Weierstraß-Institut
für Angewandte Analysis und Stochastik
Leibniz-Institut im Forschungsverbund Berlin e. V.

Preprint ISSN 0946 – 8633

Optimal control of multiphase steel production

Dietmar Hömberg[1], Klaus Krumbiegel[2], Nataliya Togobytska[1]

submitted: June 25, 2014

[1] Weierstrass Institute
Mohrenstr. 39
10117 Berlin
Germany
E-Mail: dietmar.hoemberg@wias-berlin.de
nataliya.togobytska@wias-berlin.de

[2] IAV GmbH
Carnotstr. 1
10587 Berlin
Germany
E-Mail: klaus.krumbiegel@iav.de

No. 1971
Berlin 2014

2010 *Mathematics Subject Classification.* 35K05, 49M37, 49N90.

Key words and phrases. hot rolling, dual phase steels, optimal control.

The work on this paper has been partially supported by the Deutsche Forschungsgemeinschaft (DFG) within the priority program 1204 – *Algorithms for fast, material specific process-chain design and analysis in metal forming.*

Edited by
Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS)
Leibniz-Institut im Forschungsverbund Berlin e. V.
Mohrenstraße 39
10117 Berlin
Germany

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

Abstract

An optimal control problem for the production of multiphase steel is investigated, where the state equations are a semilinear heat equation and an ordinary differential equation, which describes the evolution of the ferrite phase fraction. The optimal control problem is analyzed and the necessary and sufficient optimality conditions are derived. For the numerical solution of the control problem reduced sequential quadratic programming (rSQP) method with a primal-dual active set strategy (PDAS) was applied. The numerical results are presented for the optimal control of a cooling line for production of hot rolled Mo-Mn dual phase steel.

1 Introduction

We consider an optimal control problem that describes the hot rolling process of multiphase steel, in particular the dual phase (DP) steel. Dual phase steels have shown high potential for automotive applications due to their remarkable property combination with high strength and good formability. The

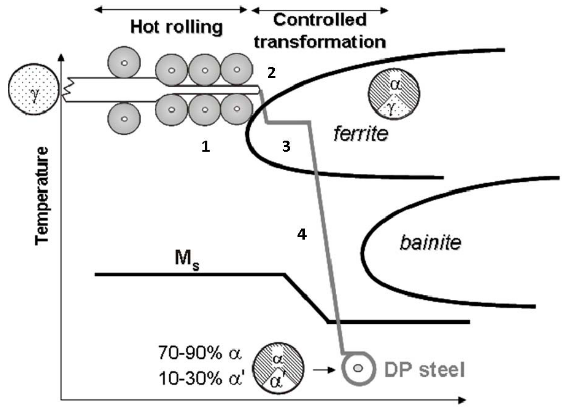


Figure 1: A sketch of the processing scheme for hot rolled dual phase steel.

hot rolling process of dual phase steel consists of 4 steps:
Rolling in roughing and finishing stands, which results in the refinement of austenite grain size due to the repeating static recrystallization (1), laminar cooling into two phase region (2), isothermal holding at ferrite transformation region temperatures, where the temperatures remain relatively constant (3), and finally, fast continuous cooling to the required coiling temperature, during which martensite transformation takes place and bainite transformation can be avoided (4).

The controlled cooling of stages (2)-(4) happens on the so-called run out table (ROT). The biggest challenge in producing DP steel in this way is that the process window is very tight as only very short time in order of less than 10 s is allowed on the run out table according to its limited length. Hence, there is a strong demand for the online control of the process parameters such as the time and temperature on ROT as well as the cooling rate during cooling down to coiling (step 4 in Figure 1).

The goal of this paper is the analysis of a mathematical optimal control problem to compute the desired ferrite fraction and temperature at the end of step 3 of the process. Existing optimal control approaches for run out tables up to now solely focus on the evolution of temperature, see, e.g., [20],[16]. The heat transfer coefficient in the Newton type cooling boundary condition acts as the control parameter. In a previous paper [3] we have shown how to relate this coefficient to the flow rate of coolant in a real cooling process. The scope of this paper is to analyze the resulting boundary coefficient control problem subject to a semilinear heat equation and rate law to describe the evolution of ferrite phase.

We investigate the existence of a solution and derive the first-oder necessary and second-order sufficient optimality conditions. An extended analysis of the state system of coupled partial and ordinary differential equations is presented in e.g Hömberg and Sokolowski [11] and Hömberg,Volkwein [12]. In [12] the existence and first-oder necessary optimality conditions have been discussed for the optimal control problem of laser surface hardening. Second order optimality conditions for control problems governed by instationary equations have been discussed e.g in [6] and [18]. In comparison to the very general and abstract setting of the latter contribution the main novelty of this paper is that we can allow for mixed boundary conditions and a control of coefficient function.

To solve the control problem numerically, we use a reduced sequential quadratic programming (SQP) method, which has proved to be very effective in many areas of application, such as optimal control. For an overview about reduced-Hessian SQP methods in finite dimensional spaces we refer to e.g. [17]. A prospective look at SQP methods, in particular rSQP, for semilinear parabolic control problems is given by Kupfer and Sachs [14]. A numerical application of the reduced SQP method to parabolic control problems was considered by Kupfer and Sachs [15], Hintermüller, Volkwein and Diwoky [10].

In each iteration of rSQP method the quadratic optimal control problem (QP^k) with control constraints has to be solved. To treat the (QP^k) problems we apply a primal-dual active set strategy as for instance proposed by Bergonioux, Ito and Kunisch [2] for control constrained optimal control problems.

The paper is organized as follows: In Section 2 we analyze the optimal control problem and derive optimality conditions. In Section 3 we discuss the numerical optimization algorithms, i.e. the reduced SQP method with the active set strategy. The last section is devoted to numerical results.

2 The optimal control problem

2.1 Problem formulation and assumptions

The system of state equations consists of a semilinear heat equation coupled with an initial-value problem for the phase transition of ferrite.

$$
\begin{aligned}
f_t &= G(\theta, f), && \text{in } Q = \Omega \times (0,T) && \text{(1a)}\\
f(0) &= 0, && \text{in } \Omega && \text{(1b)}\\
\rho c_p \theta_t - k\Delta\theta &= \rho L f_t, && \text{in } Q && \text{(1c)}\\
-k\frac{\partial \theta}{\partial n} &= u(t)(\theta - \theta_w), && \text{on } \Sigma_1 = \Gamma \times (0,T) && \text{(1d)}\\
-k\frac{\partial \theta}{\partial n} &= 0, && \text{on } \Sigma_2 = (\partial\Omega \setminus \Gamma) \times (0,T) && \text{(1e)}\\
\theta(0) &= \theta_0, && \text{in } \Omega && \text{(1f)}
\end{aligned}
$$

Here, f denotes the volume fraction of ferrite. The density ρ, the heat capacity c_p, the heat conductivity κ and the latent heat L are assumed to be positive constants. The term $\rho L f_t$ describes the latent heat due to the phase transformation of ferrite. $u(t)$ represents a time-dependent heat transfer coefficient, which contains information about flow rate of water in the cooling line and serves as a control variable.

The particular optimal control problem reads as follows:

$$\min \qquad J(\theta,f,u) = \frac{\alpha_1}{2}\int\limits_{\Omega}(f(x,T)-f_d(x))^2\,dx + \frac{\alpha_2}{2}\iint\limits_{Q}(\theta-\theta_d)^2dx\,dt$$
$$+\frac{\alpha_3}{2}\int\limits_0^T u^2dt \tag{P}$$
$$\text{s.t. } (\theta,\ f,\ u) \text{ satisfies (1) and } u\in U_{ad}$$

where $U_{ad} = \{u \in L^\infty(0,T) : u_a \leq u \leq u_b, u_a, u_b \geq 0\}$ and $\alpha_i,\ i = 1,\cdots,3$ are positive constants. Moreover, we require the following on the quantities of the optimal control problem and the state equations:

(A1) $\Omega \subset \mathbb{R}^3$ denotes a bounded domain with Lipschitz boundary $\partial\Omega$.

(A2) The function $G = G(\theta, f)$ is twice continuously differentiable with respect to θ and f. There is a constant $M > 0$, such that

$$|G(\theta,f)| \leq M, \quad \forall(\theta,f)\in\mathbb{R}^2.$$

The second derivative of G w.r.t. (θ, f) is uniformly Lipschitz on bounded sets, i.e. for all $M > 0$ there exists $L_M > 0$ such that G satisfies

$$|G''(\theta_1,f_1)-G''(\theta_2,f_2)| \leq L_M(|\theta_1-\theta_2|+|f_1-f_2|)$$

for all $\theta_i,\ f_i \in \mathbb{R}$ with $|\theta_i|, |f_i| \leq M,\ i = 1, 2.$

(A3) $\theta_w \in L^\infty(\Sigma_1)$, $\theta_0 \in C(\bar{\Omega})$ and $\theta_d \in L^\infty(Q)$.

(A4) $f_d \in L^\infty(\Omega),\ 0 \leq f_d \leq 1$ a.e. in Ω.

Remark 1: Assumption (A2) can be relaxed and has been chosen only to avoid technicalities when computing the derivatives. For more realistic phase transition models we refer to [5].

Remark 2: The choice of the cost functional in P is somewhat arbitrary. Mutatis mutandis, also a control of the temperature at end-time and/or a control of the distributed ferrite fraction is possible.

2.2 Analysis of the state system

Let us start with the discussion of the initial value problem in the state system. In view of the assumptions, the following result can be proven by standard arguments. For a detailed proof, we refer to [11] or [12].

Lemma 2.1. *Suppose that (A2) holds true. Then we have the following.*

(a) Let $\theta \in L^1(Q)$ be given, then (1a), (1b) *has a unique solution $f \in W^{1,\infty}(0,T;L^\infty(\Omega))$ and*

$$\|f\|_{W^{1,\infty}(0,T;L^\infty(\Omega))} \leq M_1$$

with a constant independent of θ.

(b) Let $\theta_1,\ \theta_2 \in L^p(Q)$, $1 \leq p < \infty$ and let $f_1,\ f_2$ be the corresponding solutions of (1a), (1b)*, then there exists a constant $M_2 > 0$ such that,*

$$\|f_1 - f_2\|_{W^{1,p}(0,T;L^p(\Omega))} \leq M_2 \|\theta_1 - \theta_2\|_{L^p(Q)}.$$

Before considering the heat equation, we recall the following results from the theory of linear parabolic equations. We consider the following linear parabolic problem

$$\rho c_p \theta_t - k\Delta\theta = r, \qquad \text{in } Q \tag{2a}$$

$$-k\frac{\partial\theta}{\partial n} = u(\theta - \theta_w), \qquad \text{on } \Sigma_1 \tag{2b}$$

$$-k\frac{\partial\theta}{\partial n} = 0, \qquad \text{on } \Sigma_2 \tag{2c}$$

$$\theta(0) = \theta_0, \qquad \text{in } \Omega. \tag{2d}$$

It is well known that a suitable function space for the solution of linear parabolic partial differential equations is

$$W(0,T) = \{\theta \in L^2(0,T;H^1(\Omega)) : \theta_t \in L^2(0,T;H^1(\Omega)^*\}.$$

Under additional assumptions on the data r, u, θ_w, θ_0 the following result can be found,e.g., in Tröltzsch [22], Theorem 5.5:

Lemma 2.2. *Suppose that (A3) holds true, and $r \in L^{s_1}(Q)$, $u \in L^\infty(0,T), u \geq 0$. Let $s_1 > 5/2$, $s_2 > 4$, then the initial value problem* (2a)-(2d) *admits a unique solution $\theta \in W(0,T) \cap C(\bar{Q})$ satisfying the a priori estimate with a constant $C > 0$*

$$\|\theta\|_{W(0,T)} + \|\theta\|_{C(\bar{Q})} \leq C(\|r\|_{L^{s_1}(Q)} + \|u\|_{L^{s_2}(0,T)} + \|\theta_0\|_{C(\bar{Q})}). \tag{3}$$

It is a useful result for the proof of solvability of the state system (1), which is discussed below.

