Numer. Math. 71: 289–315 (1995)

Numerische Mathematik

Analysis and finite element approximation of an optimal control problem in electrochemistry with current density controls

L. Steven Hou[1,*], **James C. Turner**[2,**]

[1] Department of Mathematics and Statistics, York University, North York, Ontario M3J 1P3, Canada
e-mail: hou@mathstat.yorku.ca.
[2] Department of Mathematics, The Ohio State University, Columbus, Ohio 43210-1174, USA

Received March 10, 1993 / Revised version received July 4, 1994

Summary. An optimal control problem for impressed cathodic systems in electrochemistry is studied. The control in this problem is the current density on the anode. A matching objective functional is considered. We first demonstrate the existence and uniqueness of solutions for the governing partial differential equation with a nonlinear boundary condition. We then prove the existence of an optimal solution. Next, we derive a necessary condition of optimality and establish an optimality system of equations. Finally, we define a finite element algorithm and derive optimal error estimates.

Mathematics Subject Classification (1991): 49J20, 49K20, 65K10, 65N15, 65N30

1. Introduction

We consider an optimal control problem for impressed cathodic systems. A typical example of an impressed cathodic system is a metal container filled with an electrolyte. The painted portion of the container surface is usually treated as insulated. The unpainted part is divided into the cathode and the anode which are connected to the negative and positive poles of an electrical source, respectively. By adjusting the current density on the anode we could effectively alter the potential distribution on the entire bounding surface or in the entire flow domain. The potential distribution, of course, has a direct effect on the chemical reaction process occurring inside the flow domain. The reaction process in turn affects on the rate of corrosion of the metal container. Thus the current density on the anode can be used as a practical control variable for generating a desired poten-

* Work supported in part by the Natural Science and Engineering Research Council of Canada under Grant OGP-0137436
** Work supported in part by US Army Research Office under Grant DAAL03-91-G0237

tial field. This idea can be conveniently formulated as optimal control problems for the potential equation with appropriate boundary conditions. Optimal control problems of this sort have been studied in [20] and [21] where the goal was to match a desired potential distribution on the cathode. The models analyzed in [20] and [21] are essentially linear. [14] discussed, mainly from an algorithmic point of view, several control mechanisms including adjusting the positions of anodes and/or the current density on the anodes in order to match a desired potential on the structure surface; nonlinear models were employed as well as linear ones. [15] analyzed a "location control" problem, i.e., the control variable is the location of anodes, wherein nonlinear models with boundary conditions of polynomial or exponential growth type were considered. In this article, we will attempt to analyze mathematically optimal control problems with current density controls. The nonlinear model used involves an exponentially growing boundary condition.

We assume the electrolyte occupies a physical domain $\Omega \in \mathbb{R}^2$ with a boundary Γ. The domain is assumed to be finite in this paper, although infinite domain problems can be handled if appropriate limits at infinity are assumed. If $\Omega \subset \mathbb{R}^3$, we will need to work with a non-Hilbert space $W^{1,r}(\Omega)$ with, e.g., $r = 3$; similar results can still be obtained.

The electrical potential ϕ in Ω is governed by the differential equation

$$-\operatorname{div}(\sigma \operatorname{grad} \phi) = 0 \quad \text{in } \Omega\,,$$

where the conductivity σ is a continuous function with a positive lower bound.

The boundary Γ is divided into three components: the anode Γ_A, the cathode Γ_C and the insulated part Γ_0. On the cathode Γ_C, ϕ satisfies the relation

$$\sigma \frac{\partial \phi}{\partial n} = -f(\phi) \quad \text{on } \Gamma_C\,,$$

where f is an empirical function that depends on the electrode materials (see [4]). In particular, we will assume f is given by the Butler-Volmer function:

$$f(\phi) = C_3[e^{C_1\phi} - e^{-C_2\phi}] \tag{1.1}$$

where C_1, C_2 and C_3 are positive constants (see [4]). Throughout this paper, f will be assumed to be defined by (1.1). For notational convenience, we will mainly use $f(\phi)$ rather than the explicit expression given in (1.1).

On the anode Γ_A, we have the boundary condition

$$\sigma \frac{\partial \phi}{\partial n} = u \quad \text{on } \Gamma_A\,,$$

which corresponds to the specification of the current density on the anode. Adjusting the current density on Γ_A amounts to treating u as a control variable. On the insulated part Γ_0,

$$\sigma \frac{\partial \phi}{\partial n} = 0 \quad \text{on } \Gamma_0\,.$$

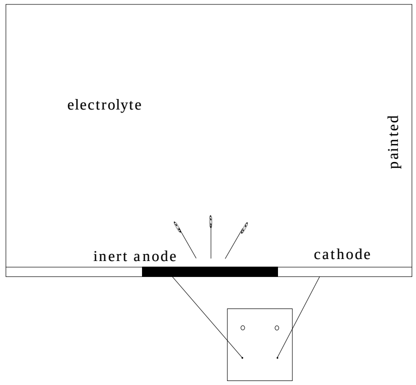

Fig. 1. A typical impressed cathodic system: an electrolyte container connected with an electrical current source

We are concerned with the following optimal control problem: seek a state ϕ and a control u such that the functional

$$\mathscr{J}(\phi, u) = \frac{1}{2\epsilon_0} \int_\Omega (\phi - \phi_0)^2 \, d\Omega + \frac{\delta_0}{2} \int_{\Gamma_A} u^2 \, d\Gamma \,, \tag{1.2}$$

is minimized subject to the the constraint equations

$$- \operatorname{div} (\sigma \operatorname{grad} \phi) = 0 \quad \text{in } \Omega \tag{1.3}$$

$$\sigma \frac{\partial \phi}{\partial n} = u \quad \text{on } \Gamma_A \,, \tag{1.4}$$

$$\sigma \frac{\partial \phi}{\partial n} = 0 \quad \text{on } \Gamma_0 \tag{1.5}$$

and

$$\sigma \frac{\partial \phi}{\partial n} = -f(\phi) \quad \text{on } \Gamma_C \,. \tag{1.6}$$

In (1.2) ϕ_0 is a desired potential distribution in Ω and ϵ_0 and δ_0 are positive constants. Physically, this problem amounts to matching a desired potential in the entire domain Ω by adjusting the (normal) electrical current density on the anode Γ_A. Many other objectives can be similarly treated.

We will utilize standard notations for Sobolev spaces $H^m(\Omega)$, $H^s(\Gamma_A)$, $H^s(\Gamma_C)$, $H^s(\Gamma_0)$ and $H^s(\Gamma)$. The corresponding norms on these spaces will be denoted by, e.g., $\|\cdot\|_m$, $\|\cdot\|_{s,\Gamma_A}$, etc. For details, see [1] and [8]. A weak formulation for the nonlinear boundary value problem (1.3)–(1.6) is given as follows: seek a $\phi \in H^1(\Omega)$ such that

$$\int_{\Omega} \sigma \operatorname{grad} \phi \cdot \operatorname{grad} \psi \, d\Omega + \int_{\Gamma_C} f(\phi)\psi \, d\Gamma = \int_{\Gamma_A} u\psi \, d\Gamma \quad \forall\, \psi \in H^1(\Omega)\,. \tag{1.7}$$

A solution ϕ to the nonlinear boundary value problem (1.3)–(1.6) will be understood in the sense of (1.7). We mention that second order elliptic differential equations with exponentially growing coefficients were studied in, among others, [9], [12]. [13] and [16]. An elliptic equation with mixed Dirichlet-Neumann type boundary conditions that have an exponentially growing coefficient in the boundary condition was studied in [7]. Some of the techniques in these articles are useful for the mathematical and numerical analysis of the state equation (1.7).

We restate the minimization problem as follows:

(1.8) seek a state $\phi \in H^1(\Omega)$ and a $u \in U$ such that the functional (1.2) is minimized subject to (1.7),

where

(1.9) U is a non-empty, closed, convex subset of $L^2(\Gamma_A)$.

Now we state a few useful facts. We set $\alpha = C_3 \min\{C_1, C_2\}$. We obtain by elementary calculus that

$$f(x)x \geq C_3(\mathrm{e}^{C_1 x} - 1)x \geq C_3 C_1 x^2 \qquad \forall\, x \geq 0$$

and

$$f(x)x \geq C_3(\mathrm{e}^{-C_2 x} - 1)(-x) \geq C_3 C_2 x^2 \qquad \forall\, x < 0$$

so that

$$f(x)x \geq \alpha x^2 \qquad \forall\, x \in \mathbb{R}\,. \tag{1.10}$$

It is also easy to see that

$$f'(x) = C_3(C_1 \mathrm{e}^{C_1 x} + C_2 \mathrm{e}^{-C_2 x}) \geq \alpha \qquad \forall\, x \in \mathbb{R}\,. \tag{1.11}$$

The norm $|||\cdot|||_1$ on $H^1(\Omega)$ defined by

$$|||\phi|||_1 = \left\{ \int_{\Omega} \sigma |\operatorname{grad} \phi|^2 \, d\Omega + \alpha \int_{\Gamma_C} \phi^2 \, d\Gamma \right\}^{1/2} \qquad \forall\, \phi \in H^1(\Omega)$$

is equivalent to the usual $H^1(\Omega)$-norm $\|\cdot\|_1$, i.e., there exist constants $\rho > 0$ and $\gamma > 0$ such that

$$\rho\, \|\phi\|_1^2 \geq \int_{\Omega} \sigma |\operatorname{grad} \phi|^2 \, d\Omega + \alpha \int_{\Gamma_C} \phi^2 \, d\Gamma \geq \gamma\, \|\phi\|_1^2 \qquad \forall\, \phi \in H^1(\Omega)\,. \tag{1.12}$$

A proof of (1.12) can be found in, e.g., [17]. We also state the trace result for functions in $H^1(\Omega)$:

(1.13) $$\|\phi\|_{0,\Gamma} \le \|\phi\|_{1/2,\Gamma} \le \beta\|\phi\|_1 \qquad \forall\, \phi \in H^1(\Omega)$$

where $\beta > 0$ is a constant independent of ϕ.

