

[2] J.-J. Alibert and J.-P. Raymond. Boundary control of semilinear elliptic equations with discontinuous leading coefficients and unbounded controls. *Numer. Funct. Anal. and Optimization*, 3&4:235–250, 1997.

[3] K. Atkinson and G. Chandler. The collocation method for solving the radiosity equation for unoccluded surfaces. *J. Int. Eqn. Appl.*, 10:253–290, 1998.

[4] M. Bergounioux, K. Ito, and K. Kunisch. Primal-dual strategy for constrained optimal control problems. *SIAM J. Control and Optimization*, 37:1176–1194, 1999.

[5] M. Bergounioux and K. Kunisch. Primal-dual active set strategy for state-constrained optimal control problems. *Computational Optimization and Applications*, 22:193–224, 2002.

[6] E. Casas. Control of an elliptic problem with pointwise state constraints. *SIAM J. Control and Optimization*, 4:1309–1322, 1986.

[7] E. Casas. Boundary control of semilinear elliptic equations with pointwise state constraints. *SIAM J. Control and Optimization*, 31:993–1006, 1993.

[8] E. Casas, J.C. De Los Reyes, and F. Tröltzsch. Sufficient second order optimality conditions for semilinear control problems with pointwise state constraints. Submitted, 2007.

[9] E. Casas and F. Tröltzsch. Error estimates for the finite-element approximation of a semilinear elliptic control problem. *Control and Cybernetics*, 31:695–712, 2002.

[10] J. de los Reyes and K. Kunisch. A semismooth Newton method for control constrained boundary optimal control of the navier-stokes equations. *Nonlinear Analysis*, 62:1289–1316, 2005.

[11] J. Elschner, J. Rehberg, and G. Schmidt. Optimal regularity for elliptic transmission problems including c^1 interfaces. *Interfaces and Free Boundaries*, 2:233–252, 2007.

[12] K. Gröger. A $W^{1,p}$-Estimate for Solutions to Mixed Boundary Value Problems for Second Order Elliptic Differential Equations. *Math. Ann.*, 283:679–687, 1989.

[13] M. Hintermüller, K. Ito, and K. Kunisch. The primal-dual active set strategy as a semismooth Newton method. *SIAM J. Optim.*, 13:865–888, 2003.

[14] M. Hintermüller and K. Kunisch. Feasible and non-interior path-following in constrained minimization with low multiplier regularity. Report 01-05, Department of Mathematics and Scientific Computing, University of Graz, Heinrichstraße 36, A-8010 Graz, Austria, October 2005.

[15] K. Ito and K. Kunisch. Augmented Lagrangian methods for nonsmooth, convex optimization in Hilbert spaces. *Nonlinear Analysis TMA*, 41:591–616, 2000.

[16] K. Ito and K. Kunisch. Semi-smooth Newton methods for state-constrained optimal control problems. *Systems and Control Letters*, 50:221–228, 2003.

[17] K. Ito and K. Kunisch. The primal-dual active set method for nonlinear optimal control problems with bilateral constraints. *SIAM J. Control and Optimization*, 43:357–376, 2004.

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

[19] A. Konstantinov. Sublimation growth of SiC. In *Properties of Silicon Carbide*, Ch. 8.2, pp. 170-203 in G. Harris, ed., *Properties of Silicon Carbide*, No. 13, in EMIS Datareview Series, Institution of Electrical Engineers, INSPEC, London, UK, 1995.

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

[21] C. Meyer. *Optimal control of semilinear elliptic equations with applications to sublimation crystal growth.* Dissertation, 2006.

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

[23] C. Meyer and I. Yousept. State-constrained optimal control of semilinear elliptic equations with nonlocal radiation interface conditions. 2007, Submitted.

[24] P. Philip. *Transient Numerical Simulation of Sublimation Growth of SiC Bulk Single Crystals. Modeling, Finite Volume Method, Results.* PhD thesis, Department of Mathematics, Humboldt University of Berlin, 2003.

[25] 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.*, 61–62:68–72, 1999.

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