Theorem 2.3. *Let (A1)-(A4) be satisfied. Then, the state system* (1) *admits for every control $u \in U_{ad}$ a unique solution*

$$(\theta,\ f) \in W(0,T) \cap C(\bar{Q}) \times W^{1,\infty}(0,T;L^\infty(\Omega))$$

satisfying

$$\|\theta\|_{W(0,T)} + \|\theta\|_{C(\bar{Q})} + \|f\|_{W^{1,\infty}(0,T;L^\infty(\Omega))} \leq M_3.$$

Proof. If not otherwise stated, c denotes a generic constant, not to be confused with the heat capacity c_p. To prove the existence of a local unique solution to (1c)-(1f), we apply the Banach's fixed point theorem. For that purpose we define an operator $F : K \subset W(0,T) \to W(0,T)$ that maps $\hat{\theta} \in W(0,T)$ to the solution θ of

$$\rho c_p \theta_t - k\Delta\theta = \rho L \hat{f}_t, \qquad \text{in } Q \tag{4a}$$

$$-k\frac{\partial\theta}{\partial n} = u(\theta - \theta_w), \qquad \text{on } \Sigma_1 \tag{4b}$$

$$-k\frac{\partial\theta}{\partial n} = 0, \qquad \text{on } \Sigma_2 \tag{4c}$$

$$\theta(0) = \theta_0 \qquad \text{in } \Omega, \tag{4d}$$

where $\hat{f}$ solves (1a)-(1b) with $\hat{\theta}$. From Lemma 2.1 we find that $\hat{f} \in W^{1,\infty}(0,T;L^\infty(\Omega))$ is uniquely determined. It follows from the theory of the linear parabolic equations that the problem (4a)-(4d) possesses a unique solution in $W(0,T)$ (see e.g. [22], Chap. 3.4.4). Hence, we can conclude that F is well-defined. Furthermore, the following a priori estimate with a constant $C_1 > 0$ is valid

$$\|\theta\|_{W(0,T)} \leq C_1(\|\hat{f}\|_{L^2(Q)} + \|u\theta_w\|_{L^2(\Sigma_1)} + \|\theta_0\|_{L^2(\Omega)}) \leq C_2,$$

where C_2 depends only on θ_0 and the constant M_1 from Lemma 2.1. Hence, if M is chosen big enough, F is a self mapping on

$$K = \{\eta \in W(0,T) : \ \|\eta\|_{W(0,T)} \leq M\}.$$

Now, we want to show that F is a contraction. Let $\hat{\theta}_i \in K, \ i = 1,2, \ \theta_i = F(\hat{\theta}_i)$ and $\hat{\theta} = \hat{\theta}_1 - \hat{\theta}_2$. Then $\theta = \theta_1 - \theta_2$ solves

$$\begin{aligned}
\rho c_p \theta_t - k\Delta\theta &= \rho L(G(\hat{\theta}_1, f_1) - G(\hat{\theta}_2, f_2)), && \text{in } Q \\
-k\frac{\partial\theta}{\partial n} &= u(t)\theta, && \text{on } \Sigma_1 \\
-k\frac{\partial\theta}{\partial n} &= 0, && \text{on } \Sigma_2 \\
\theta(0) &= 0 && \text{in } \Omega
\end{aligned}$$

Here again, we use the a priori estimate

$$\|\theta\|_{W(0,T)} \leq c\|G(\hat{\theta}_1, f_1) - G(\hat{\theta}_2, f_2)\|_{L^2(Q)}. \tag{6}$$

Due to the Lipschitz continuity of G in both variables (Assumption (A2)) and Lemma 2.1 (b) we obtain

$$\|\theta\|_{W(0,T)} \leq c(\|\hat{\theta}\|_{L^2(Q)} + \|f_1 - f_2\|_{L^2(Q)}) \leq c\|\hat{\theta}\|_{L^2(Q)} \tag{7}$$

Further, we use the fact that $W(0,T) \hookrightarrow C(0,T,L^2(\Omega))$

$$\|\theta\|_{W(0,T)} \leq c\|\hat{\theta}\|_{L^2(Q)} \leq cT^{1/2}\|\hat{\theta}\|_{L^\infty(0,T;L^2(\Omega))} \leq cT^{1/2}\|\hat{\theta}\|_{W(0,T)}. \tag{8}$$

Hence, choosing $T^+ < T$ small enough, we conclude that F is a contraction on $W(0,T^+)$. Since F is also a self-mapping on K, we can apply the Banach's fixed point theorem to conclude that F has a unique fixed point θ, which is a local solution to (1c)-(1f). By a bootstrapping argument, the solution can be extended to the time interval $[0,T]$.
Moreover, in view of Lemma 2.1 we can apply Lemma 2.2 and obtain the additional regularity for θ. □

In view of the analysis of the state system, we define

$$Y = W(0,T) \cap C(\bar{Q})$$

and introduce the control to state mapping

$$S = (S_\theta, \, S_f) : L^\infty(0,T) \to Y \times W^{1,p}(0,T;L^p(\Omega)), \quad 1 \leq p < \infty, \tag{9}$$

which assigns to every control $u(t) \in L^\infty(0,T)$ the solution of the state system (1). Moreover, the mapping is Lipschitz continuous:

Corollary 2.4. *Suppose that (A1)-(A4) hold and let $(\theta_1, \, f_1), \, (\theta_2, \, f_2)$ be the solutions of* (1) *corresponding to $u_1, \, u_2 \in L^\infty(0,T)$. Then, there exists a constant $C > 0$, such that*

$$\|\theta_1 - \theta_2\|_{C(\bar{Q})} + \|f_1 - f_2\|_{W^{1,p}(0,T;L^p(\Omega))} \leq C\|u_1 - u_2\|_{L^\infty(0,T)}.$$

Proof. Defining $\theta = \theta_1 - \theta_2$ and $f = f_1 - f_2$, one finds that $(\theta,\ f)$ solves

$$f_t = G(\theta_1, f_1) - G(\theta_2, f_2), \qquad \text{in } Q \tag{10a}$$

$$f(0) = 0, \qquad \text{in } \Omega \tag{10b}$$

$$\rho c_p \theta_t - k\Delta\theta = \rho L f_t, \qquad \text{in } Q \tag{10c}$$

$$-k\frac{\partial \theta}{\partial n} = u_1(t)\theta + (u_1 - u_2)(\theta_2 - \theta_w), \qquad \text{on } \Sigma_1 \tag{10d}$$

$$-k\frac{\partial \theta}{\partial n} = 0, \qquad \text{on } \Sigma_2 \tag{10e}$$

$$\theta(0) = 0, \qquad \text{in } \Omega. \tag{10f}$$

Further, we prove the Lipschitz continuity regarding the $L^\infty(Q)$-norm. The multiplication of (10c) by θ^{2k-1}, for an arbitrary $k \in \mathbb{N}$ and Integration over Ω and over $(0, t)$ yields

$$\begin{aligned} \frac{\rho c_p}{2k}\int_\Omega \theta^{2k}(t)\,dx + \kappa(2k-1)\int_0^t\int_\Omega \theta^{2k-2}|\nabla\theta|^2\,dxds + \int_0^t\int_{\Sigma_1} u_1(t)\theta^{2k}\,dxds \\ = -\int_0^t\int_{\Sigma_1}(u_1 - u_2)(\theta_2 - \theta_w)\theta^{2k-1}\,dxds + \int_0^t\int_\Omega f_t\theta^{2k-1}\,dxds \end{aligned} \tag{11}$$

Due to Lemma 2.1(b) and applying Hölder's inequality

$$\int_0^t\int_\Omega |f_t\theta^{2k-1}|\,dxds \le C_1\int_0^t\int_\Omega \theta^{2k}\,dxds \tag{12}$$

Using Young's inequality

$$|ab| \le \frac{\varepsilon^p|a|^p}{p} + \frac{\varepsilon^{-q}|b|^q}{q}, \quad \frac{1}{p} + \frac{1}{p} = 1$$

with $b = (\theta_2 - \theta_w)(u_1 - u_2)\beta(x),\ a = \theta^{2k-1},\ p = \frac{2k}{2k-1},\ q = 2k,\ \varepsilon > 0$
and applying the trace theorem we obtain

$$\begin{aligned} \int_0^t\int_{\Sigma_1} |(u_1 - u_2)(\theta_2 - \theta_w)\theta^{2k-1}|\,dxds &\le \frac{\varepsilon^p}{p}\int_0^t\int_{\Sigma_1}\theta^{2k}\,dxds \\ &+ \frac{\varepsilon^{-q}}{q}\int_0^t\int_{\Sigma_1}(u_1 - u_2)^{2k}(\theta_2 - \theta_w)^{2k}\,dxds \\ &\le C_2\frac{\varepsilon^p}{p}\int_0^t\int_\Omega \theta^{2k}\,dxds + C_2 k\frac{\varepsilon^p}{p}\int_0^t\int_\Omega \theta^{2k-2}|\nabla\theta|^2\,dxds \\ &+ C_3\frac{\varepsilon^{-q}}{q}\|u_1 - u_2\|^{2k}_{L^\infty(0,T)}\|\theta_2 - \theta_w\|^{2k}_{L^\infty(\Sigma_1)} \end{aligned} \tag{13}$$

Choosing $\varepsilon = (\frac{p\kappa}{2C_2})^{1/p}$ we have

$$\begin{aligned} \int_0^t\int_{\Sigma_1} |(u_1 - u_2)(\theta_2 - \theta_w)\theta^{2k-1}|\,dxds \le &\frac{\kappa}{2}\int_0^t\int_\Omega \theta^{2k}\,dxds + \frac{\kappa k}{2}\int_0^t\int_\Omega \theta^{2k-2}|\nabla\theta|^2\,dxds \\ &+ \frac{C_5}{2k}C_4^{2k}\|u_1 - u_2\|^{2k}_{L^\infty(0,T)} \end{aligned} \tag{14}$$

Inserting (12) and (14) into (11) we conclude

$$\int_\Omega \theta^{2k}(t)\,dx \le C_5 C_4^{2k} \|u_1 - u_2\|^{2k}_{L^\infty(0,T)} + C_6 2k \int_0^t \int_\Omega \theta^{2k}\,dxds \tag{15}$$

Gronwall's Lemma yields

$$\|\theta(t)\|^{2k}_{L^{2k}} \le C_5 C_4^{2k} \|u_1 - u_2\|^{2k}_{L^\infty(0,T)} exp(C_6 2kt), \qquad \forall t \in [0,T],$$

Taking the $(2k)$-th root,

$$\sup_{0\le t\le T} \|\theta(t)\|_{L^{2k}} \le C_7 \|u_1 - u_2\|_{L^\infty(0,T)}.$$

Letting $k \to \infty$, we obtain the Lipschitz continuity of the solution operator in L^∞-norm. The coincidence of $L^\infty(Q)$ and $C(\bar{Q})$ norms implies the Lipschitz stability of the solution operator in $C(\bar{Q})$ space. The estimate for $\|f_1 - f_2\|_{W^{1,p}(0,T;L^p(\Omega))}$ follows from Lemma 2.1. □

Now, let us discuss differentiability of the solution operator.

Theorem 2.5. *Let Assumptions (A1)-(A4) be satisfied. Then, the solution operator S is twice Frechét-differentiable from $L^\infty(0,T)$ to $Y \times W^{1,p}(0,T;L^p(\Omega))$, $\quad 1 \le p < \infty$. The directional derivative $(\theta_h,\ f_h) = S'(u)h = (S'_\theta(u)h, S'_f(u)h)$ at point $u \in L^\infty(0,T)$ in direction $h \in L^\infty(0,T)$ is given by the solution of*

$$\begin{aligned}
(f_h)_t &= G_\theta(\theta,f)\theta_h + G_f(\theta,f)f_h, && \textit{in } Q && \text{(16a)}\\
f_h(0) &= 0, && \textit{in } \Omega && \text{(16b)}\\
\rho c_p(\theta_h)_t - k\Delta\theta_h &= \rho L(f_h)_t, && \textit{in } Q && \text{(16c)}\\
-k\frac{\partial\theta_h}{\partial n} &= u(t)\theta_h + h(t)(\theta - \theta_w), && \textit{on } \Sigma_1 && \text{(16d)}\\
-k\frac{\partial\theta_h}{\partial n} &= 0, && \textit{on } \Sigma_2 && \text{(16e)}\\
\theta_h(0) &= 0, && \textit{in } \Omega, && \text{(16f)}
\end{aligned}$$

with $(\theta,\ f) = S(u)$. Furthermore, $(\theta_{h_1h_2}, f_{h_1h_2}) = S''(u)[h_1,h_2]$ is the solution of

$$\begin{aligned}
(f_{h_1h_2})_t &= G_\theta(\theta,f)\theta_{h_1h_2} + G_f(\theta,f)f_{h_1h_2}, && \textit{in } Q && \text{(17a)}\\
&\quad + G''(\theta,f)[(\theta_{h_1},f_{h_1}),(\theta_{h_2},f_{h_2})] && &&\\
f_{h_1h_2}(0) &= 0, && \textit{in } \Omega && \text{(17b)}\\
\rho c_p(\theta_{h_1h_2})_t - k\Delta\theta_{h_1h_2} &= \rho L(f_{h_1h_2})_t && \textit{in } Q && \text{(17c)}\\
-k\frac{\partial\theta_{h_1h_2}}{\partial n} &= u(t)\theta_{h_1h_2} + h_1(t)\theta_{h_2} + h_2(t)\theta_{h_1}, && \textit{on } \Sigma_1 && \text{(17d)}\\
-k\frac{\partial\theta_{h_1h_2}}{\partial n} &= 0, && \textit{on } \Sigma_2 && \text{(17e)}\\
\theta_{h_1h_2}(0) &= 0, && \textit{in } \Omega, && \text{(17f)}
\end{aligned}$$

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

Proof. The existence of a unique solution (θ_h, f_h) of the linearized state system (16) in $W(0,T) \times W^{1,\infty}(0,T; L^{10/3}(\Omega))$ can be proved along the lines of Theorem 2.3. Moreover, the terms on the right-hand side of (16c),(16d) have enough regularity, namely

$$h(t)(\theta - \theta_w) \in L^\infty(\Sigma_1),\ G_f(\theta, f) f_h \in L^\infty(0,T; L^{10/3}(\Omega)),\ G_\theta(\theta, f)\theta_h \in L^{10/3}(Q).$$

The latter is true due to the fact, that $G_\theta(\theta, f) \in L^\infty(Q)$, $\theta_h \in W(0,T)$ and therefore $\theta_h \in L^{10/3}(Q)$ (see Lemma 6.7 in [11]). Then the continuity of θ_h follows from Lemma 2.2.