The rest of the paper is organized as follows. In Sect. 2 we prove the existence and uniqueness of solutions to (1.7) so that the constraint equation is well-posed. In Sect. 3 we show the existence of an optimal pair $(\hat{\phi}, \hat{u})$ that minimizes (1.1) subject to (1.7). In Sect. 4 we derive an optimality condition. In Sect. 5 we discuss the regularity of optimal solutions. Finally in Sect. 6 we define a finite element algorithm for solving the optimality system and derive optimal error estimates.

2. Existence and uniqueness of solutions to the constraint equations

We first examine the existence of a solution to the nonlinear Neumann type boundary value problems (1.7).

Lemma 2.1. *Assume $\phi \in H^1(\Omega)$ and $s > 0$. Then $\mathrm{e}^{s|\phi|} \in L^1(\Gamma)$. Moreover, there exists a constant κ, independent of ϕ, such that*

$$\int_\Gamma \mathrm{e}^{s|\phi|}\, d\Gamma \le 1 + |\Gamma| + \mathrm{e}^{s^2\kappa^2\|\phi\|_1^2}\,|\Gamma| < \infty\,,$$

where $|\Gamma|$ is the measure of Γ.

Proof. Let $\phi \in H^1(\Omega)$ and $s > 0$ be given. Then $\phi \in H^{1/2}(\Gamma)$. Using embedding results for Orlicz-Sobolev spaces (see [1], [10] and [18]) (recall $\Omega \subset \mathbb{R}^2$), we have $H^{1/2}(\Gamma) \hookrightarrow L_{\mathrm{A}}(\Gamma)$ where the N-function $A(t) = \mathrm{e}^{t^2} - 1$. Thus there exists a constant $\kappa > 0$ such that

$$\|\phi\|_{L_{\mathrm{A}}(\Gamma)} \equiv \inf\left\{ r : \int_\Gamma \mathrm{e}^{\frac{|\phi|^2}{r^2}}\, d\Gamma \le 1 \right\} \le \kappa\|\phi\|_1 < \infty\,.$$

Hence for each sufficiently small $\epsilon > 0$, the constant $r \equiv \|\phi\|_{L_{\mathrm{A}}(\Gamma)} + \epsilon$ satisfies

$$\int_\Gamma [\mathrm{e}^{\frac{|\phi|^2}{r^2}} - 1]\, d\Gamma \le 1$$

so that

$$\int_\Gamma \mathrm{e}^{\frac{|\phi|^2}{r^2}}\, d\Gamma \le 1 + |\Gamma|\,.$$

We set $M = sr^2$. An elementary calculation yields

$$\mathrm{e}^{sx} < \mathrm{e}^{\frac{x^2}{r^2}} \qquad \forall\, |x| > M\,.$$

Setting $K = \mathrm{e}^{sM}$, i.e., $K = \mathrm{e}^{s^2r^2} < \infty$, we obtain

$$\int_\Gamma e^{s|\phi|}\,d\Gamma = \int_{\{\mathbf{X}\in\Gamma:|\phi(\mathbf{X})|\geq M\}} e^{s|\phi|}\,d\Gamma + \int_{\{\mathbf{X}\in\Gamma:|\phi(\mathbf{X})|<M\}} e^{s|\phi|}\,d\Gamma$$
$$\leq \int_\Gamma e^{\frac{|\phi|^2}{r^2}}\,d\Gamma + K\,|\Gamma| \quad \leq 1 + |\Gamma| + e^{s^2(\|\phi\|_{L_A(\Gamma)}+\epsilon)^2}\,|\Gamma|$$
$$\leq 1 + |\Gamma| + e^{s^2(\kappa\|\phi\|_1+\epsilon)^2}\,|\Gamma| \quad < \infty\,.$$

Letting $\epsilon \to 0$ yield the desired result. □

Theorem 2.2. *Assume $u \in L^2(\Gamma_A)$. Then there exists a unique $\phi \in H^1(\Omega)$ that satisfies* (1.7). *Furthermore, ϕ satisfies the estimate*

$$\|\phi\|_1 \leq \frac{\beta}{\gamma}\|u\|_{0,\Gamma_A}\,, \tag{2.1}$$

where β and γ are constants independent of ϕ as introduced in (1.12) *and* (1.13).

Proof. We introduce the functional

$$j_u(\psi) = \frac{1}{2}\int_\Omega \sigma|\operatorname{grad}\psi|^2\,d\Omega + \int_{\Gamma_C} F(\psi)\,d\Gamma - \int_{\Gamma_A} u\,\psi\,d\Gamma \qquad \forall\,\psi \in H^1(\Omega)\,,$$

where $F : \mathbb{R} \to \mathbb{R}$ is defined by

$$F(x) = \frac{C_3}{C_1}e^{C_1 x} + \frac{C_3}{C_2}e^{-C_2 x}\,.$$

Thanks to Lemma 2.1, the term $\int_{\Gamma_C} F(\psi)\,d\Gamma$ is finite so that $j_u(\psi) < \infty$ for all $\psi \in H^1(\Omega)$. It is clear that $\phi \in H^1(\Omega)$ is a solution of (1.7) if and only if ϕ is a solution of the minimization problem

$$j_u(\phi) = \min_{\psi\in H^1(\Omega)} j_u(\psi)\,. \tag{2.2}$$

Note that $F''(x) = C_3(C_1e^{C_1x} + C_2e^{-C_2x}) \geq C_3\min\{C_1, C_2\} = \alpha > 0$. Therefore we have that

$$F(\psi+\tau) + F(\psi-\tau) - 2F(\psi) = F''(\xi)\tau^2 \geq \alpha\tau^2$$

where ξ is between $(\psi - \tau)$ and $(\psi + \tau)$, so that we obtain the strict convexity property for the functional $j_u(\cdot)$:

$$j_u(\psi+\tau) + j_u(\psi-\tau) - 2j_u(\psi) \geq \int_\Omega \sigma|\operatorname{grad}\tau|^2\,d\Omega + \alpha\int_{\Gamma_A}\tau^2\,d\Gamma$$
$$\geq \gamma\|\tau\|_1^2 \qquad \forall\,\psi,\tau \in H^1(\Omega)\,.$$

It follows that

$$j_u(\xi) + j_u(\zeta) - 2j_u\big((\xi+\zeta)/2\big) \geq \frac{\gamma}{4}\|\xi-\zeta\|_1^2 \qquad \forall\,\xi,\zeta \in H^1(\Omega)$$

so that

(2.3) $$j_u(\xi) + j_u(\zeta) - 2 \inf_{\psi \in H^1(\Omega)} j_u(\psi) \geq \frac{\gamma}{4} \|\xi - \zeta\|_1^2 \qquad \forall\, \xi, \zeta \in H^1(\Omega)\,.$$

Now, let $\{\psi_k\} \subset H^1(\Omega)$ be a minimizing sequence for (2.2), i.e.,

$$\lim_{k\to\infty} j_u(\psi_k) = \inf_{\psi \in H^1(\Omega)} j_u(\psi)\,.$$

Then, from (2.3), $\{\psi_k\}$ is a Cauchy sequence in $H^1(\Omega)$. Let ϕ be the $H^1(\Omega)$-strong limit of $\{\psi_k\}$. We may choose a subsequence (still denoted by $\{\psi_k\}$) such that $\{\psi_k\}$ converges to ϕ pointwise almost everywhere in Ω. Using Fatou's Lemma for the limit in the term $\int_{\Gamma_C} F(\psi_k)\, d\Gamma$, we obtain

$$j_u(\phi) \leq \liminf_{k\to\infty} j_u(\psi_k) = \inf_{\psi \in H^1(\Omega)} j_u(\psi)\,.$$

Hence, ϕ is a solution of (2.2), or equivelently, (1.7). The uniqueness of the solution for (1.7) follows directly from the strict convexity of $j_u(\cdot)$ (or from (2.3)).

Finally we prove (2.1). By setting $\psi = \phi$ in (1.7) and using (1.10) and (1.12), we obtain that

$$\gamma\, \|\phi\|_1^2 \leq \int_{\Gamma_A} u\phi\, d\Gamma \leq \|u\|_{0,\Gamma_A}\, \|\psi_u\|_{0,\Gamma_A} \leq \beta\, \|u\|_{0,\Gamma_A}\, \|\psi_u\|_1$$

so that

$$\|\phi_u\|_1 \leq \frac{\beta}{\gamma} \|u\|_{0,\Gamma_A}\,. \qquad \square$$

3. Existence of an optimal solution

Having shown that the constraint equation (1.7) is well posed, we are now prepared to study the existence of an optimal solution $(\hat{\phi}, \hat{u})$ that minimizes the functional (1.2) subject to (1.7). We introduce the admissible set

$$\mathscr{U}_{\text{ad}} = \{(\phi, u) \in H^1(\Omega) \times U : (\phi, u) \text{ satisfies } (1.7)\}\,,$$

where U is given by (1.9). Then the goal of this section is to show the existence of a solution $(\hat{\phi}, \hat{u})$ for the minimization problem:

$$\mathscr{J}(\hat{\phi}, \hat{u}) = \min_{(\phi,u)\in \mathscr{U}_{\text{ad}}} \mathscr{J}(\phi, u)\,.$$

We first establish a useful result.