For given control $u \in L^\infty(0,T)$ and direction $h \in L^\infty(0,T)$ we define $(\theta, f) = S(u)$ and $(\theta^h, f^h) = S(u+h)$, respectively. Furthermore, let (θ_h, f_h) be the unique solution of (16). Considering the remainder terms

$$r_\theta = \theta^h - \theta - \theta_h, \qquad r_f = f^h - f - f_h,$$

it remains to show the a priori estimate

$$\|r_\theta\|_{C(\bar{Q})} + \|r_f\|_{W^{1,p}(0,T;L^p(\Omega))} = o(\|h\|_{L^\infty(0,T)}).$$

Due to Assumption (A2), this can be proven similarly to the estimates in Corollary 2.4 by the use of a first-order Taylor expansion of the function G. Furthermore, one can analogously show Lipschitz continuity of the first derivative of the solution operator, i.e. for all $u_1,\ u_2,\ h \in L^\infty(0,T)$ there exist a constant $C > 0$ such that

$$\|(S_\theta'(u_1) - S_\theta'(u_2))h\|_{C(\bar{Q})} + \|(S_f'(u_1) - S_f'(u_2))h\|_{W^{1,p}(0,T;L^p(\Omega))} \le C\|u_1 - u_2\|_{L^\infty(0,T)}.$$

holds true. By means of this and again Assumption (A2), one can show that the unique solution of the linear system (17) represents the second derivative of the solution operator. To prove this one has to derive the remainder term of second order and proceed as before, which we omit here for reasons of space. □

2.3 Existence and optimality conditions of optimal solutions

Since the state system is nonlinear, we can not expect uniqueness of an optimal control and we have to deal with local optimal controls. We have the following result.

Theorem 2.6. *Let Assumption (A1)-(A4) be satisfied. Then there exists at least one solution of the optimal control problem* (P).

To prove Theorem 2.6 we need the following auxiliary result:

Lemma 2.7. *Assume* $\{\theta_k\}$ *is bounded in* $L^2(0,T; H^1(\Omega)) \cap L^\infty(Q)$ *and*

$$\theta_k \to \theta \qquad \text{strongly in } L^2(0,T; L^2(\Omega)) \tag{18}$$
$$\text{and weakly in } L^2(0,T; H^1(\Omega))\,. \tag{19}$$

Then, it also holds

$$\theta_k \to \theta \quad \text{strongly in } L^2(0,T; L^2(\partial\Omega))\,.$$

Proof. We define the operator $A : L^2(0,T;H^1(\Omega)) \to L^2(0,T)$ by

$$A\theta = \int_{\partial\Omega} \theta(x,t)dx.$$

A is linear and also continuous, since application of the trace theorem yields

$$\begin{aligned}
\|A\theta\|^2_{L^2(0,T)} &= \int_0^T \left(\int_{\partial\Omega} \theta(x,t)dx \right)^2 dt \\
&\leq |\partial\Omega| \int_0^T \int_{\partial\Omega} \theta^2(x,t)dt \leq c\|\theta\|^2_{L^2(0,T;H^1(\Omega))} .
\end{aligned}$$

In view of (19), we can infer

$$A\theta_k \rightharpoonup A\theta \quad \text{in } L^2(0,T) .$$

Utilizing the boundedness of $\{\theta_k\}$ in $L^\infty(Q) \cap L^2(0,T;H^1(\Omega))$ we see that

$$\|\theta_k^2\|^2_{L^2(0,T;H^1(\Omega))} = \int_0^T \int_\Omega \theta_k^4 dxdt + 2\int_0^T \int_\Omega |\theta_k \nabla\theta_k|^2 dxdt \leq c . \tag{20}$$

Now we take smooth functions $\varphi(x)$ and $\chi(t)$, then

$$\begin{aligned}
&\int_0^T \left(\int_\Omega \theta_k^2 \varphi dx \right) \chi(t)dt + \int_0^T \left(\int_\Omega \nabla(\theta_k^2)\nabla\varphi dx \right) \chi(t)dt \\
&= \int_0^T \left(\int_\Omega \theta_k^2 \varphi dx \right) \chi(t)dt + 2\int_0^T \left(\int_\Omega \theta_k \nabla\theta_k \nabla\varphi dx \right) \chi(t)\, dt .
\end{aligned}$$

Since φ and χ are smooth, using (19) we see that

$$\langle \theta_k^2, \varphi\chi \rangle_{L^2(0,T;H^1(\Omega))} \to \langle \theta^2, \varphi\chi \rangle_{L^2(0,T;H^1(\Omega))} .$$

Together with (20), we have shown

$$\theta_k^2 \rightharpoonup \theta^2 \quad \text{weakly in } L^2(0,T;H^1(\Omega)) .$$

Since the limit does not depend on the extracted subsequence the whole sequence converges. From this, we infer

$$A\theta_k^2 \rightharpoonup A\theta^2 \quad \text{which means}$$

$$\|\theta_k\|_{L^2(0,T;L^2(\partial\Omega))} \to \|\theta_k\|_{L^2(0,T;L^2(\partial\Omega))}$$

and thus $\theta_k \to \theta$ strongly in $L^2(0,T;L^2(\partial\Omega))$. □

With Lemma 2.7 at hand, we are now able to prove the existence of optimal solution of control problem (P).

Proof of Theorem 2.6:
Due to Theorem 2.3, there exist a unique solution $(\theta, f) \in W(0,T) \cap C(\bar{Q}) \times W^{1,p}(0,T;L^p(\Omega))$ of the state system (1) for every control $u \in U_{ad}$. Since the set of admissible controls is bounded in $L^\infty(0,T)$, the set of respective solutions (θ, f) of the state system is bounded in $W(0,T) \cap$

$C(\bar{Q}) \times W^{1,p}(0,T;L^p(\Omega))$, see Lemma 2.1 and Theorem 2.3. By means of boundedness of the cost functional, there exists a minimizing sequence $\{\theta_k, f_k, u_k\}$ such that

$$j = \lim_{k\to\infty} J(\theta_k, f_k, u_k) = \inf J(\theta, f, u),$$

where $(\theta_k, f_k) = S(u_n)$ is the solution of the state system w.r.t. to the control u_k.

Since U_{ad} is bounded, closed and convex, there exists a subsequence $\{u_{k'}\}$ such that

$$u_{k'} \rightharpoonup \bar{u} \quad \text{weakly in } \; L^2(0,T)\,.$$

In view of Theorem 2.3, extracting possibly a further subsequence still indexed by k', we have

$$\theta_{k'} \rightharpoonup \theta \qquad \text{weakly in } \; W(0,T) \tag{21}$$

$$\text{strongly in } \; L^2(Q)\,. \tag{22}$$

Applying Lemma 2.1 we obtain

$$f_{k'} \to f \quad \text{strongly in } \; W^{1,2}(0,T;L^2(\Omega))\,,$$

where f is the solution corresponding to θ. We use test functions $\varphi \in H^1(\Omega)$ and $\chi \in C^1[0,T]$ such that $\chi(T) = 0$ and consider the weak formulation of (1c)-(1f) for $(\theta_{k'}, f_{n'}, u_{n'})$

$$\begin{aligned}\rho c_p \int_0^T \int_\Omega \theta_{k',t}\varphi\chi dxdt + k\int_0^T\int_\Omega \nabla\theta_{k'}\nabla\varphi\chi dxdt + \int_0^T \left(\int_{\Gamma_1} \theta_{k'}\varphi ds\right) u_{k'}(t)\chi dt \\ = \int_0^T \left(\int_{\Gamma_1} \theta_w \varphi ds\right) u_{k'}(t)\chi dt + \int_0^T \int_\Omega f_{k'}\varphi\chi dxdt\,.\end{aligned} \tag{23}$$

Except of the third term in (23) we can pass to the limit by standard arguments. To pass to the limit in the remaining term we define

$$\alpha_k(t) = \left(\int_{\Gamma_1} \theta_k \varphi ds\right)\chi(t)$$

and estimate

$$\int_0^T (\alpha_{k'} - \alpha)^2 dt = \int_0^T \left(\int_{\Gamma_1} (\theta_{k'} - \theta)\varphi dx\right)^2 \chi^2(t)dt \le c\int_0^T \|\theta_{k'} - \theta\|^2_{L^2(\Gamma_1)} dt\,.$$

Now we apply Lemma 2.7 and obtain

$$\alpha_{k'} \to \alpha \quad \text{strongly in } \; L^2(\Gamma_1)\,,$$

which enables us to pass to the limit in the remaining term in (23). Since the solution to the state equation is unique, we can infer

$$\theta = \theta(\bar{u}) =: \bar{\theta} \quad \text{and} \quad f = f(\bar{\theta}) =: \bar{f}\,.$$

The optimality of $(\bar{\theta}, \bar{f}, \bar{u})$ follows by standard arguments using the lower semicontinuity of the cost functional w.r.t. u.

□

In the following theorem first order necessary optimality conditions are characterized by respective adjoint equations.

Theorem 2.8. *Let $\bar{u} \in U_{ad}$ be an optimal control of problem* (P) *and* $(\bar{\theta},\ \bar{f}) = S(\bar{u})$ *the associated solution of the state system* (1). *Then there exists a unique solution* $(\bar{p},\ \bar{q}) \in Y \times W^{1,\infty}(0,T; L^\infty(\Omega))$ *such that*

$$
\begin{aligned}
-\bar{q}_t &= G_f(\bar{\theta},\bar{f})(\bar{q}+\rho L\bar{p}), && \text{in } Q && \text{(24a)}\\
\bar{q}(T) &= \alpha_1(\bar{f}(T)-f_d), && \text{in } \Omega && \text{(24b)}\\
-\rho c_p \bar{p}_t - k\Delta\bar{p} &= G_\theta(\bar{\theta},\bar{f})(\rho L\bar{p}+\bar{q}) + \alpha_2(\bar{\theta}-\theta_d), && \text{in } Q && \text{(24c)}\\
-k\frac{\partial\bar{p}}{\partial n} &= \bar{u}(t)\bar{p}, && \text{on } \Sigma_1 && \text{(24d)}\\
-k\frac{\partial\bar{p}}{\partial n} &= 0, && \text{on } \Sigma_2 && \text{(24e)}\\
\bar{p}(T) &= 0, && \text{in } \Omega. && \text{(24f)}
\end{aligned}
$$

Moreover, the following variational inequality is valid

$$\iint_{\Sigma_1} (-\bar{p}(\bar{\theta}-\theta_w) + \frac{\alpha_3}{|\Gamma|}\bar{u})(u-\bar{u})d\sigma dt \geq 0 \quad \forall u \in U_{ad}. \tag{25}$$

Proof. First observe that the system (24) is a linear backward-in-time system of the parabolic equation and ODE. After the time transformation $t \mapsto T-t$ one can proceed as in the proof of Theorem 2.5 in order to prove the existence of the unique solution $(\bar{p},\bar{q}) \in W(0,T)\cap C(\bar{Q}) \times W^{1,\infty}(0,T; L^\infty(\Omega))$ of the system (24).
By means of the control to state mapping (9), the reduced cost functional of problem (P) is given by

$$
\begin{aligned}
\min_{u\in U_{ad}} j(u) = J(S(u),u) =& \frac{\alpha_1}{2}\int_\Omega (S_f(u)(T)-f_d)^2\,dx\\
&+\frac{\alpha_2}{2}\iint_Q (S_\theta(u)-\theta_d)^2 dx\,dt + \frac{\alpha_3}{2}\int_0^T u^2 dt
\end{aligned}
$$