Lemma 3.1. *Assume $\{\phi_n\} \subset L^2(\Gamma_C)$ is a sequence such that $\phi_n \to \phi$ a.e. on Γ_C and*

(3.1) $$\int_{\Gamma_C} f(\phi_n)\phi_n\, d\Gamma \leq B \quad \forall\, n$$

where f is defined by (1.1) *and $B > 0$ is a constant independent of n. Then*

$$\int_{\Gamma_C} f(\phi)\phi \, d\Gamma \leq \liminf_{n\to\infty} \int_{\Gamma_C} f(\phi_n)\phi_n \, d\Gamma$$

and

$$\lim_{n\to\infty} \int_{\Gamma_C} |f(\phi_n) - f(\phi)| \, d\Gamma = 0 \, .$$

Proof. The proof follows the ideas of [13], pp. 21–22. Since f is continuous and $\phi_n \to \phi$ a.e. on Γ_C, we deduce that $f(\phi_n) \to f(\phi)$ a.e. on Γ_C. Note that $f(\phi)\phi \geq 0$ on Γ_C so that we may use Fatou's Lemma to obtain

$$\int_{\Gamma_C} f(\phi)\phi \, d\Gamma \leq \liminf_{n\to\infty} \int_{\Gamma_C} f(\phi_n)\phi_n \, d\Gamma \leq B \, .$$

Hence $f(\phi)\phi \in L^1(\Omega)$. By setting $K = \sup_{|x|\leq 1} |f(x)|$ we easily conclude from the identity

$$|f(t)| = |t|^{-1} f(t)t \quad \forall\, t \neq 0 \tag{3.2}$$

that

$$|f(t)| \leq f(t)t + K \quad \forall\, t \in \mathbb{R} \, .$$

Thus

$$|f(\phi)| \leq |f(\phi)| \, |\phi| + K \quad \text{on } \Gamma_C \, ,$$

i.e., $f(\phi) \in L^1(\Gamma_C)$. Utilizing (3.2) again, we deduce that for each $\delta > 0$ and for a.e. $\mathbf{x} \in \Gamma_C$, we have either

$$|\phi_n| \leq \delta^{-1}$$

or

$$|f(\phi)| \leq \delta f(\phi_n)\, \phi_n$$

so that

$$|f(\phi)| \leq C_\delta + \delta f(\phi_n)\, \phi_n \quad \text{on } \Gamma_C \, ,$$

where $C_\delta = \sup\limits_{|x|\leq \delta^{-1}} |f(x)|$. For every measurable subset $S \subset \Gamma_C$ we have

$$\int_{\Gamma_C} |f(\phi_n)| \, d\Gamma \leq C_\delta |S| + \delta \int_{\Gamma_C} f(\phi_n)\phi_n \, d\Gamma \, .$$

Equation (2.1) implies

$$\int_S f(\phi_n)\phi_n \, d\Gamma \leq 2B$$

for n greater than some $N_0 > 0$. Thus

$$\int_S |f(\phi_n)| \, d\Gamma \leq C_\delta |S| + 2B\delta \quad \forall\, n > N_0 \, ,$$

where $|S|$ is the measure of S. Hence, the sequence of functions $\{f(\phi_n)\}$ has equi-absolutely continuous integrals. By Vitali's Convergence Theorem,

$$\lim_{n\to\infty}\int_{\Gamma_C} |f(\phi_n) - f(\phi)|\, d\Gamma = 0\,. \qquad \square$$

We are now prepared to prove the existence of an optimal solution.

Theorem 3.2. *There exists a* $(\hat{\phi}, \hat{u}) \in H^1(\Omega) \times U$ *that minimizes* (1.2) *subject to* (1.7).

Proof. Theorem 2.2 implies an element $(\phi, u) \in \mathscr{U}_{ad}$ exists such that $\mathscr{J}(\phi, u) < \infty$. Thus we may choose a minimizing sequence $\{(\phi_n, u_n)\} \subset \mathscr{U}_{ad}$ such that

$$\lim_{n\to\infty} \mathscr{J}(\phi_n, u_n) = \inf_{(\phi,u)\in\mathscr{U}_{ad}} \mathscr{J}(\phi, u) \tag{3.3}$$

and

(3.4)
$$\int_\Omega \sigma \operatorname{grad} \phi_n \cdot \operatorname{grad} \psi\, d\Omega + \int_{\Gamma_C} f(\phi_n)\psi\, d\Gamma = \int_{\Gamma_A} u_n\psi\, d\Gamma\,, \quad \forall\, \psi \in H^1(\Omega)\,.$$

Using (1.2) and (3.3) we deduce that $\{u_n\}$ is bounded in $L^2(\Gamma_A)$. Then (2.1) implies $\{\|\phi_n\|_1\}$ is bounded. Hence we may extract a subsequence $\{(\phi_n, u_n)\}$ such that

$$\phi_n \rightharpoonup \hat{\phi} \quad \text{in } H^1(\Omega) \qquad \text{and} \qquad u_n \rightharpoonup \hat{u} \quad \text{in } L^2(\Gamma_A)\,.$$

Furthermore, trace theorems and compact imbedding results imply $\phi_n \to \phi$ in $L^2(\Gamma_C)$; this in turn implies $\phi_n \to \phi$ pointwise a.e. on Γ_C (after extracting subsequences if necessary). By setting $\psi = \phi_n$ in (3.4) we obtain

$$\int_\Omega \sigma |\operatorname{grad} \phi_n|^2\, d\Omega + \int_{\Gamma_C} f(\phi_n)\phi_n \le \|u_n\|_{0,\Gamma_A} \|\phi_n\|_{0,\Gamma_A} \le \beta\, \|u_n\|_{0,\Gamma_A} \|\phi_n\|_1\,.$$

Hence we deduce

$$\int_{\Gamma_C} f(\phi_n)\phi_n \le M$$

where M is a constant independent of n. By Lemma 3.1,

$$\int_{\Gamma_C} f(\hat{\phi})\hat{\phi}\, d\Gamma \le \liminf_{n\to\infty} \int_{\Gamma_C} f(\phi_n)\phi_n\, d\Gamma$$

and

$$\lim_{n\to\infty}\int_{\Gamma_C} |f(\phi_n) - f(\hat{\phi})|\, d\Gamma = 0\,. \tag{3.5}$$

For each $\psi \in C^\infty(\overline{\Omega})$, (3.5) allows us to pass to the limit in (3.4) to obtain

$$\int_\Omega \sigma \operatorname{grad} \hat{\phi} \cdot \operatorname{grad} \psi \, d\Omega + \int_{\Gamma_C} f(\hat{\phi})\psi \, d\Gamma = \int_{\Gamma_A} \hat{u}\psi \, d\Gamma \qquad \forall\, \psi \in C^\infty(\overline{\Omega}) \,.$$

Then using the denseness of $C^\infty(\overline{\Omega})$ in $H^1(\Omega)$ and the fact that $f(\hat{\phi}) \in L^2(\Gamma_C)$ (due to Lemma 2.1), we obtain

$$\int_\Omega \sigma \operatorname{grad} \hat{\phi} \cdot \operatorname{grad} \psi \, d\Omega + \int_{\Gamma_C} f(\hat{\phi})\psi \, d\Gamma = \int_{\Gamma_A} \hat{u}\psi \, d\Gamma \qquad \forall\, \psi \in H^1(\Omega) \,.$$

Thus $(\hat{\phi}, \hat{u}) \in \mathscr{U}_{ad}$. Finally using the weak lower semi-continuity of $\mathscr{J}(\cdot,\cdot)$, we conclude that $(\hat{\phi}, \hat{u})$ is indeed an optimal solution, i.e.,

$$\mathscr{J}(\hat{\phi}, \hat{u}) = \inf_{(\phi,u)\in \mathscr{U}_{ad}} \mathscr{J}(\phi, u) \,. \qquad \square$$

4. A necessary condition of optimality

In this section we will derive a necessary condition that an optimal solution must satisfy. (The existence of an optimal solution has been established in Sect. 3.)

In Sect. 2 we have shown that for each $u \in L^2(\Gamma_A)$, there exists a unique ϕ satisfying (1.7). Thus the state ϕ is a well-defined function of u and will be denoted by $\phi = \phi(u)$. In Sect. 3 we have proved that there exists a $\hat{u} \in U$ such that $(\phi(\hat{u}), \hat{u}) \in \mathscr{U}_{ad}$ is a minimizer for the problem (1.8). Introducing

$$\mathscr{G}(u) = \mathscr{J}\big(\phi(u), u\big) \qquad \forall\, u \in U \,,$$

we see that $\hat{u}$ is a minimizer for the problem

$$\mathscr{G}(\hat{u}) = \min_{u\in U} g(u)$$

so that formally, $\hat{u}$ necessarily satisfies

$$\mathscr{G}'(\hat{u}) \cdot (u - \hat{u}) \geq 0 \qquad \forall\, u \in U \,.$$

Our task is to justify this necessary condition rigorously and express it in a more practical form.

We first study the differentiability of the mapping $u \mapsto \phi(u)$ from $L^2(\Gamma_A)$ to $H^1(\Omega)$. (But remember we need to come back later to the case where the mapping $u \mapsto \phi$ is from U to $H^1(\Omega)$.)