Due Theorem 2.5, j is differentiable and the set of admissible controls U_{ad} bounded, closed and convex. Hence, the first order necessary optimality conditions for a (local) optimal solution $\bar{u} \in U_{ad}$ is given by $j'(\bar{u})(u-\bar{u}) \geq 0\,\forall u \in U_{ad}$. For given direction $h \in L^\infty(0,T)$ we have

$$
\begin{aligned}
j'(\bar{u})h = \alpha_1 &\int_\Omega (S_f(\bar{u})(T)-f_d)S_f'(\bar{u})h\,dx\\
&+\alpha_2\iint_Q (S_\theta(\bar{u})-\theta_d)S_\theta'(\bar{u})h dx\,dt + \alpha_3\int_0^T \bar{u}h dt.
\end{aligned} \tag{26}
$$

We will rewrite the directional derivative with the help of $(\bar{p},\bar{q})$ which solves the adjoint system (24). The existence of a unique solution of (24) can be proven similar to Theorem 2.3. For brevity we introduce $f_h = S_f'(\bar{u})h$ and $\theta_h = S_\theta'(\bar{u})h$ as the solution of the linearized system (16). We start by multiplying (16a) with $\bar{q}$ and integrate over Q:

$$
\begin{aligned}
0 &= \iint_Q ((f_h)_t - G_\theta(\bar{\theta},\bar{f})\theta_h - G_f(\bar{\theta},\bar{f})f_h)\bar{q} dx\,dt\\
&= \iint_Q -\bar{q}_t f_h - \bar{q}(G_\theta(\bar{\theta},\bar{f})\theta_h + G_f(\bar{\theta},\bar{f})f_h)dx\,dt + \int_\Omega f_h(T)\bar{q}(T)dx.
\end{aligned}
$$

Due to end-time condition for $\bar{q}$, one can obtain for the first term in (26)

$$\alpha_1 \int_\Omega (f_h(T) - f_d) f_h(T)\, dx = \iint_Q \bar{q}_t f_h + \bar{q}(G_\theta(\bar{\theta}, \bar{f})\theta_h + G_f(\bar{\theta}, \bar{f}) f_h) dx\, dt$$
$$= \iint_Q -\rho L G_f(\bar{\theta}, \bar{f}) \bar{p} f_h + \bar{q} G_\theta(\bar{\theta}, \bar{f})\theta_h.$$

Next, we test (24c) with θ_h, integrate over Q such that

$$\begin{aligned}
\alpha_2 \iint_Q (\bar{\theta} - \theta_d)\theta_h dx\, dt &= -\int_0^T \rho c_p \bar{p}_t \theta_h dt - \kappa \iint_Q \Delta \bar{p} \theta_h dx\, dt - \iint_Q G_\theta(\bar{\theta}, \bar{f})(\rho L \bar{p} + \bar{q})\theta_h dx\, dt \\
&= \int_0^T \rho c_p \bar{p} (\theta_h)_t dt - \kappa \iint_Q \Delta \theta_h \bar{p} dx\, dt - \iint_Q G_\theta(\bar{\theta}, \bar{f})(\rho L \bar{p} + \bar{q})\theta_h dx\, dt \\
&- \iint_{\Sigma_2} h(\bar{\theta} - \theta_w)\bar{p} d\sigma dt \\
&= -\iint_{\Sigma_1} h(\bar{\theta} - \theta_w)\bar{p} d\sigma dt - \iint_Q G_\theta(\bar{\theta}, \bar{f})(\rho L \bar{p} + \bar{q})\theta_h dx\, dt \\
&\quad + \iint_Q \rho L (G_\theta(\bar{\theta}, \bar{f})\theta_h + G_f(\bar{\theta}, \bar{f}) f_h)\bar{p} dx dt
\end{aligned}$$

Summarizing, one replace (26) by

$$j'(\bar{u})h = -\iint_{\Sigma_1} h(\bar{\theta} - \theta_w)\bar{p} d\sigma dt + \alpha_3 \int_0^T \bar{u} h dt.$$

Thus, the first order optimality conditions for a (local) optimal solution $\bar{u}$ are represented by the variational inequality (25). $\square$

Next, we will formulate second order sufficient optimality conditions regarding the optimal control problem (P). Therefore, we provide the second derivative of the reduced cost functional $j(u) = J(S(u), u)$. Straightforward computation and the use of the adjoint variables introduced in Theorem 2.8 yields

$$\begin{aligned}
j''(u)[h_1, h_2] = \alpha_1 \int_\Omega f_{h_1}(T) f_{h_2}(T) dx + \alpha_2 \iint_Q \theta_{h_1}\theta_{h_2} dx dt \\
+ \alpha_3 \int_0^T h_1 h_2 dt - \iint_{\Sigma_1} (\theta_{h_1} h_2 + \theta_{h_2} h_1) p d\sigma dt \\
+ \iint_Q G''(\theta(u), f(u))[(\theta_{h_1}, f_{h_1}), (\theta_{h_2}, f_{h_2})](\rho L p + q) dx dt,
\end{aligned} \tag{27}$$

with $(\theta_{h_i}, f_{h_i}) = S'(u) h_i,\ i = 1, 2$ and (p, q) is the solution of the adjoint system (24).

In all what follows we denote by $\bar{u}$ an admissible control of problem (P) with associated solution $(\bar{\theta}, \bar{f}) = S(\bar{u})$ of the state system (1). We suppose that the first order optimality conditions given in Theorem 2.8 are satisfied with respective adjoint states $(\bar{p}, \bar{q})$. Let us define the strongly active set associated to $\bar{u}$. For fixed $\tau > 0$ we set

$$A_\tau(\bar{u}) = \left\{ t \in (0,T) : \left| \int\limits_\Gamma -\bar{p}(x,t)(\bar{\theta}(x,t) - \theta_w(x,t))d\sigma + \alpha_3 \bar{u}(t) \right| > \tau \right\}.$$

Next, we shall assume a coercivity condition on the second derivative of the cost functional for directions associated to the previous strongly active set, henceforth called second order sufficient optimality conditions:

$$\left.\begin{array}{c} \text{There exist } \tau > 0 \text{ and } \delta > 0 \text{ such that} \\ j''(\bar{u})h^2 \geq \delta \|h\|^2_{L^2(0,T)} \\ \text{holds for all } h = \bar{u} - u,\ u \in U_{ad} \text{ with } h = 0 \text{ on } A_\tau(\bar{u}) \end{array}\right\} \tag{SSC}$$

Theorem 2.9. *Let $\bar{u}$ be an admissible control of problem* (P) *with associated state $(\bar{\theta}, \bar{f}) = S(\bar{u})$ satisfying the first order necessary optimality conditions given in Theorem 2.8 with associated adjoint states $(\bar{p}, \bar{q})$. Further, it is assumed that (SSC) holds at $\bar{u}$. Then there exist a $\tilde{\delta} > 0$ and $\rho > 0$ such that*

$$J(\theta, f, u) \geq J(\bar{\theta}, \bar{f}, \bar{u}) + \tilde{\delta}\|u - \bar{u}\|^2_{L^2(0,T)} \tag{28}$$

holds for all $u \in U_{ad}$ with $\|u - \bar{u}\|_{L^\infty(0,T)} \leq \rho$ with associated states $(\theta, f) = S(u)$.

Proof. The proof closely resembles that of Theorem 5.17 in [22], therefore we will not give here all details and refer to [22]. We only indicate some important arguments that need a bit more explanation. The crutial point in the proof is the fact that the quadratic form $j''(u)[h_1, h_2]$ has to depend continiously on $h_i,\ i = 1, 2$ in the L^2-norm, i.e we have to ensure the following continuity estimate

$$|\ j''(u)[h_1, h_2]\ | \leq c\|h_1\|_{L^2(0,T)}\|h_2\|_{L^2(0,T)}. \tag{29}$$

The first two terms in $j''(u)[h_1, h_2]$ (see (27)) can be estimated with respect to the L^2-norm of $h_i,\ i = 1, 2$ by applying standard a priori estimates and Lemma 2.1 b), e.g.

$$\begin{aligned} \|\theta_{h_i}\|_{L^\infty(Q)} &\leq c\|\bar{\theta}\|_{\mathbb{C}(\bar{Q})}\|h_i\|_{L^2(0,T)}, \\ \|f_{h_i}\|_{L^\infty(Q)} &\leq c\|\bar{\theta}\|_{\mathbb{C}(\bar{Q})}\|h_i\|_{L^2(0,T)}. \end{aligned}$$

The other terms are more delicate. Here we take advantage of the regularity of the adjoint state. Using trace theorem we estimate

$$\begin{aligned} \Big| \iint\limits_{\Sigma_1} \theta_{h_i} h_j p d\sigma dt \Big| &\leq c\|p\|_{\mathbb{C}(\bar{Q})}\|\theta_{h_i}\|_{L^2(0,T;H^1(\Omega))}\|h_j\|_{L^2(0,T)}, \\ &\leq c\|p\|_{\mathbb{C}(\bar{Q})}\|\theta_{h_i}\|_{W(0,T)}\|h_j\|_{L^2(0,T)} \leq c\|p\|_{\mathbb{C}(\bar{Q})}\|h_i\|_{L^2(0,T)}\|h_j\|_{L^2(0,T)} \end{aligned}$$

for $i, j = 1, 2,\ i \neq j$. For the last term in (27) we need to estimate the second derivative of $G(\theta, f)$

$$\begin{aligned} |G''(\theta, f)[(\theta_{h_1}, f_{h_1}), (\theta_{h_2}, f_{h_2})]| &= |G_{\theta\theta}[\theta_{h_1}, \theta_{h_2}] + G_{\theta f}[\theta_{h_1}, f_{h_2}] + G_{f\theta}[f_{h_1}, \theta_{h_2}] + G_{ff}[f_{h_1}, f_{h_2}]| \\ &\leq c(\|\theta_{h_1}\|_{\mathbb{C}(\bar{Q})}\|\theta_{h_2}\|_{\mathbb{C}(\bar{Q})} + \|\theta_{h_1}\|_{\mathbb{C}(\bar{Q})}\|f_{h_2}\|_{\mathbb{C}(\bar{Q})} \\ &\quad + \|f_{h_1}\|_{\mathbb{C}(\bar{Q})}\|\theta_{h_2}\|_{\mathbb{C}(\bar{Q})} + \|f_{h_1}\|_{\mathbb{C}(\bar{Q})}\|f_{h_2}\|_{\mathbb{C}(\bar{Q})}). \end{aligned}$$

The last step of the estimation is valid due to the uniformly boundedness of the partial derivatives of $G(\theta, f)$ up to the order two on the bounded sets (it follows from assumption (A2)).
The next important issue is to estimate the second order remainder term of the reduced cost functional j. We denote $h = u - \bar{u}$. It follows from Taylor's theorem with integral remainder (see, e.g. Theorem 8.14.3 ,p.186 in [4]) that

$$j(u) = j(\bar{u}) + j'(\bar{u})h + \frac{1}{2}j''(\bar{u})h^2 + r_2^j(\bar{u}, h)$$

with the remainder

$$r_2^j(\bar{u}, h) = \int_0^1 (1-s)(j''(\bar{u}+sh) - j''(\bar{u}))h^2 ds.$$

Let $(\bar{\theta}, \bar{f}) = S(\bar{u}),\ (\theta, f) = S(\bar{u}+sh)$ and $(\bar{\theta}_h, \bar{f}_h) = S'(\bar{u})h,\ (\theta_h, f_h) = S'(\bar{u}+sh)h$. Further, we consider

$$\begin{aligned}(j''(\bar{u}+sh) - j''(\bar{u}))h^2 = {} & \alpha_1 \int\limits_\Omega f_h^2(T) - \bar{f}_h^2(T)dx + \alpha_2 \int\limits_\Omega \theta_h^2(T) - \bar{\theta}_h^2(T)dx \\ & - 2 \iint\limits_{\Sigma_1} (\theta_h p - \bar{\theta}_h \bar{p}) h d\sigma dt \\ & + \iint\limits_Q G''(\theta, f)(\theta_h, f_h)^2(\rho L p + q) - G''(\bar{\theta}, \bar{f})(\bar{\theta}_h, \bar{f}_h)^2(\rho L\bar{p} + \bar{q}) dx dt,\end{aligned} \tag{30}$$

In order to estimate the terms in (30), we need the following estimates

$$\begin{aligned}&\|f_h - \bar{f}_h\|_{W^{1,p}(0,T;L^p(\Omega))} + \|\theta_h - \bar{\theta}_h\|_{\mathbb{C}(\bar{Q})} \le cs\|h\|_{L^\infty(0,T)}\|h\|_{L^2(0,T)}, \\ &\|q - \bar{q}\|_{W^{1,p}(0,T;L^p(\Omega))} + \|p - \bar{p}\|_{\mathbb{C}(\bar{Q})} \le cs\|h\|_{L^\infty(0,T)},\end{aligned} \tag{31}$$

which can be obtained by the standard a priori estimates and Lipschitz continuity of the solution operator. Using (31) and Lipschitz continuity of $G''(\theta, f)$, we can estimate the remainder term r_2^j as follows

$$|r_2^j(\bar{u}, h)| \le c\int_0^1 (1-s)s\|h\|_{L^\infty(0,T)}\|h\|^2_{L^2(0,T)} ds \le c\|h\|_{L^\infty(0,T)}\|h\|^2_{L^2(0,T)}.$$

From this point, we can argue along exactly the same lines as on pages 292-294 in the proof of Theorem 5.17 in [22] to conclude the validity of the assertion. □

Such kind of sufficient optimality conditions is an indispensable tool basis for carrying out numerical analysis of optimal control problems, e.g. convergence analysis of the sequential quadratic programming method in order to solve optimal control problems numerically.