Lemma 4.1. *The mapping $u \mapsto \phi(u)$ is differentiable from $L^2(\Gamma_A)$ to $H^1(\Omega)$.*

Proof. Let $u \in L^2(\Gamma_A)$ be given. We define a linear operator $K : L^2(\Gamma_A) \to H^1(\Omega)$ as follows: $Kw = \xi$ for $w \in L^2(\Gamma_A)$ and $\xi \in H^1(\Omega)$ if and only if

(4.1)
$$\int_\Omega \sigma \operatorname{grad} \xi \cdot \operatorname{grad} \psi \, d\Omega + \int_{\Gamma_C} f'(\phi_u)\,\xi\psi \, d\Gamma = \int_{\Gamma_C} w\psi \, d\Gamma \qquad \forall\, \psi \in H^1(\Omega) \,.$$

Lemma 2.1 ensures the term $\int_{\Gamma_C} f'(\phi_u)\,\xi\psi\,d\Gamma$ is finite; also, (1.11)–(1.12) and Lax-Milgram Lemma guarantees the operator K is well defined. We now show that $\phi(u)$ is differentiable and $K = \phi'(u)$. For each $v \in L^2(\Gamma_A)$, by subtracting the defining equations for $\phi(v)$ and $\phi(u)$ (see (1.7)) and then subtracting the defining equation for $\zeta = K(u - v)$ (see (4.1)), we obtain

$$\int_\Omega \sigma \operatorname{grad}\left[\phi(v) - \phi(u) - \zeta\right] \cdot \operatorname{grad}\psi\, d\Omega + \int_{\Gamma_C}\left[f\left(\phi(v)\right) - f\left(\phi(u)\right) - f'\left(\phi(u)\right)\zeta\right]\psi\, d\Gamma = 0 \qquad \forall\,\psi \in H^1(\Omega)\,.$$

Setting $\psi = \phi(v) - \phi(u) - \zeta$ and using the Taylor expansion $f\left(\phi(v)\right) = f\left(\phi(u)\right) + f'\left(\phi(u)\right)[\phi(v) - \phi(u)] + f''(\eta)[\phi(v) - \phi(u)]^2/2$ where η is between $\phi(v)$ and $\phi(u)$, we have that

$$\begin{aligned}
&\int_\Omega \sigma|\operatorname{grad}\left(\phi(v) - \phi(u) - \zeta\right)|^2\, d\Omega + \int_{\Gamma_C} f'\left(\phi(u)\right)\left[\phi(v) - \phi(u) - \zeta\right]^2 d\Gamma \\
&\quad = \frac{1}{2}\int_{\Gamma_C} f''(\eta)[\phi(v) - \phi(u)]^2\left[\phi(v) - \phi(u) - \zeta\right] d\Gamma \\
&\quad \le \frac{1}{2}\left\{\int_{\Gamma_C} |f''(\eta)|^4\, d\Gamma\right\}^{1/4} \|\phi(v) - \phi(u)\|^2_{L^4(\Gamma_C)}\, \|\phi(v) - \phi(u) - \zeta\|_{L^4(\Gamma_C)} \\
&\quad \le \frac{C}{2} B_1(\|\eta\|_1)\, \|\phi(v) - \phi(u)\|_1^2\, \|\phi(v) - \phi(u) - \zeta\|_1
\end{aligned}$$

where in the last inequality we used Lemma 2.1 to estimate the first factor with $B_1(\cdot)$ a continuous positive function, and used trace theorems to estimate the other two factors. Using (1.11)–(1.12), we derive from the last relation that

$$\|\phi(v) - \phi(u) - K(v - u)\|_1 \le \frac{C}{2\gamma}\, B_1\left(\|\phi(u)\|_1 + \|\phi(v)\|_1\right) \|\phi(v) - \phi(u)\|_1^2 \tag{4.2}$$

for all $v \in L^2(\Gamma_A)$. By subtracting the defining equations for $\phi(u)$ and $\phi(v)$ and setting $\psi = \phi(u) - \phi(v)$ we obtain

$$\int_\Omega |\operatorname{grad}[\phi(u) - \phi(v)]|^2\, d\Omega + \int_{\Gamma_C}\left[f\left(\phi(u)\right) - f\left(\phi(v)\right)\right][\phi(u) - \phi(v)]\, d\Gamma = \int_{\Gamma_A} (u - v)\,[\phi(u) - \phi(v)]\, d\Gamma\,.$$

Since $f\left(\phi(u)\right) - f\left(\phi(v)\right) = f'(\xi)\,[\phi(u) - \phi(v)]$ where ξ is between $\phi(u)$ and $\phi(v)$, we have that, using (1.11) and (1.12),

$$\gamma\,\|\phi(u) - \phi(v)\|_1^2 \le \int_{\Gamma_A} (u - v)\,[\phi(u) - \phi(v)]\, d\Gamma \le \beta\,\|u - v\|_{0,\Gamma_A}\, \|\phi(u) - \phi(v)\|_1$$

so that

$$\|\phi(u) - \phi(v)\|_1 \le \frac{\beta}{\gamma}\|u - v\|_{0,\Gamma_A}\,. \tag{4.3}$$

By plugging this last relation into (4.2) and using (2.1), we have that

$$\|\phi(v) - \phi(u) - K(v-u)\|_1 \leq \frac{C\beta}{2\gamma^2} B_1\big(\|\phi(u)\|_1 + 1\big)\, \|v-u\|^2_{0,\Gamma_A}$$

for all $v \in L^2(\Gamma_A)$ with $\|v\|_{0,\Gamma_A} \leq \frac{\gamma}{\beta}$. Hence we have proved that the mapping $u \mapsto \phi(u)$ is differentiable from $L^2(\Gamma_A)$ to $H^1(\Omega)$ and that $\phi'(u) = K$ where K is defined by (4.1). □

Remark. We may use boodstrap techniques to show that the mapping $u \mapsto \phi(u)$ is infinitely differentiable from $L^2(\Gamma_C) \to H^1(\Omega)$.

Remark. From (1.4)–(1.6) we obtain

$$\Big\|\sigma \frac{\partial \phi(u)}{\partial n}\Big\|_{0,\Gamma} \leq \|f(\phi_u)\|_{0,\Gamma_C} + \|u\|_{0,\Gamma_A}$$

and using Lemma 2.1,

$$\Big\|\sigma \frac{\partial \phi(u)}{\partial n}\Big\|_{0,\Gamma} \leq B_2(\|u\|_{0,\Gamma_A})$$

where $B_2(\cdot)$ is a continuous, positive function. This last estimate together with (1.2) and elliptic regularity results yields

$$\|\sigma \operatorname{grad} \phi(u)\|_{1/2} \leq B_3\big(\|u\|_{0,\Gamma_A}\big)$$

where $B_3(\cdot)$ equals $B_2(\cdot)$ times a positive constant. Sobolev imbedding results imply that

$$\|\operatorname{grad} \phi(u)\|_{L^4(\Omega)} \leq B_4\big(\|u\|_{0,\Gamma_A}\big)$$

and

$$\|\phi(u)\|_{L^\infty(\Omega)} \leq B_5\big(\|u\|_{0,\Gamma_A}\big)$$

where $B_4(\cdot)$ and $B_5(\cdot)$ are both equal to $B_2(\cdot)$ times a corresponding positive constant. There estimates together with (2.1) and (4.3) allow us to show that the mapping $u \mapsto \phi(u)$ is infinitely differentiable from $L^2(\Gamma_A)$ to $W^{1,4}(\Omega)$.

Now we are prepared to derive a necessary condition that an optimal solution for (1.8) satisfies. Noting that we consider the functional $\mathscr{G}(u) = \mathscr{J}\big(\phi(u), u\big)$ only for $u \in U$ and U in general is not an open set, we need to be careful in making use of the derivative $\phi'(u)$.

Theorem 4.2. *Assume* $(\hat{\phi}, \hat{u}) \in \mathscr{U}_{ad}$ *is an optimal solution to the minimization problem* (1.8). *Then there exists a* $\lambda \in H^1(\Omega)$ *such that*

$$\int_\Omega \sigma \operatorname{grad} \psi \cdot \operatorname{grad} \lambda \, d\Omega + \int_{\Gamma_C} f'(\hat{\phi})\, \psi \lambda \, d\Gamma = \frac{1}{\epsilon_0} \int_\Omega (\hat{\phi} - \phi_0)\psi \, d\Omega \qquad \forall\, \psi \in H^1(\Omega)\,. \tag{4.4}$$

and

$$\int_{\Gamma_A} (\delta_0 \hat{u} + \lambda)(u - \hat{u})\, d\Gamma \geq 0 \qquad \forall\, u \in U\,. \tag{4.5}$$

Proof. For an arbitrary $u \in U$, we define $g(t) = \mathscr{J}\left(\phi(tu + (1-t)\hat{u}), tu + (1-t)\hat{u}\right)$ for $t \in [0,1]$. Due to the convexity of U we have that $tu + (1-t)\hat{u} \in U$ for all $t \in [0,1]$ so that $g(\cdot)$ attains a minimum at $t = 0$. From Lemma 4.1 we easily see that $g(\cdot)$ is right-differentiable at $t = 0$ (we denote this right-derivative by $g'(0)$) and $g'(0) \geq 0$. Using chain rules we obtain

$$g'(0) = \frac{1}{\epsilon_0} \int_\Omega \left[\phi(\hat{u}) - \phi_0\right] \left[\phi'(\hat{u})(u - \hat{u})\right] d\Omega + \delta_0 \int_{\Gamma_A} \hat{u}\, (u - \hat{u})\, d\Gamma \geq 0\,. \tag{4.6}$$

We set $\lambda \in H^1(\Omega)$ to be the solution of (4.4) (the existence of such a λ is guaranteed by (1.11)–(1.12) and Lax-Milgram Lemma.) We set $\zeta = \phi'(u)(u - \hat{u})$. Then by the definition of $\phi'(u)$ (see the proof of Lemma 4.1 and (4.1)) we have that

$$\begin{aligned} \int_\Omega \sigma \operatorname{grad} \zeta \cdot \operatorname{grad} \psi\, d\Omega + \int_{\Gamma_C} f'(\hat{\phi})\, \zeta\psi\, d\Gamma \\ = \int_{\Gamma_A} (u - \hat{u})\psi\, d\Gamma \qquad \forall\, \psi \in H^1(\Omega)\,. \end{aligned} \tag{4.7}$$

By setting $\psi = \zeta$ in (4.4) and $\psi = \lambda$ in (4.7) and then comparing the two equations we obtain

$$\begin{aligned} \int_{\Gamma_A} (u - \hat{u})\lambda\, d\Gamma &= \frac{1}{\epsilon_0} \int_\Omega (\hat{\phi} - \phi_0)\zeta\, d\Omega \\ &= \frac{1}{\epsilon_0} \int_\Omega \left[\phi(\hat{u}) - \phi_0\right] \left[\phi'(\hat{u})(u - \hat{u})\right] d\Omega\,. \end{aligned}$$

Plugging this last relation into (4.4) yields (4.5). □

5. An optimality system and the regularity of its solutions

In the sequel we will treat the special case $U = L^2(\Gamma_A)$. From (4.5) we easily obtain

$$\hat{u} = -\frac{1}{\delta_0}\lambda\,. \tag{5.1}$$

From (4.4), (5.1) and the original constraint equation (1.7), we form the following system of equations (dispensing with the hat notations to denote optimal solutions):

(5.2)
$$\int_{\Omega} \sigma \operatorname{grad} \phi \cdot \operatorname{grad} \psi \, d\Omega + \int_{\Gamma_C} f(\phi)\psi \, d\Gamma = -\frac{1}{\delta_0} \int_{\Gamma_A} \lambda \psi \, d\Gamma , \quad \forall \psi \in H^1(\Omega)$$

and

(5.3)
$$\int_{\Omega} \sigma \operatorname{grad} \lambda \cdot \operatorname{grad} \omega \, d\Omega + \int_{\Gamma_C} f'(\phi)\lambda \omega \, d\Gamma = \frac{1}{\epsilon_0} \int_{\Omega} (\phi - \phi_0) \omega \, d\Omega , \quad \forall \omega \in H^1(\Omega) .$$

This system of equations will be called the *optimality system*.

Integrations by parts may be used to show that the system (5.2)–(5.3) constitutes a weak formulation of the problem

(5.4)
$$-\operatorname{div}(\sigma \operatorname{grad} \phi) = 0 \quad \text{in } \Omega ,$$

(5.5)
$$\sigma \frac{\partial \phi}{\partial n} = -\frac{1}{\delta_0}\lambda \quad \text{on } \Gamma_A , \quad \sigma \frac{\partial \phi}{\partial n} = 0 \quad \text{on } \Gamma_0 \quad \text{and} \quad \sigma \frac{\partial \phi}{\partial n} = -f(\phi) \quad \text{on } \Gamma_C ,$$

(5.6)
$$-\operatorname{div}(\sigma \operatorname{grad} \lambda) = \frac{1}{\epsilon_0}(\phi - \phi_0) \quad \text{in } \Omega ,$$

(5.7)
$$\sigma \frac{\partial \lambda}{\partial n} = 0 \quad \text{on } \Gamma_A \cup \Gamma_0 \qquad \text{and} \qquad \sigma \frac{\partial \lambda}{\partial n} = -f'(\phi)\lambda \quad \text{on } \Gamma_C ,$$

Now we examine the regularity of solutions of the optimality system (5.2)–(5.3), or equivalently, (5.4)–(5.7).

Theorem 5.1. *Suppose that $\Omega \subset \mathbb{R}^2$ is convex or of class $C^{1,1}$ and $\sigma \in C^1(\overline{\Omega})$. Assume $(\phi, \lambda) \in H^1(\Omega) \times H^1(\Omega)$ is a solution to the optimality system* (5.2)–(5.3), *or equivalently,* (5.4)–(5.7), *then we have that $(\phi, \lambda) \in W^{3/2,r}(\Omega) \times W^{3/2,r}(\Omega)$ for $r \in [1, \infty)$.*

Proof. Since ϕ, $\lambda \in H^1(\Omega)$, Lemma 2.1 implies $f(\phi) \in L^r(\Gamma_C)$ and $f'(\phi) \in L^r(\Gamma_C)$ for all $r \in [1, \infty)$. We infer from trace theorems that $\lambda \in L^q(\Gamma_C)$ for all $q > 1$. Hence we have $\sigma \frac{\partial \phi}{\partial n} \in L^q(\Gamma)$ and $\sigma \frac{\partial \lambda}{\partial n} \in L^q(\Gamma)$ for each $q > 1$. By applying elliptic regularity results to equations (5.4)–(5.7), we obtain $\phi \in W^{3/2,q}(\Omega)$ and $\lambda \in W^{3/2,q}(\Omega)$ for each $q > 1$. □

Remark. In general the possible discontinuity of the normal derivative on the intersection of Γ_C, Γ_0 and Γ_A prohibits us from obtaining further regularity. However, if ϕ and λ vanish on the entire intersection of Γ_C, Γ_0 and Γ_A, then we could in fact show that $\phi \in C^2(\Omega) \cap C(\overline{\Omega})$ and $\lambda \in C^2(\Omega) \cap C(\overline{\Omega})$, i.e., ϕ and

λ are in fact classical solutions of the optimality system. Also, $H^2(\Omega)$-regularity for ϕ and λ is expected.

6. Finite element approximations

6.1 Finite element discretizations

A finite element discretization of the optimality system (5.2)–(5.3) is defined in the usual manner. For simplicity we assume the domain Ω is a convex polygon. We first choose families of finite dimensional subspaces $V^h \subset H^1(\Omega)$ satisfying the approximation property: there exists a constant C and an integer k such that

$$\|v - v^h\|_1 \le C h^m \|v\|_{m+1}\,, \quad \forall\, v \in H^{m+1}(\Omega)\,,\ 1 \le m \le k\,. \tag{6.1}$$

One may consult, *e.g.*, [3] or [6] for a catalogue of finite element spaces satisfying (6.1). Then, we may formulate the approximate problem for the optimality system (5.2)–(5.3): seek $\phi^h \in V^h$ and $\lambda^h \in V^h$ such that

$$\begin{aligned} \int_\Omega \sigma \operatorname{grad} \phi^h \cdot \operatorname{grad} \psi^h \, d\Omega + \int_{\Gamma_C} f(\phi^h)\psi^h \, d\Gamma \\ = -\frac{1}{\delta_0} \int_{\Gamma_A} \lambda^h \psi^h \, d\Gamma\,, \quad \forall\, \psi^h \in V^h \end{aligned} \tag{6.2}$$

and

$$\begin{aligned} \int_\Omega \sigma \operatorname{grad} \lambda^h \cdot \operatorname{grad} \omega^h \, d\Omega + \int_{\Gamma_C} f'(\phi^h)\lambda^h \omega^h \, d\Gamma \\ = \frac{1}{\epsilon_0} \int_\Omega (\phi^h - \phi_0)\, \omega^h \, d\Omega\,, \quad \forall\, \omega^h \in V^h\,. \end{aligned} \tag{6.3}$$

6.2 Quotation of Brezzi-Rappaz-Raviart approximation theory

The error estimate to be derived in Sect. 6.3 makes use of results developed by Brezzi et al. (see [5], also [7] and [8]) concerning the approximation of a class of nonlinear problems. Here, for the sake of completeness, we will state the relevant results, specialized to our needs.

The nonlinear problems considered in [5] (also [7] and [8]) are of the type

$$F(\psi) \equiv \psi + TG(\psi) = 0 \tag{6.4}$$

where X and Y are Banach spaces and $T \in \mathscr{L}(Y; X)$, G is a C^2 mapping from X into Y. A solution ψ to the equation $F(\psi) = 0$ is called a *nonsingular solution* if we have that $F'(\psi)$ is an isomorphism from X into X. (Here, $F'(\cdot)$ denotes the Frechet derivative of $F(\cdot)$.)

Approximations are defined by introducing a family of finite dimensional subspaces $X^h \subset X$ and for each $h > 0$ an approximating operator $T^h \in \mathscr{L}(Y;X^h)$. Then, we seek $\psi^h \in X^h$ such that

$$F^h(\psi^h) \equiv \psi^h + T^h G(\psi^h) = 0\,. \tag{6.5}$$

We will assume that there exists another Banach space Z, contained in Y, with continuous imbedding, such that

$$G'(\psi) \in \mathscr{L}(X;Z) \quad \forall\, \psi \in X\,. \tag{6.6}$$

Concerning the operator T^h, we assume the approximation properties

$$\lim_{h\to 0} \|(T^h - T)y\|_X = 0 \quad \forall\, y \in Y \tag{6.7}$$

and

$$\lim_{h\to 0} \|(T^h - T)\|_{\mathscr{L}(Z;X)} = 0\,. \tag{6.8}$$

Note that (6.6) and (6.8) imply that the operator $G'(\psi) \in \mathscr{L}(X;X)$ is compact. Morevover, (6.8) follows from (6.7) whenever the imbedding $Z \subset Y$ is compact.

We can now state the first result that will be used in the sequel. In the statement of the theorem, G'' represents the second order Frechet derivative of G.