3 Numerical implementation

In this section we introduce numerical algorithms for the solution of optimal control problem (P) analyzed in the previous section. This problem belongs to the class of the nonlinear boundary control problems with control constraints. The SQP (Sequential Quadratic Programming) method has turned out to be one of the most successful methods in nonlinear optimization (see e.g. [17], [1]). The principal idea is to linearize the nonlinear equality constraints and to replace the cost functional by a quadratic approximation of the Lagrangian. It is well known that the SQP algorithm exhibits local quadratic convergence in finite-dimensional spaces. The convergence analysis for nonlinear parabolic boundary control problems was presented in the works of Tröltzsch [7], [21].

In this work we focus on the reduced SQP method (rSQP), where the reduction onto the control space takes place when solving the (QP^k)-subproblems. We also introduce the primal-dual active set (PDAS) strategy, used for the treatment of the quadratic (QP^k) problems in each iteration of rSQP method. The conjugate gradient (CG) method has been applied to solve the linear system of equations arising in the (PDAS) algorithm.

3.1 Reduced SQP-method

We introduce the Lagrange functional

$$\mathcal{L}(\theta, f, u, p, q) : Y \times W^{1,\infty}(0,T; L^\infty) \times L^\infty(0,T) \times Y \times W^{1,\infty}(0,T; L^\infty) \to \mathbb{R}$$

with $Y := W(0,T) \cap C(\bar{Q})$ and

$$\mathcal{L}(\theta, f, u, p, q) = J(\theta, f, u) - \Bigg(\int_0^T \rho c_p \langle \theta_t, p \rangle_{H^1(\Omega)^*, H^1(\Omega)} dt + a(u)[\theta, p] - (u(t)\theta_w, p)_{\Sigma_1} - (\rho L G(\theta, f), p)_Q + (f_t - G(\theta, f), q)_Q \Bigg),$$

with a bilinear form

$$a(u)[\theta, v] := \iint_Q k \nabla\theta \cdot \nabla v dx dt + \iint_{\Sigma_1} u\theta v d\sigma dt.$$

and $(\cdot,\cdot)_Q$, $(\cdot,\cdot)_{\Sigma_1}$ denote the scalar products in $L^2(Q)$ and $L^2(\Sigma_1)$, respectively.

At each iteration of the SQP-method a quadratic approximation of the Lagrangian is minimized under linearized constraints, where it is assumed that the current iterate $x^k = (\theta^k, f^k, u^k)$ is sufficiently close to a local optimal solution $(\bar{\theta}, \bar{f}, \bar{u})$:

$$\begin{aligned} \min \quad & \frac{1}{2}\mathcal{L}''(x^k, p^k, q^k)[\delta x, \delta x] + J'(x^k)\delta x \\ \delta f_t &= G_f(\theta^k, f^k)\delta f + G_\theta(\theta^k, f^k)\delta\theta \\ & \quad - f_t^k + G(\theta^k, f^k), && \text{in } Q \\ \delta f(0) &= -f^k(0), && \text{in } \Omega \\ \rho c_p \delta\theta_t - k\Delta\delta\theta &= \rho L \delta f_t - (\rho c_p \theta_t^k - k\Delta\theta^k - \rho L f_t^k), && \text{in } Q \\ -k\frac{\partial \delta\theta}{\partial n} - \chi_{\Sigma_1} u^k(t)\delta\theta &= \chi_{\Sigma_1}\delta u(t)(\theta^k - \theta_w) \\ & \quad + k\frac{\partial\theta^k}{\partial n} + \chi_{\Sigma_1} u^k(t)(\theta^k - \theta_w), && \text{on } \Sigma \\ \delta\theta(0) &= \theta_0 - \theta^k(0), && \text{in } \Omega \\ u_a \le \delta u + u^k &\le u_b \quad \text{in } (0,T) \end{aligned} \tag{QP^k}$$

Note that

$$J'(x^k)\delta x = \alpha_1(f^k(T) - f_d, \delta f)_\Omega + \alpha_2(\theta^k - \theta_d, \delta\theta)_Q + \alpha_3(u^k, \delta u)_{(0,T)}$$

and

$$\begin{aligned}\mathcal{L}''(x^k, p^k, q^k)[\delta x, \delta x] = \alpha_1(\delta f, \delta f)_\Omega + \alpha_2(\delta\theta, \delta\theta)_Q + \alpha_3(\delta u, \delta u)_{(0,T)} \\ - 2(\delta u \delta\theta, p^k)_{\Sigma_1} + (G''(\theta^k, f^k)[\delta\theta, \delta f]^2, \rho L p^k + q^k)_Q\end{aligned} \tag{32}$$

In order to prescribe the resulting optimality system in a preferably compact way, we will introduce an abstract description of the state equation and its linearization. The state system can be written as a mapping

$$e(\theta, f, u) = \begin{pmatrix} e_1(\theta, f, u) \\ e_2(\theta, f, u) \end{pmatrix} : Y \times L^\infty(0,T) \to L^2(0,T; H^1(\Omega)^*) \times L^r(Q)$$

and

$$e(\theta, f, u) = 0.$$

Moreover, the mapping is defined by using test functions $p \in L^2(0,T; H^1(\Omega)),\ q \in L^s(Q)$:

$$e_1(\theta, f, u)(p) := \int_0^T \rho c_p \langle \theta_t, p\rangle_{H^1(\Omega)^*, H^1(\Omega)} dt + a(u)[\theta, p] - (\rho L G(\theta, f), p)_Q - (u(t)\theta_w, p)_{\Sigma_1} \tag{33}$$

$$e_2(\theta, f, u)(q) := \iint_Q f_t q - G(\theta, f) q \, dx dt. \tag{34}$$

By means of this, the linearized state system in problem (QP^k) is given by

$$e_x(x^k)(\delta\theta, \delta f, \delta u) = \begin{pmatrix} e_{1,\theta}(x^k)\delta\theta + e_{1,f}(x^k)\delta f + e_{1,u}(x^k)\delta u \\ e_{2,\theta}(x^k)\delta\theta + e_{2,f}(x^k)\delta f \end{pmatrix} = -e(x^k).$$

Note that $e_{2,u}(\cdot)$ is zero. The partial derivatives are defined as follows:

$$\begin{aligned}(e_{1,\theta}(\theta^k, f^k, u^k)\delta\theta)(v) &= \int_0^T \rho c_p \langle \delta\theta_t, v\rangle_{H^1(\Omega)^*, H^1(\Omega)} dt + a(u^k)[\delta\theta, v] - (\rho L G_\theta(\theta^k, f^k)\delta\theta, v)_Q \\ (e_{1,f}(\theta^k, f^k, u^k)\delta f)(v) &= -(\rho L G_f(\theta^k, f^k)\delta f, v)_Q \\ (e_{1,u}(\theta^k, f^k, u^k)\delta u)(v) &= (\delta u(t)(\theta^k - \theta_w), v)_{\Sigma_1} \\ (e_{2,\theta}(\theta^k, f^k, u^k)\delta\theta)(q) &= (-G_\theta(\theta^k, f^k)\delta\theta, q)_Q \\ (e_{2,f}(\theta^k, f^k, u^k)\delta f)(q) &= (\delta f_t - G_f(\theta^k, f^k)\delta f, q)_Q\end{aligned} \tag{35}$$

Hence, problem (QP^k) can be written as

$$\begin{aligned} \min \quad & \frac{1}{2}\mathcal{L}''(x^k, p^k, q^k)[\delta x, \delta x] + J'(x^k)\delta x \\ & e_x(x^k)(\delta\theta, \delta f, \delta u) = -e(x^k) \\ & \delta u \in U_{ad} - \{u^k\} \end{aligned} \tag{QP^k}$$

Introducing adjoint variables with respect to the linearized state system and neglecting the inequality constraints for a moment, the optimality system is given in the following compact form

$$\begin{pmatrix} \mathcal{L}''_{\theta\theta} & \mathcal{L}''_{\theta f} & \mathcal{L}''_{\theta u} & e^*_{1,\theta} & e^*_{2,\theta} \\ \mathcal{L}''_{f\theta} & \mathcal{L}''_{ff} & \mathcal{L}''_{fu} & e^*_{1,f} & e^*_{2,f} \\ \mathcal{L}''_{u\theta} & \mathcal{L}''_{uf} & \mathcal{L}''_{uu} & e^*_{1,u} & 0 \\ e_{1,\theta} & e_{1,f} & e_{1,u} & 0 & 0 \\ e_{2,\theta} & e_{2,f} & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \delta\theta \\ \delta f \\ \delta u \\ p \\ q \end{pmatrix} = \begin{pmatrix} -J_\theta \\ -J_f \\ -J_u \\ \\ -e \end{pmatrix} \tag{36}$$

For simlicity, function arguments are now omitted. Unless otherwise stated, all functions are to be evaluated at $k-$th iterate. Introducing the notation $\mathcal{L}''_{(\theta,f)}$ - the second derivative of the Lagrangian $\mathcal{L}$ with respect to the state pair variable (θ, f), we can rewrite the KKT matrix as 3×3 block matrix. Since the linearized state system is uniquely solvable for every right hand side (it can be shown along the lines of Theorem 2.3), we can derive the following decomposition of the full KKT matrix in (36) by Gaussian block elimination

$$\begin{pmatrix} \mathcal{L}''_{(\theta,f)} & \mathcal{L}''_{(\theta,f)u} & e^*_{(\theta,f)} \\ \mathcal{L}''_{u(\theta,f)} & \mathcal{L}''_{uu} & e^*_u \\ e_{(\theta,f)} & e_u & 0 \end{pmatrix} = \begin{pmatrix} \mathcal{L}''_{(\theta,f)} e^{-1}_{(\theta,f)} & 0 & I \\ \mathcal{L}''_{u(\theta,f)} e^{-1}_{(\theta,f)} & I & e^*_u e^{-*}_{(\theta,f)} \\ I & 0 & 0 \end{pmatrix} \begin{pmatrix} e_{(\theta,f)} & e_u & 0 \\ 0 & H & 0 \\ 0 & W & e^*_{(\theta,f)} \end{pmatrix}$$

The so called reduced Hessian H is defined by

$$H = \mathcal{L}''_u + e^*_u e^{-*}_{(\theta,f)} (\mathcal{L}''_{(\theta,f)} e^{-1}_{(\theta,f)} e_u - \mathcal{L}''_{(\theta,f)u}) - \mathcal{L}''_{u(\theta,f)} e^{-1}_{(\theta,f)} e_u. \tag{37}$$

Moreover, we have

$$W = -\mathcal{L}''_{(\theta,f)} e^{-1}_{(\theta,f)} e_u + \mathcal{L}''_{(\theta,f)u}.$$

By means of this decomposition, (36) can be treated by:

(i) Solve the reduced Hessian system:

$$H\delta u = \underbrace{-J_u + e^*_u e^{-*}_{(\theta,f)} (J_{(\theta,f)} - L''_{(\theta,f)} e^{-1}_{(\theta,f)} e) + L''_{u(\theta,f)} e^{-1}_{(\theta,f)} e}_{:=r} \tag{38}$$

(ii) Solve the linearized state system, i.e.

$$e_{(\theta,f)} \begin{pmatrix} \delta\theta \\ \delta f \end{pmatrix} = -e_u \delta u - e$$

(iii) Solve the adjoint state system, i.e.

$$e^*_{(\theta,f)} \begin{pmatrix} p \\ q \end{pmatrix} = -J_{(\theta,f)} - \mathcal{L}''_{(\theta,f)} \begin{pmatrix} \delta\theta \\ \delta f \end{pmatrix} - \mathcal{L}''_{(\theta,f)u} \delta u$$

Based on this arguments and taking the control constraints into account, the reduced optimality conditions of the linear quadratic problem (QP^k) are given by

$$(H(x^k, p^k, q^k)\delta u - r(x^k, p^k, q^k), \delta v - \delta u)_{(0,T)} \geq 0 \qquad \forall \delta v \in U_{ad} - \{u^k\}, \tag{39}$$

where H is defined as in (37) and the residuum r has to be evaluated by

$$r := -J_u + e^*_u e^{-*}_{(\theta,f)} (J_{(\theta,f)} - L''_{(\theta,f)} e^{-1}_{(\theta,f)} e) + L''_{u(\theta,f)} e^{-1}_{(\theta,f)} e$$

Concluding, we state the rSQP algorithm for tackling the problem (P) in Algorithm 1.