Theorem 6.1. *Let X and Y be Banach spaces. Assume that G is a second order Frechet differentiable mapping from X into Y and that G'' is bounded on all bounded sets of X. Assume that* (6.6)–(6.8) *hold and that ψ is a nonsingular solution of* (6.4). *Then, there exists a $\delta > 0$ and an $h_0 > 0$ such that for $h \le h_0$, there exists a unique $\psi^h \in X^h$ satisfying ψ^h is a nonsingular solution of* (6.5) *and $\|\psi^h - \psi\|_X \le \delta$. Moreover, there exists a constant $C > 0$, independent of h, such that*

$$\|\psi^h - \psi\|_X \le C\,\|(T^h - T)G(\psi)\|_X\,. \tag{6.9}$$

For the second result, we need to introduce two other Banach spaces H and W, such that $W \subset X \subset H$, with continuous imbeddings, and assume that

(6.10) for all $w \in W$, the operator $G'(w)$ may be extended as a linear operator of $\mathscr{L}(H;Y)$, the mapping $w \to G'(w)$ being continuous from W onto $\mathscr{L}(H;Y)$.

We also suppose that

$$\lim_{h\to 0} \|T^h - T\|_{\mathscr{L}(Y;H)} = 0\,. \tag{6.11}$$

Then we may state the following additional result.

Theorem 6.2. *Assume that the hypotheses of Theorem* 6.1 *hold and that* (6.10) *and* (6.11) *hold. Assume further that*

(6.12) $$F'(\psi) \text{ is an isomorphism of } H\,.$$

Then, for $h \le h_1$ sufficiently small, there exists a constant C, independent of h, such that

(6.13) $$\|\psi^h - \psi\|_H \le C\,\|(T^h - T)G(\psi)\|_H + \|\psi^h - \psi\|_X^2\,. \qquad \square$$

6.3 Error estimates for the approximations of solutions of the optimality system

In order to derive error estimates, we begin by recasting the optimality system (5.2)–(5.3) and its discretization (6.2)–(6.3) into a form that fits into the framework of *Brezzi-Rappaz-Raviart* theory summarized in Sect. 6.2.

We define

$$X = H^1(\Omega) \times H^1(\Omega)\,,$$

$$Y = H^{-1/2}(\Gamma) \times H^1(\Omega)^* \times H^{-1/2}(\Gamma)\,,$$

$$Z = L^2(\Gamma) \times L^2(\Omega) \times L^2(\Gamma)$$

and

$$X^h = V^h \times V^h\,,$$

where $H^1(\Omega)^*$ denotes the dual space of $H^1(\Omega)$. Note that using Sobolev imbedding theorems, $Z \subset Y$ with a compact imbedding.

Let the operator $T \in \mathscr{L}(Y;X)$ be defined in the following manner: $T(\zeta,\eta,\theta) = (\phi,\lambda)$ for $(\zeta,\eta,\theta) \in Y$ and $(\phi,\lambda) \in X$ if and only if

(6.14) $$\int_\Omega \sigma \operatorname{grad} \phi \cdot \operatorname{grad} \psi \, d\Omega + \alpha \int_{\Gamma_C} \phi\psi \, d\Gamma = \langle \zeta, \psi\rangle_\Gamma\,, \quad \forall\, \psi \in H^1(\Omega)$$

and

(6.15) $$\int_\Omega \sigma \operatorname{grad} \lambda \cdot \operatorname{grad} \omega \, d\Omega + \alpha \int_{\Gamma_C} \lambda\,\omega \, d\Gamma = \langle \eta, \omega\rangle + \langle \theta, \omega\rangle_\Gamma\,, \quad \forall\, \omega \in H^1(\Omega)\,.$$

Clearly, (6.14)–(6.15) consists of two *uncoupled* elliptic equations with mixed Robin-Neumann type boundary conditions and T is its solution operator.

Analogously, the operator $T^h \in \mathscr{L}(Y;X^h)$ is defined as follows: $T^h(\zeta,\eta,\theta) = (\phi^h,\lambda^h)$ for $(\zeta,\eta,\theta) \in Y$ and $(\phi^h,\lambda^h) \in X^h$ if and only if

(6.16) $$\int_\Omega \sigma \operatorname{grad} \phi^h \cdot \operatorname{grad} \psi^h \, d\Omega + \alpha \int_{\Gamma_C} \phi^h\psi^h \, d\Gamma = \langle \zeta, \psi^h\rangle_\Gamma\,, \quad \forall\, \psi^h \in V^h$$

and

$$\int_{\Omega} \sigma \operatorname{grad} \lambda^h \cdot \operatorname{grad} \omega^h \, d\Omega + \alpha \int_{\Gamma_{\mathrm{C}}} \lambda^h \omega^h \, d\Gamma = \langle \eta, \omega^h \rangle + \langle \theta, \omega^h \rangle_{\Gamma} , \quad \forall\, \omega^h \in V^h . \tag{6.17}$$

Clearly, (6.16)–(6.17) consists of two discrete Poisson-type equations that are discretizations of the equations (6.14)–(6.15); also, T^h is the solution operator for these two discrete equations.

By the well-known results concerning the approximation of elliptic equations (see, *e.g.*, [3] or [6]), we obtain:

$$\|(T - T^h)(\zeta, \eta, \theta)\|_X \to 0 \quad \text{as } h \to 0 , \tag{6.18}$$

for all $(\zeta, \eta, \theta) \in Y$ and, in addition, if $T(\zeta, \eta, \theta) \in H^{m+1}(\Omega) \times H^{m+1}(\Omega)$, then

$$\|(T - T^h)(\zeta, \eta, \theta)\|_X \le Ch^m \|T(\zeta, \eta, \theta)\|_{H^{m+1}(\Omega) \times H^{m+1}(\Omega)} . \tag{6.19}$$

Also, because $Z \subset Y$ with a compact imbedding, we have that

$$\|(T - T^h)\|_{\mathscr{L}(Z;X)} \to 0 \quad \text{as } h \to 0 . \tag{6.20}$$

Next, we define the *nonlinear* mapping $G : X \to Y$ as follows: $G\big(\phi, \lambda\big) = (\zeta, \eta, \theta)$ for $(\phi, \lambda) \in X$ and $(\zeta, \eta, \theta) \in Y$ if and only if

$$\langle \zeta, \pi \rangle_{\Gamma} = \frac{1}{\delta_0} \int_{\Gamma_{\mathrm{A}}} \lambda \pi \, d\Gamma + \int_{\Gamma_{\mathrm{C}}} (f(\phi) - \alpha\phi)\pi \, d\Gamma \quad \forall\, \pi \in H^{1/2}(\Gamma) , \tag{6.21}$$

$$\langle \eta, \omega \rangle = -\frac{1}{\epsilon_0} \int_{\Omega} (\phi - \phi_0) \, \omega \, d\Omega \quad \forall\, \omega \in H^1(\Omega) \tag{6.22}$$

and

$$\langle \theta, \tau \rangle_{\Gamma} = \int_{\Gamma_{\mathrm{C}}} (f'(\phi) - \alpha)\lambda \, \tau \, d\Gamma \quad \forall\, \tau \in H^{1/2}(\Gamma) . \tag{6.23}$$

(6.21)–(6.23) is equivalent to

$$\zeta = \begin{cases} \frac{1}{\delta_0}\lambda & \text{on } \Gamma_{\mathrm{A}} ; \\ f(\phi) - \alpha\phi & \text{on } \Gamma_{\mathrm{C}} ; \\ 0 & \text{on } \Gamma_0 , \end{cases} \tag{6.24}$$

$$\eta = -\frac{1}{\epsilon_0}(\phi - \phi_0) \quad \text{in } \Omega \tag{6.25}$$

and

$$\theta = \begin{cases} (f'(\phi) - \alpha)\lambda & \text{on } \Gamma_{\mathrm{C}} ; \\ 0 & \text{on } \Gamma_0 \cup \Gamma_{\mathrm{A}} . \end{cases} \tag{6.26}$$

Recall $f(\phi) = C_3(\mathrm{e}^{C_1\phi} - \mathrm{e}^{C_2\phi})$ so that $f'(\phi) = C_3(C_1\mathrm{e}^{C_1\phi} + C_2\mathrm{e}^{C_2\phi})$. Using Lemma 2.1 and trace theorems we infer that if $(\phi, \lambda) \in H^1(\Omega) \times H^1(\Omega)$, then for all

$q > 1$, $\phi|_\Gamma \in L^q(\Gamma)$, $\lambda|_\Gamma \in L^q(\Gamma)$, $f(\phi) \in L^q(\Gamma)$ and $f'(\phi) \in L^q(\Gamma)$. Hence we see that the triplet (ζ, η, θ) defined by (6.24)–(6.26) is indeed in Y, i.e., G is well-defined.

It is easily seen that the optimality system (5.2)–(5.3) is equivalent to

$$(\phi, \lambda) + TG\,(\phi, \lambda) = 0 \tag{6.27}$$

and that the discrete optimality system (6.2)–(6.3) is equivalent to

$$(\phi^h, \lambda^h) + T^h G\left(\phi^h, \lambda^h\right) = 0\,. \tag{6.28}$$

We have thus recast our continuous and discrete optimality problems into a form that enables us to apply the theories of Sect. 6.2. It remains to verify the hypotheses in Theorem 6.1. This will be the task of the next two propositions.

Proposition 6.3. *The operator $G : X \to Y$ defined by* (6.21)–(6.23) *is second order Frechet differentiable. Furthermore,* (6.6) *holds and G'' is bounded on all bounded sets of X.*

Proof. In showing the differentiability of G, the linear terms appearing in the definition of G does not pose any difficulty. Furthermore the nonlinear terms in (6.21) and (6.23) can be dealt with in a similar way. For clarity, we will only analyse the differentiability of the nonlinear term $\tau \mapsto \int_{\Gamma_C} f'(\phi)\lambda\tau\,d\Gamma$. We define a mapping $Q : X \to H^{-1/2}(\Gamma)$ by $\langle Q(\phi,\lambda),\tau\rangle \equiv \int_{\Gamma_C} f'(\phi)\lambda\tau\,d\Gamma$ for all $(\phi,\lambda) \in X$ and $\tau \in H^{1/2}(\Gamma)$. For each given $(\phi,\lambda) \in X$ we have that

$$\begin{aligned}
&\Big\langle Q(\phi+\delta\phi,\lambda+\delta\lambda) - Q(\phi,\lambda),\tau\Big\rangle \\
&\qquad\qquad - \int_{\Gamma_C} f''(\phi)(\delta\phi)\,\lambda\tau\,d\Gamma - \int_{\Gamma_C} f'(\phi)(\delta\lambda)\tau\,d\Gamma \\
&= \int_{\Gamma_C} [f'(\phi+\delta\phi) - f'(\phi) - f''(\phi)(\delta\phi)]\,\lambda\tau\,d\Gamma \\
&\qquad\qquad + \int_{\Gamma_C} [f'(\phi+\delta\phi) - f'(\phi)](\delta\lambda)\tau\,d\Gamma \\
&= \int_{\Gamma_C}\int_0^1 [f''\big((1-t)\phi + t(\phi+\delta\phi)\big) - f''(\phi)]\,dt\,(\delta\phi)\,\lambda\tau\,d\Gamma \\
&\qquad + \int_{\Gamma_C}\int_0^1 f''\big((1-t)\phi + t(\phi+\delta\phi)\big)\,dt\,(\delta\phi)(\delta\lambda)\tau\,d\Gamma \\
&= \int_{\Gamma_C}\int_0^1\int_0^1 t\,f'''\big(s(1-t)\phi + st(\phi+\delta\phi) + (1-s)\phi\big)\,ds\,dt\,|\delta\phi|^2\,\lambda\tau\,d\Gamma \\
&\quad + \int_{\Gamma_C}\int_0^1 f''\big((1-t)\phi + t(\phi+\delta\phi)\big)\,dt\,(\delta\phi)(\delta\lambda)\tau\,d\Gamma \quad \forall\,(\delta\phi,\delta\lambda)\in X.
\end{aligned} \tag{6.29}$$

Note that $f(\phi) = C_3(\mathrm{e}^{C_1\phi} - \mathrm{e}^{-C_2\phi})$, $f'(\phi) = C_3(C_1\mathrm{e}^{C_1\phi} + C_2\mathrm{e}^{-C_2\phi})$, $f''(\phi) = C_3(C_1^2\mathrm{e}^{C_1\phi} - C_2^2\mathrm{e}^{-C_2\phi})$ and $f'''(\phi) = C_3(C_1^3\mathrm{e}^{C_1\phi} + C_2^3\mathrm{e}^{-C_2\phi})$. By Lemma 2.1 we have that for all real number $m > 1$,

$$\|f'(\phi)\|_{L^m(\Gamma_{\mathrm{C}})} \le C \left\{1 + |\Gamma| + \mathrm{e}^{\,m^2C\,\|\phi\|_1^2}\,|\Gamma|\right\}^{\frac{1}{m}} ,$$

$$\|f''(\phi)\|_{L^m(\Gamma_{\mathrm{C}})} \le C \left\{1 + |\Gamma| + \mathrm{e}^{\,m^2C\,\|\phi\|_1^2}\,|\Gamma|\right\}^{\frac{1}{m}}$$

and

$$\|f'''(\phi)\|_{L^m(\Gamma_{\mathrm{C}})} \le C \left\{1 + |\Gamma| + \mathrm{e}^{\,m^2C\,\|\phi\|_1^2}\,|\Gamma|\right\}^{\frac{1}{m}} ,$$

where C is a generic constant independent of ϕ. Trace theorems for $\Omega \subset \mathbb{R}^2$ implies that for all $p > 1$, $q > 1$ and $r > 1$,

$$\|\delta\phi\|_{L^p(\Gamma_{\mathrm{C}})} \le C\,\|\delta\phi\|_1 \quad \forall\ \delta\phi \in H^1(\Omega)\,,$$

$$\|\delta\lambda\|_{L^q(\Gamma_{\mathrm{C}})} \le C\,\|\delta\lambda\|_1 \quad \forall\ \delta\lambda \in H^1(\Omega)$$

and

$$\|\tau\|_{L^r(\Gamma_{\mathrm{C}})} \le C\,\|\tau\|_{1/2,\Gamma} \quad \forall\ \tau \in H^{1/2}(\Gamma)\,.$$

We fix some $m > 1$, $p > 1$, $q > 1$ and $r > 1$ with $\frac{1}{m} + \frac{1}{p} + \frac{1}{q} + \frac{1}{r} = 1$. Then for every $(\delta\phi, \delta\lambda) \in X$ we have that

$$\begin{aligned}
&\int_{\Gamma_{\mathrm{C}}}\int_0^1 f''\big((1-t)\phi + t(\phi+\delta\phi)\big)\,dt\,(\delta\phi)(\delta\lambda)\tau\,d\Gamma \\
&\quad\le \sup_{0\le t\le 1}\|f''\big((1-t)\phi + t(\phi+\delta\phi)\big)\|_{L^m(\Gamma_{\mathrm{C}})}\,\|\delta\phi\|_{L^p(\Gamma_{\mathrm{C}})}\,\|\delta\lambda\|_{L^q(\Gamma_{\mathrm{C}})}\,\|\tau\|_{L^r(\Gamma_{\mathrm{C}})} \\
&\quad\le C\left\{1 + |\Gamma| + \mathrm{e}^{m^2 2C\,\|\phi\|_1^2}\,|\Gamma|\right\}^{\frac{1}{m}}\ \|\delta\phi\|_1\,\|\delta\lambda\|_1\,\|\tau\|_{1/2,\Gamma} \quad \forall\ \tau \in H^{1/2}(\Gamma)\,.
\end{aligned}$$

Similarly, we have that for every $\delta\phi \in H^1(\Omega)$ and every $\tau \in H^{1/2}(\Gamma)$,

$$\begin{aligned}
&\int_{\Gamma_{\mathrm{C}}}\int_0^1\int_0^1 t\,f'''\big(s(1-t)\phi + st(\phi+\delta\phi) + (1-s)\phi\big)\,ds\,dt\,|\delta\phi|^2\,\lambda\tau\,d\Gamma \\
&\quad\le C\left\{1 + |\Gamma| + \mathrm{e}^{m^2 3C\,\|\phi\|_1^2}\,|\Gamma|\right\}^{\frac{1}{m}}\ \|\delta\phi\|_1^2\,\|\lambda\|_1\,\|\tau\|_{1/2,\Gamma}\,.
\end{aligned}$$

Returning to (6.29) we obtain that for all $\tau \in H^{1/2}(\Gamma)$ and $(\delta\phi, \delta\lambda) \in X$,

$$\begin{aligned}
&\Big\langle Q(\phi+\delta\phi, \lambda+\delta\lambda) - Q(\phi,\lambda), \tau\Big\rangle - \int_{\Gamma_{\mathrm{C}}} f''(\phi)(\delta\phi)\,\lambda\tau\,d\Gamma - \int_{\Gamma_{\mathrm{C}}} f'(\phi)(\delta\lambda)\tau\,d\Gamma \\
&\quad\le C\left\{1 + |\Gamma| + \mathrm{e}^{m^2 3C\,\|\phi\|_1^2}\,|\Gamma|\right\}^{\frac{1}{m}}\ \left\{\|\delta\phi\|_1\,\|\delta\lambda\|_1 + \|\delta\phi\|_1^2\,\|\lambda\|_1\right\}\ \|\tau\|_{1/2,\Gamma}\,,
\end{aligned}$$

so that we conclude Q as a mapping from X to $H^{-1/2}(\Gamma)$ is Frechet differentiable and its derivative $Q'(\phi,\lambda)$ is given by

$$\left\langle Q'(\phi,\lambda)(\tilde{\psi},\tilde{\omega}),\tau\right\rangle = \int_{\Gamma_C} [f''(\phi)\tilde{\psi}\lambda\tau + f'(\phi)\tilde{\omega}\tau]\,d\Gamma \quad \forall\,\tau\in H^{1/2}(\Gamma)\,.$$