Algorithm 1 *SQP method (outer loop)*

1: Choose initial variables $x^0 = (\theta^0, f^0, u^0)$ sufficiently close to $(\bar{\theta}, \bar{f}, \bar{u})$ and set $k := 0$
2: Evaluate (p^k, q^k) as the solution of the adjoint system of (P)
3: **repeat**
4: *Primal-dual active set strategy (inner loop)*
Solve (QP^k), i.e. determine δu such that

$$(H(x^k, p^k, q^k)\delta u - r(x^k, p^k, q^k), \delta v - \delta u)_{(0,T)} \geq 0 \qquad \forall \delta v \in U_{ad} - \{u^k\}$$

is satisfied
5: Solve linearized state system

$$e_{(\theta,f)}(x^k)\begin{pmatrix}\delta\theta\\ \delta f\end{pmatrix} = -e_u(x^k)\delta u - e(x^k)$$

6: Solve the adjoint state system of (QP^k), i.e.

$$e^*_{(\theta,f)}(x^k)\begin{pmatrix}p\\ q\end{pmatrix} = -J_{(\theta,f)}(x^k) - \mathcal{L}''_{(\theta,f)}(x^k, p^k, q^k)\begin{pmatrix}\delta\theta\\ \delta f\end{pmatrix} - \mathcal{L}''_{(\theta,f)u}(x^k, p^k, q^k)\delta u$$

7: Update iterates

$$u^{k+1} = u^k + \delta u, \quad \theta^{k+1} = \theta^k + \delta\theta, \quad f^{k+1} = f^k + \delta f, \quad p^{k+1} := p, \quad q^{k+1} := q$$

8: Set $k := k + 1$
9: **until**

$$\begin{aligned}\tau :=& \frac{1}{5}\Big(\frac{\| u^{k+1} - u^k \|_{L^2(0,T)}}{\| u^k \|_{L^2(0,T)}} + \frac{\| \theta^{k+1} - \theta^k \|_{L^2(Q)}}{\| \theta^k \|_{L^2(Q)}} + \frac{\| f^{k+1} - f^k \|_{L^2(Q)}}{\| f^k \|_{L^2(Q)}}\\ &+ \frac{\| p^{k+1} - p^k \|_{L^2(Q)}}{\| p^k \|_{L^2(Q)}} + \frac{\| q^{k+1} - q^k \|_{L^2(Q)}}{\| q^k \|_{L^2(Q)}}\Big) < tol\end{aligned}$$

3.2 Primal-Dual Active Set (PDAS) Strategy

In a next step we have to specify how to solve the reduced linear quadratic optimal control problems arising in the iterations of the above SQP-method. To this end, we will use an Primal-dual active set strategy. Let us assume that the active sets of the optimal solution of problem (QP^k) are known, i.e. we can define

$$\begin{aligned}A^- &= \{t \in (0,T) \,|\, \delta u = u_a - u^k\}\\ A^+ &= \{t \in (0,T) \,|\, \delta u = u_b - u^k\}\\ I &= (0,T) \setminus (A^- \cup A^+).\end{aligned}$$

Furthermore, we decompose the control $\delta u = \delta u_I + \delta u_A$ in an active part δu_A and inactive part δu_I according to the previous sets:

$$\delta u_A = \begin{cases} u_a - u^k, & t \in A^- \\ u_b - u^k, & t \in A^+ \\ 0, & \text{else} \end{cases} \quad \delta u_I = \begin{cases} 0, & t \in A^- \\ 0, & t \in A^+ \\ \text{unknown}, & t \in I \end{cases}$$

The problem (QP^k) can be interpreted as an free optimal control problem, where δu_I serves as control variable. For a given active part δu_A, then the variational inequality (39) simplifies to:

$$H(x^k, p^k, q^k)\delta u_I = r(x^k, p^k, q^k) - H(x^k, p^k, q^k)\delta u_A$$

Now, the idea of the active set strategy is to iterate with respect to the active sets based on initial sets A_0^-, A_0^+ and I_0. Suppose that for given active sets A_l^- and A_l^+ the solution of the respective free optimal control problem is denoted by δu_I^l and we set $\delta u^l = \delta u_I^l + \delta u_A^l$. Based on the variational inequality, an update of the active sets for a fixed constant $c > 0$ can be defined as follows

$$\begin{aligned} A_{l+1}^- &:= \{t \in (0,T) | c(\delta u_I^l - u_a + u^k) - H(x^k, p^k, q^k)\delta u_I^l + r(x^k, p^k, q^k) < 0\} \\ A_{l+1}^+ &:= \{t \in (0,T) | c(\delta u_I^l - u_b + u^k) - H(x^k, p^k, q^k)\delta u_I^l + r(x^k, p^k, q^k) > 0\} \\ I_{l+1} &= (0,T) \setminus (A_{l+1}^- \cup A_{l+1}^+). \end{aligned}$$

A usual stopping criterion is the coincidence of subsequent active sets $A_{l+1}^- = A_l^-$ and $A_{l+1}^+ = A_l^+$. One can easily check, that if the previous condition is satisfied the optimal active sets are determined such that the variational inequality (39) is fulfilled and problem (QP^k) is solved. Summarized, the active set strategy for solving the linear quadratic subproblems (QP^k) of the SQP-method is in Algorithm 2.

In a last step, we have to provide a method for solving the linear system of equations in step 4 of the primal dual active set strategy. Due to the definition of the reduced Hessian in (37), the system matrix H is not explicitly given after choosing a discretization strategy for the underlying partial differential equations. Hence, an iterative solver has to be established for tackling the reduced Hessian system, e.g. Conjugate gradient method (CG-method) or Generalized minimal residual method (GMRES). In view of second order sufficient optimality conditions for the original problem, we have applied the CG method for solving

$$\tilde{H}\delta u_l = (E_{I_l} H E_{I_l} + E_{A_l})\delta u_{l,I} = E_{I_l}(r - H\delta u_{l,A}) =: b.$$

4 Numerical results

In this section we discuss the numerical solution of the control problem (P). Firstly, we construct a test control problem in order to check the convergence of the reduced SQP method with a primal-dual active set strategy described above. Then we solve the optimal control problem for the hot rolling of DP steel. Here, for a globalization of the rSQP method, we use a projected gradient algorithm (see e.g. [13]) with a line search according to the Armijo rule to find suitable initial values for the rSQP method. The numerical algorithms have been implemented in *WIAS-pdelib* software. For the solving the state and adjoint system the finite element toolbox *pdelib* was used.

Algorithm 2 *Active set strategy for solving* (QP^k) *(inner loop)*

1: Choose initial active sets according to current iterate of SQP-method, i.e.

$$A_0^- = \{t \,|\, u^k(t) = u_a\},\; A_0^+ = \{t \,|\, u^k(t) = u_b\},\; I_0 = (0,T) \setminus (A_0^- \cup A_0^+).$$

2: Set l=0 and

$$\delta u_{0,A} = \begin{cases} u_a - u^k, & t \in A_0^- \\ u_b - u^k, & t \in A_0^+ \\ 0, & \text{else} \end{cases}$$

3: Define operators $E_{I_l} : L^\infty(0,T) \to L^\infty(0,T), u \mapsto \chi_{I_l} u$ and $E_{A_l} := I - E_{I_l}$, where χ_{I_l} is the characteristic function w.r.t. I_l

4: Determine $\delta u_{l,I}$ by solving

$$(E_{I_l} H(x^k,p^k,q^k) E_{I_l} + E_{A_l}) \delta u_{l,I} = E_{I_l}(r(x^k,p^k,q^k) - H(x^k,p^k,q^k)\delta u_{l,A})$$

and set $\delta u_l = \delta u_{l,I} + \delta u_{l,A}$

5: Determine state variables $(\delta\theta_l, \delta f_l)$

$$e_{(\theta,f)}(x^k,p^k,q^k) \begin{pmatrix} \delta\theta_l \\ \delta f_l \end{pmatrix} = -e_u(x^k,p^k,q^k)\delta u_l - e(x^k,p^k,q^k)$$

6: Evaluate adjoint variables (p_l, q_l) by

$$e^*_{(\theta,f)}(x^k,p^k,q^k) \begin{pmatrix} p_l \\ q_l \end{pmatrix} = -J_{(\theta,f)}(x^k,p^k,q^k) - \mathcal{L}''_{(\theta,f)}(x^k,p^k,q^k) \begin{pmatrix} \delta\theta_l \\ \delta f_l \end{pmatrix} - \mathcal{L}''_{(\theta,f)u}(x^k,p^k,q^k)\delta u_l$$

7: Determine

$$\lambda^- := \delta u_l - u_a + u^k - \left(\mathcal{L}''_u \delta u_l + e^*_{1,u} p_l + \mathcal{L}''_{u(\theta,f)} \begin{pmatrix} \delta\theta_l \\ \delta f_l \end{pmatrix} + J_u \right)$$
$$\lambda^+ := \delta u_l - u_b + u^k - \left(\mathcal{L}''_u \delta u_l + e^*_{1,u} p_l + \mathcal{L}''_{u(\theta,f)} \begin{pmatrix} \delta\theta_l \\ \delta f_l \end{pmatrix} + J_u \right)$$

and update active sets

$$A_{l+1}^- = \{t \,|\, \lambda^-(t) < 0\},\; A_{l+1}^+ = \{t \,|\, \lambda^+(t) > 0\},\; I_{l+1} = (0,T) \setminus (A_0^- \cup A_0^+).$$

8: **if** $A_{l+1}^- = A_l^-$ and $A_{l+1}^+ = A_l^+$ **then**

9: STOP

10: **else**

11:

$$\delta u_{(l+1),A} = \begin{cases} u_a - u^k, & t \in A_{l+1}^- \\ u_b - u^k, & t \in A_{l+1}^+ \\ 0, & \text{else} \end{cases}$$

set $l = l + 1$ and GOTO 3

12: **end if**

4.1 A test problem

Let $\Omega = (0,1) \times (0,1)$ and $T > 0$. We apply the rSQP method discussed above to the semilinear parabolic boundary control problem

$$\min J(\theta, u) = \frac{1}{2} \int_0^T \int_\Omega (\theta - \theta_{d,\Omega})^2 dx dt + \frac{1}{2} \int_0^T \int_\Gamma (\theta - \theta_{d,\Gamma})^2 dx dt + \frac{1}{2} \int_0^T (u - u_d)^2 dt$$

subject to

$$\begin{aligned}
&\theta_t - \Delta\theta = -\theta^5 + f(x,t), && \text{in } \Omega \times (0,T) \\
&\frac{\partial \theta}{\partial \nu} + \theta = (\tilde{u}(t) - u(t)) g(x), && \text{on } \partial\Omega \times (0,T) \\
&\theta(x,0) = \theta_0(x), && \text{in } \Omega,
\end{aligned}$$

and $u_a \leq u(t) \leq u_b$ a.e. at $[0,T]$,
where

$$\begin{aligned}
&f(x,t) = e^{-5t} \cos^5 \pi x_1 \cdot \cos^5 \pi x_2 + e^{-t}(2\pi^2 - 1) \cos \pi x_1 \cdot \cos \pi x_2 \\
&\tilde{u}(t) = \bar{u} + e^{-t} \\
&g(x) = \cos \pi x_1 \cdot \cos \pi x_2 \\
&\theta_{d,\Omega} = -5e^{-4t}(t - T) \cos^5 \pi x_1 \cdot \cos^5 \pi x_2 - (2\pi^2(t-T) - e^{-t} - 1) \cos \pi x_1 \cdot \cos \pi x_2 \\
&\theta_{d,\Gamma} = (e^{-t} - t + T) \cos \pi x_1 \cdot \cos \pi x_2 \\
&u_d = -e^{-t} - 2(t - T) \\
&\theta_0 = \cos \pi x_1 \cdot \cos \pi x_2 \\
&T = 1,\ u_a = -0.85, u_b = -0.4.
\end{aligned}$$

The optimal solution to this problem with corresponding adjoint variable is given as

$$\begin{aligned}
&\bar{u} = \Pi_{[u_a,u_b]}(-e^{-t}) \\
&\bar{\theta} = e^{-t} \cos \pi x_1 \cdot \cos \pi x_2 \\
&\bar{p} = (t - T) \cos \pi x_1 \cdot \cos \pi x_2
\end{aligned}$$

The triple of functions $(\bar{u}, \bar{\theta}, \bar{p})$ is chosen a priori, such that the first-order necessary optimality conditions are fulfilled.

To prove local optimality, we show that the second-order sufficient optimality condition is satisfied. We write down the formal Lagrange function

$$\begin{aligned}
\mathcal{L}(\theta, u, p) = J(\theta, u) &- \int_0^T \int_\Omega (\theta_t - \Delta\theta + \theta^5 - f(x,t)) p dx dt \\
&- \int_0^T \int_\Gamma (\frac{\partial \theta}{\partial t} + \theta - (\tilde{u} - u) g(x)) p ds dt - \int_\Omega (\theta(x,0) - \theta_0) p dx
\end{aligned}$$

with

$$\mathcal{L}''(\bar{\theta}, \bar{u}, \bar{p})(\theta, u) = \int_0^T \int_\Omega \theta^2 dx dt + \int_0^T \int_\Gamma \theta^2 ds dt + \int_0^T u^2 dt - 20 \int_0^T \int_\Omega \bar{\theta}^3 \theta^2 \bar{p} dx dt \qquad (41)$$

The last term in (41) is nonnegative due to $\bar{\theta}^3\bar{p} = (t-T)cos^4\pi x_1 cos^4\pi x_2 \le 0$ for all $t \in [0,T]$. Hence,

$$\mathcal{L}''(\bar{\theta},\bar{u},\bar{p})(\theta,u) \ge \|u\|^2_{L^2(0,T)}.$$

The sufficient optimality condition holds in the entire control-state space, i.e. it is satisfied in a strong form.

We choose the initial point for the rSQP method

$$u^0(t) \equiv -0.8, \ ,\theta^0(x,t) \equiv 1 \ p^0(x,t) \equiv 1.$$

The parabolic problem was solved numerically by applying the semi-discretization approach, where the elliptic system in each time increment was solved by the finite element method. The controls were chosen as piecewise constant functions on the time grid. The spatial domain is discretized with triangular finite elements with a maximal edge length of $h = 0.0125$. The time interval is discretized uniformly with stepsize $\Delta t = 0.001$.

The sequence of controls u^k produced by the rSQP algorithm is depicted in the Figure 2. The corresponding state and adjoint variables are displayed in Figure 3.

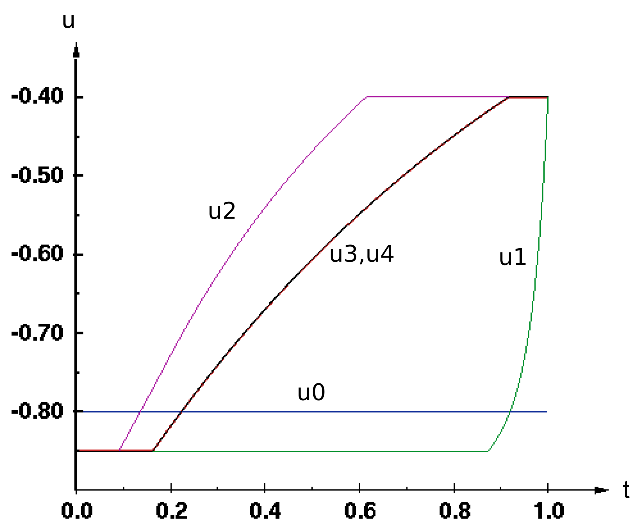


Figure 2: Controls $u^k(t)$.

Iter	J_k	e_k	τ_k	#PDAS-Loops
1	21.8504	0.94	0.22	3
2	20.3691	0.45	0.33	4
3	20.3517	0.0085	0.0938	3
4	20.3515	140.7	$5 \cdot 10^{-4}$	1

Table 1: Iterations history of the rSQP method with primal-dual active set strategy.

Table 4.1 illustrates the convergence behavior of the rSQP method. It contains the value of objective

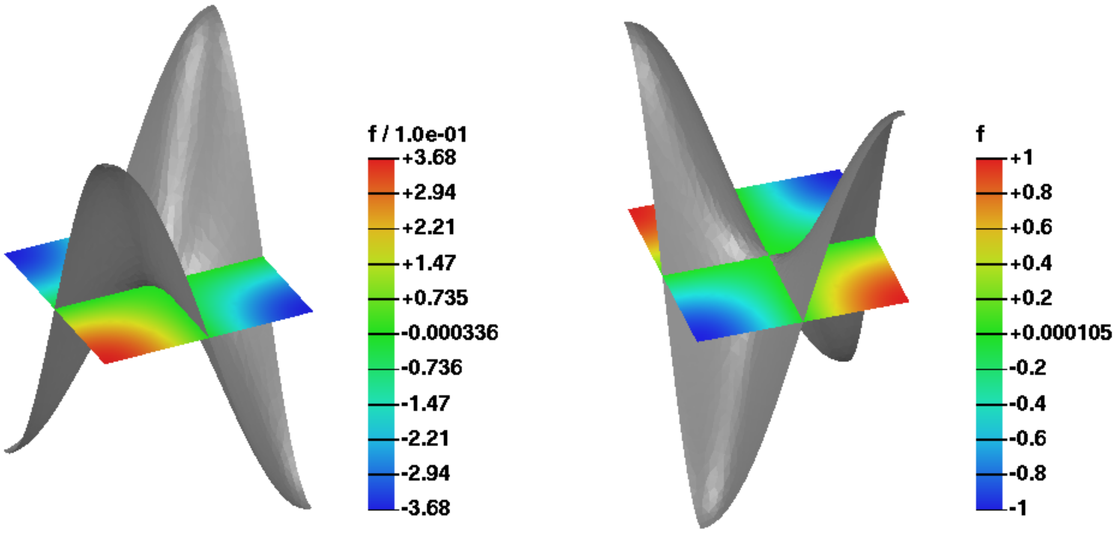


Figure 3: State variable $\bar{\theta}$ (left) and adjoint variable $\bar{p}$ (right) at the end time $T = 1$.

function J_k, the rate of convergence e_k and the error τ_k in k-iteration of rSQP method:

$$e_k = \frac{\|u^k - \bar{u}\|_{L^2(0,T)} + \|\theta^k - \bar{\theta}\|_{L^2(Q)} + \|p^k - \bar{p}\|_{L^2(Q)}}{\|u^{k-1} - \bar{u}\|^2_{L^2(0,T)} + \|\theta^{k-1} - \bar{\theta}\|^2_{L^2(Q)} + \|p^{k-1} - \bar{p}\|^2_{L^2(Q)}},$$
$$\tau_k = \|u^k - u^{k-1}\|_{L^2(0,T)}.$$

The last column in the table gives the number of PDAS-Loops in k-iteration of rSQP method. The rSQP method shows a good convergence to the exact optimal solution $\bar{u}$. Only 4 iterations were needed to get this result.

As has been reported in [7],[8], the quadratic convergence of SQP method is assured, if the quadratic subproblems (QP^k) are solved with a quite high precision. The mesh size h has to be proportional to the current accuracy of the SQP step. In our test example, we observe that the speed of convergence of rSQP method is limited after the 3^{rd} iteration by the discretization error of FEM.

4.2 Optimal control problem for dual phase steel

In this subsection we present a numerical solution of the optimal control problem (P) formulated for the production of Mo-Mn dual phase (DP) steel.

Let us choose a two-dimensional domain $\Omega = (0, 7.5) \times (0, 0.69)\, cm^2$. This corresponds to the vertical cross section of the steel slab moving through the cooling segment with a fixed strip speed. The aim is to compute the optimal cooling strategy for a DP-steel with desired ferrite fraction $f_d(x) = 85\%$ and a temperature $\theta_d(x) = 660^oC$ at the final time $T = 7s$. Thus, the optimal control problem reads as follows:

$$\min \quad J(\theta, f, u) = \frac{\alpha_1}{2} \int_\Omega (f(x,T) - f_d(x))^2\, dx + \frac{\alpha_2}{2} \int_\Omega (\theta(x,T) - \theta_d(x))^2\, dx$$
$$+ \frac{\alpha_3}{2} \int_0^T u^2 dt$$

s.t. $(\theta,\ f,\ u)$ satisfies (1) and $0 \le u(t) \le 0.3$ a.e. in $[0, T]$.

The function $G(\theta, f)$, which describes the ferrite growth is given by

$$G(\theta, f) = (f_{eq}(\theta) - f)\mathcal{H}(f_{eq}(\theta) - f)g_1(\theta)g_2, \tag{42}$$

where $\mathcal{H}$ is a monotone approximation of the Heaviside function

$$\mathcal{H}(x) = \begin{cases} 1, & \text{for } x \geq \delta, \\ 10(\frac{x}{\delta})^6 - 24(\frac{x}{\delta})^5 + 15(\frac{x}{\delta})^4, & \text{for } \delta > x \geq 0, \\ 0, & \text{for } x < 0. \end{cases}$$

with $\delta = 0.01$. Since $\mathcal{H}$ is a regularized Heaviside function, the term $x\mathcal{H}(x)$ is a regularization of the positive part function $[x]_+$. The equilibrium volume fraction $f_{eq}(\theta)$ and temperature dependent factor $g_1(\theta)$ are cubic spline functions interpolating the pointwise data as shown in Figure 4. The factor $g_2 = 9.67$. The model (42) for the austenite-ferrite phase transformation in the hot rolling process has been discussed in [19]. For further details about the modeling we refer to this article. We note, that assumption (A2) is too strong for the function $G(\theta, f)$. Nevertheless, the existence and uniqueness of the solution to state system can be also shown for this function and all other theoretical and numerical considerations remain unchanged.

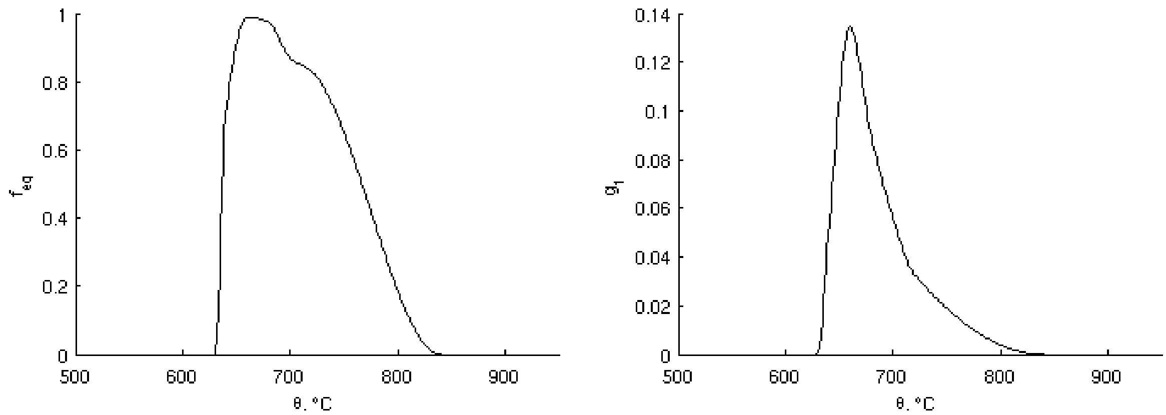


Figure 4: The functions $f_{eq}(\theta)$ (left) and $g_1(\theta)$ (right).

The physical parameters for the heat equation are given by

$$\rho = 7.85 \, \frac{g}{cm^3}, \; c = 0.5096 \, \frac{J}{g \cdot K}, \; k = 0.5 \, \frac{J}{s \cdot cm \cdot K}, \; L_1 = 77.0 \, \frac{J}{g}.$$

The initial condition for the θ-variable is $\theta_0 = 860$ and $\theta_w = 20$. Notice that (A3) is satisfied.

It should be mentioned that a choice of weighting factors $\alpha_1, \alpha_2, \alpha_3$ in the cost functional of optimal control problem (P) is of crucial importance for the numerical computations. The volume phase fraction $f \in [0, 1]$, while the temperature θ is in the range of $20 - 1200°C$. Therefore, in order to obtain useful results the equilibrating of this two terms in cost functional is necessary. In the subsequent computations we set $\alpha_1 = 1, \alpha_2 = 5 \cdot 10^{-6}$. The factor α_3 is a Tikhonov regularization parameter and was chosen as 0.1.

The nonlinear state system (1) as well the corresponding adjoint system in each iteration of projected gradient method can be solved numerically using semi-implicit Euler scheme. The rSQP method requires a solving of the linearized problems (QP^k). Here, the linear parabolic equation was discretized in a standard way using method of lines and ODE for the phase transition was treated numerically by explicit Euler scheme.

The FE triangulation of the computational domain Ω is done by a uniform mesh with $N = 561$ degrees of freedom. For the time grids we take $\Delta t = 0.0125$. We approximate the control function $u(t)$ with piecewise constant functions such that the unknown control function is represented as $u = (u_1, ..., u_{n-1})^T,\ u_i = u(t_i), i = 1, ..., n-1.$

As explained above, we use the projected gradient method for the globalization of the rSQP algorithm. As an initial guess for the projected gradient method we take $u_0 \equiv 0$. After 7 iterations the termination criteria for the projected gradient method has been realized.

The obtained control function $\hat{u}$ with corresponding state variables $\hat{\theta}$ and $\hat{f}$ and adjoint variables $\hat{p}, \hat{q}$ serve as the initial iteration of the rSQP method. Table 4.2 shows the convergence history of the rSQP steps. As would be expected, the rSQP method converges in few steps to the optimal solution with $tol = 10^{-3}$ in termination condition.

Iter	J_k	τ_k	# PDAS-Loops
1	0.01437	0.2488	9
2	0.012752	0.01462	3
3	0.012750	$1.8 \cdot 10^{-4}$	2

Table 2: Value of objective function J_k, relative error τ_k and number of PDAS-Loops in k-iteration of rSQP method.

In Figure 5 some iterations of projected gradient algorithm and SQP method are represented.

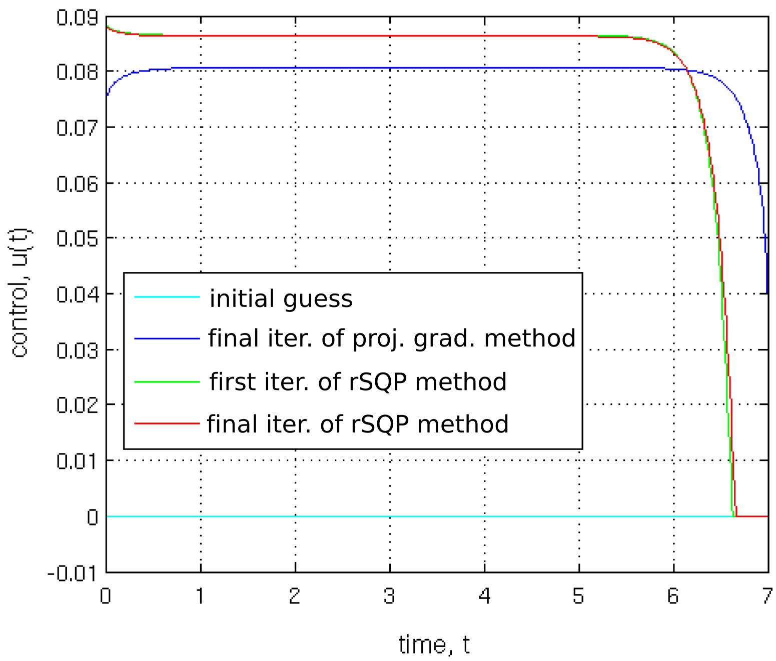


Figure 5: Some iterations of optimization procedure. The final iteration of the projected gradient method $\hat{u}$ is plotted in the blue color.

The optimal control $u(t)$ is depicted in Figure 6. Closer to the end of the time interval the optimal

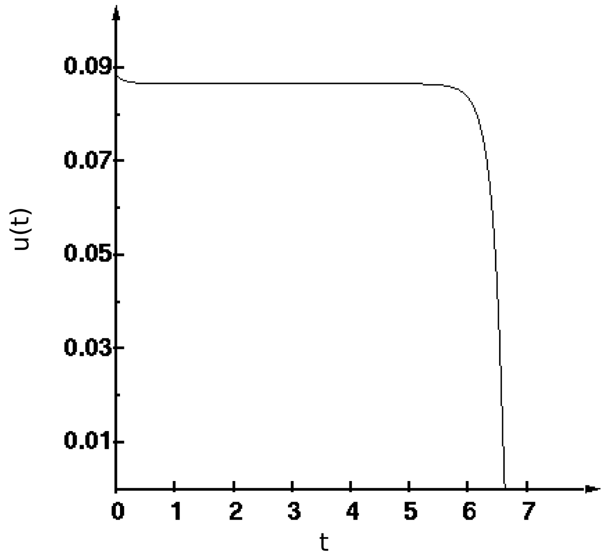


Figure 6: Optimal control $u(t)$.

control decreases to zero, which is the lower bound of the control. This fact also reflects the presence of the box constraints and the functioning of the active set method.

Figure 7 shows the simulated final temperature (left) and phase distribution (right) in the cross section of the steel slab according to the selected iterations of optimization procedure.

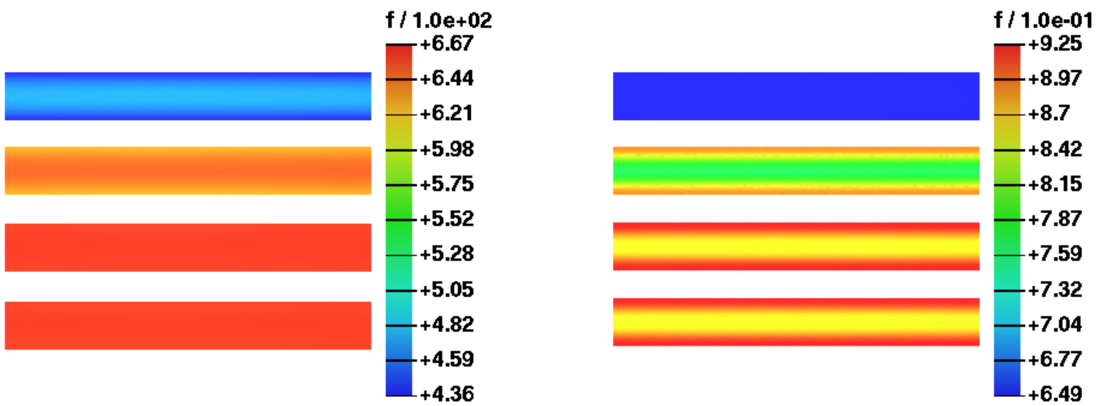
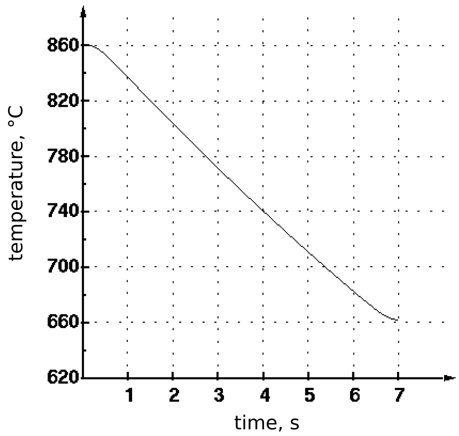


Figure 7: The simulated final temperature (left) and phase distribution (right) in the cross section of the steel slab. Both pictures show the 1^{st} and 7^{th}(final) iteration of projected gradient method, and 1^{st} and 3^{rd}(final) iterations of rSQP method in order from top to bottom.

With each iteration of rSQP method the temperature distribution in the steel slab becomes more homogeneous and closer to the desired value $\theta_d = 660°C$. On the other hand, the maximal difference between the ferrite values at the final time is about of 8%. However, in each iteration of rSQP method the ferrite phase fraction in the largest part of the cross section is closed to 85%. We additionally plot the temperature and ferrite growth during the cooling in the middle of the cross section of the steel



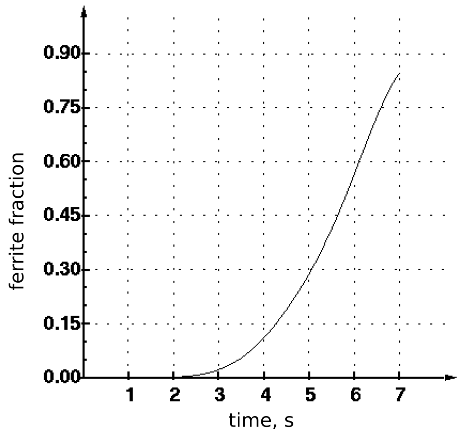


Figure 8: The simulated temperature (left) and phase growth (right) in the middle of the cross section of the steel slab.

slab. The simulation results are shown in Figure 8. The desired temperature of $660°C$ and ferrite fraction of 85% are reached very accurately in the middle of the cross section.

Conclusions

We have studied the optimal control problem that describes the hot rolling process of multiphase steel. The nonlinear boundary control problem was analyzed and the first-order necessary and second order sufficient optimality conditions were derived. The control problem was solved numerically by a reduced SQP method with active set strategy.

The approach has already been tested in an industrial setting. The results of the optimal control of the cooling line have been verified in hot rolling experiments at the pilot hot rolling mill at the Institute for Metal Forming (IMF), TU Bergakademie Freiberg. For more details we refer to a recent paper [3].

The challenging topic for the future research will be the real time control of the hot rolling process, which is an important task for the industrial employment of this approach. Here, recent developments in model reduction techniques seem to be a promising tool and will be subject of futher work of the authors.

References

[1] W. Alt. *Nichtlineare Optimierung: Eine Einführung in Theorie, Verfahren und Anwendungen*. Vieweg Studium: Aufbaukurs Mathematik. Vieweg+Teubner Verlag, 2002.

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

[3] W. Bleck, D. Hömberg, U. Prahl, P. Suwanpinij, and N. Togobytska. Optimal control of a cooling line for production of hot rolled dual phase steel. *Steel Research Int.*, to appear.

[4] J. Dieudonne. *Foundations of Modern Analysis*. Pure and Applied Mathematics. Read Books, 1960.

[5] A. Fasano, D. Hömberg, and L. Panizzi. A mathematical model for case hardening of steel. *Math. Models Methods Appl. Sci.*, 19:2101–2126, 2009.

[6] H. Goldberg and F. Tröltzsch. Second order sufficient optimality conditions for a class of nonlinear parabolic boundary control problems. *SIAM J. Contr. Opt.*, 31:1007–1025, 1993.

[7] H. Goldberg and F. Tröltzsch. On a Lagrange-Newton method for a nonlinear parabolic boundary control problem. *Optim. Methods Softw.*, 8:225–247, 1998.

[8] H. Goldberg and F. Tröltzsch. On a SQP-multigrid technique for nonlinear parabolic boundary control problems. In W. W. Hager and P. M. Pardalos, editors, *Optimal Control: Theory, Algorithms, and Applications*, pages 154–177. Kluwer Academic Publishers B.V., 1998.

[9] R. Griesse. Infinite-dimensional optimization. Short course, Bremen, 2006.

[10] M. Hintermüller, S. Volkwein, and F. Diwoky. Fast solution techniques in constrained optimal boundary control of the semilinear heat equation. In *Control of coupled partial differential equations*, volume 155 of *Internat. Series Numer. Math.*, pages 119–147. Birkhäuser, Basel, 2007.

[11] D. Hömberg and J. Sokolowski. Optimal shape design of inductor coils for surface hardening. *SIAM J. Contr. Optim.*, 42(3):1087–1117, 2003.

[12] D. Hömberg and S. Volkwein. Control of laser surface hardening by a reduced-order approach using proper orthogonal decomposition. *Math. Comput. Modelling*, 37:1003–1028, 2003.

[13] C. T. Kelley. *Iterative Methods for Optimization*. Frontiers in Applied Mathematics,SIAM, Philadelphia, 1999.

[14] F.-S. Kupfer and E. W. Sach. A prospective look at SQP methods for semilinear parabolic control problems. *Lecture Notes in Control and Inform. Sci.*, 149:143–157, 1991.

[15] F.-S. Kupfer and E. W. Sach. Numerical solution of a nonlinear parabolic control problem by a reduced SQP method. *Comput. Optim. Appl.*, 1:113–135, 1992.

[16] G. Landl and H. W. Engl. Optimal strategies for the cooling of steel strips in hot strip mills. *Inverse Problems in Engineering*, 2:103–118, 1995.

[17] J. Nocedal and S. Wright. *Numerical Optimization*. Springer Series in Operations Research and Financial Engineering. Springer, New York, second edition, 2006.

[18] J. P. Raymond and F. Tröltzsch. Second order sufficient optimality conditions for nonlinear parabolic control problems with sate constaints. *Discrete Contin. Dyn. Syst.*, 6:431–450, 2000.

[19] P. Suwanpinij, N. Togobytska, U. Prahl, W. Weiss, D. Hömberg, and W. Bleck. Numerical cooling strategy design for hot rolled dual phase steel. *Steel Research Int.*, 11:1001–1009, 2010.

[20] C. Tianyou, T. Minghao, C. Xiaoyan, and L. Hanxiong. Intelligent optimization control for laminar cooling. In *Proceedings of the 15th IFAC World Congress, 2002, Barcelona*.

[21] F. Tröltzsch. An SQP method for the optimal control of a nonlinear heat equation. *Control Cybernet.*, 23:268–288, 1994.

[22] F. Tröltzsch. *Optimal Control of Partial Differential Equations: Theory, Methods, and Applications*, volume 112 of *Graduate Studies in Mathematics*. American Mathematical Society, 2010.