Hence, taking into account the remarks in the beginning of the proof, we have justified that G is Frechet differentiable and its Frechet derivative $G'(\phi,\lambda)$ is defined as follows. For each $(\phi,\lambda)\in X$, $G'\big(\phi,\lambda\big)(\tilde{\psi},\tilde{\omega}) = (\tilde{\zeta},\tilde{\eta},\tilde{\theta})$ for $(\tilde{\psi},\tilde{\omega})\in X$ and $(\tilde{\zeta},\tilde{\eta},\tilde{\theta})\in Y$ if and only if

$$\langle\tilde{\zeta},\pi\rangle_\Gamma = \frac{1}{\delta_0}\int_{\Gamma_A}\tilde{\omega}\,\pi\,d\Gamma + \int_{\Gamma_C}(f'(\phi)\tilde{\psi}-\alpha\tilde{\psi})\pi\,d\Gamma \quad \forall\,\pi\in H^{1/2}(\Gamma)\,, \tag{6.30}$$

$$\langle\tilde{\eta},\omega\rangle = -\frac{1}{\epsilon_0}\int_\Omega\tilde{\psi}\,\omega\,d\Omega \quad \forall\,\omega\in H^1(\Omega) \tag{6.31}$$

and

$$\langle\tilde{\theta},\tau\rangle_\Gamma = \int_{\Gamma_C} f''(\phi)\tilde{\psi}\lambda\,\tau\,d\Gamma + \int_{\Gamma_C}(f'(\phi)-\alpha)\,\tilde{\omega}\,\tau\,d\Gamma \quad \forall\,\tau\in H^{1/2}(\Gamma)\,; \tag{6.32}$$

or, equivalently,

$$\tilde{\zeta} = \begin{cases} \frac{1}{\delta_0}\tilde{\omega} & \text{on } \Gamma_A\,;\\ f'(\phi)\tilde{\psi}-\alpha\tilde{\psi} & \text{on } \Gamma_C\,;\\ 0 & \text{on } \Gamma_0\,, \end{cases} \tag{6.33}$$

$$\tilde{\eta} = -\frac{1}{\epsilon_0}\tilde{\psi} \quad \text{in } \Omega \tag{6.34}$$

and

$$\tilde{\theta} = \begin{cases} f''(\phi)\lambda\tilde{\psi} + (f'(\phi)-\alpha)\tilde{\omega} & \text{on } \Gamma_C\,;\\ 0 & \text{on } \Gamma_0\cup\Gamma_A\,. \end{cases} \tag{6.35}$$

(These defining equations can be formally derived by differentiating (6.21)–(6.23).) It is easy to verify from the above equations that for each $(\tilde{\psi},\tilde{\omega})\in X$, we have $(\tilde{\zeta},\tilde{\eta},\tilde{\theta})\in Z$, i.e., $G'\big(\phi,\lambda\big)$ maps X into Z; furthermore, using trace theorems and Lemma 2.1 we obtain that

$$\begin{aligned} \|\tilde{\zeta}\|_{0,\Gamma} &\le \frac{1}{\delta_0}\|\tilde{\omega}\|_{0,\Gamma} + \|f'(\phi)\|_{L^4(\Gamma_C)}\,\|\tilde{\psi}\|_{L^4(\Gamma)} + \alpha\|\tilde{\psi}\|_{0,\Gamma}\\ &\le \frac{C}{\delta_0}\|\tilde{\omega}\|_1 + C\left\{1+|\Gamma| + \mathrm{e}^{C\|\phi\|_1^2}\,|\Gamma|\right\}^{1/4}\|\tilde{\psi}\|_1 + C\,\|\tilde{\psi}\|_1\,, \end{aligned}$$

$$\|\tilde{\eta}\|_0 \le \frac{1}{\epsilon}\|\tilde{\psi}\|_1$$

and

$$\|\tilde{\zeta}\|_{0,\Gamma} \le \|f''(\phi)\|_{L^6(\Gamma_C)} \|\tilde{\psi}\|_{L^6(\Gamma)} \|\lambda\|_{L^6(\Gamma)} + \|f'(\phi)\|_{L^4(\Gamma_C)} \|\tilde{\omega}\|_{L^4(\Gamma)} + \alpha\|\tilde{\omega}\|_{0,\Gamma}$$
$$\le C\left\{1 + |\Gamma| + e^{C\|\phi\|_1^2}|\Gamma|\right\}^{1/4} \{\|\tilde{\psi}\|_1 \|\lambda\|_1 + \|\tilde{\omega}\|_1\} + C\|\tilde{\omega}\|_1 .$$

Thus $G'\big(\phi,\lambda\big) \in \mathscr{L}(X;Z)$, i.e., we have shown that (6.6) hold.

To show the second order differentiability of G, again for clarity we will examine only one nonlinear term appearing in the definition of G', e.g., the term $\tau \mapsto \int_{\Gamma_C} f''(\phi)\tilde{\psi}\lambda\tau\, d\Gamma$. We define a mapping $R : X \to \mathscr{L}(X;H^{-1/2}(\Gamma))$ by $\big\langle R(\phi,\lambda)(\tilde{\psi},\tilde{\omega}),\tau\big\rangle \equiv \int_{\Gamma_C} f''(\phi)\tilde{\psi}\lambda\tau\, d\Gamma$ for all (ϕ,λ), $(\tilde{\psi},\tilde{\omega}) \in X$ and $\tau \in H^{1/2}(\Gamma)$. For each given $(\phi,\lambda) \in X$ we have that for all $(\delta\phi,\delta\lambda) \in X$,

$$\begin{aligned}
&\Big\langle [R(\phi+\delta\phi,\lambda+\delta\lambda) - R(\phi,\lambda)](\tilde{\psi},\tilde{\omega}),\tau\Big\rangle \\
&\qquad - \int_{\Gamma_C} f'''(\phi)(\delta\phi)\tilde{\psi}\,\lambda\tau\, d\Gamma - \int_{\Gamma_C} f''(\phi)\tilde{\psi}(\delta\lambda)\tau\, d\Gamma \\
&= \int_{\Gamma_C} [f''(\phi+\delta\phi) - f''(\phi) - f'''(\phi)(\delta\phi)]\tilde{\psi}\,\lambda\tau\, d\Gamma \\
&\qquad + \int_{\Gamma_C} [f''(\phi+\delta\phi) - f''(\phi)]\tilde{\psi}(\delta\lambda)\tau\, d\Gamma \\
&= \int_{\Gamma_C}\int_0^1\int_0^1 t\, f''''(s(1-t)\phi + st(\phi+\delta\phi) + (1-s)\phi)\, ds\, dt\, \tilde{\psi}|\delta\phi|^2\,\lambda\tau\, d\Gamma \\
&\qquad + \int_{\Gamma_C}\int_0^1 f'''((1-t)\phi + t(\phi+\delta\phi))\, dt\, (\delta\phi)(\delta\lambda)\tilde{\psi}\tau\, d\Gamma .
\end{aligned}$$

Thus similar to the analysis ensuing (6.29), we can show that the operator R is Frechet differentiable and its derivative $R'(\phi,\lambda)$ is defined by:

$$R'(\phi,\lambda)\cdot\big((\tilde{\psi},\tilde{\omega}),(\tilde{\tilde{\psi}},\tilde{\tilde{\omega}})\big) = \int_{\Gamma_C} f'''(\phi)\,\tilde{\tilde{\phi}}\,\tilde{\psi}\,\lambda\,\tau\, d\Gamma + \int_{\Gamma_C} f''(\phi)\,\tilde{\psi}\,\tilde{\tilde{\lambda}}\,\tau\, d\Gamma .$$

Hence, G is second order Frechet differentiable and $G''(\phi,\lambda)$ is defined as follows. For each $(\phi,\lambda) \in X$, $G''(\phi,\lambda)\cdot\big((\tilde{\psi},\tilde{\omega}),(\tilde{\tilde{\psi}},\tilde{\tilde{\omega}})\big) = (\tilde{\zeta},\tilde{\eta},\tilde{\theta})$ for $\big((\tilde{\psi},\tilde{\omega}),(\tilde{\tilde{\psi}},\tilde{\tilde{\omega}})\big) \in X \times X$ and $(\tilde{\zeta},\tilde{\eta},\tilde{\theta}) \in Y$ if and only if

$$\langle\tilde{\zeta},\pi\rangle_\Gamma = \int_{\Gamma_C} f''(\phi)\,\tilde{\tilde{\psi}}\,\tilde{\psi}\,\pi\, d\Gamma \quad \forall\, \pi \in H^{1/2}(\Gamma)\,,$$

$$\langle\tilde{\eta},\omega\rangle = 0 \quad \forall\, \omega \in H_0^1(\Omega)$$

and

$$\langle\tilde{\theta},\tau\rangle_\Gamma = \int_{\Gamma_C} [f'''(\phi)\,\tilde{\tilde{\psi}}\,\tilde{\psi}\,\lambda + f''(\phi)\,\tilde{\psi}\,\tilde{\tilde{\lambda}}]\,\tau\, d\Gamma + \int_{\Gamma_C} f''(\phi)\,\tilde{\tilde{\psi}}\,\tilde{\omega}\,\tau\, d\Gamma$$
$$\forall\, \tau \in H^{1/2}(\Gamma)\,;$$

or, equivalently,

$$\tilde{\zeta} = \begin{cases} 0 & \text{on } \Gamma_A\,; \\ f''(\phi)\tilde{\tilde{\psi}}\,\tilde{\psi} & \text{on } \Gamma_C\,; \\ 0 & \text{on } \Gamma_0\,, \end{cases} \tag{6.36}$$

$$\tilde{\eta} = 0 \quad \text{in } \Omega \tag{6.37}$$

and

$$\tilde{\theta} = \begin{cases} [f'''(\phi)\tilde{\tilde{\psi}}\,\tilde{\psi}\,\lambda + f''(\phi)\tilde{\psi}\,\tilde{\tilde{\lambda}}] + f''(\phi)\tilde{\tilde{\psi}}\,\tilde{\omega} & \text{on } \Gamma_C\,; \\ 0 & \text{on } \Gamma_0 \cup \Gamma_A\,. \end{cases} \tag{6.38}$$

Furthermore, using Lemma 2.1, (6.36)–(6.38) and trace theorems, we may derive a bound for $G''(\phi,\lambda)$ for each given (ϕ,λ):

$$||G''(\phi,\lambda)||_Y \le C\left\{1 + |\Gamma| + e^{C\|\phi\|_1^2}\,|\Gamma|\right\}(1 + \|\lambda\|_1)$$

for some constant C, so that G'' is bounded on every bounded subset of X. □

A solution (ϕ,λ) of the problem (5.2)–(5.3), or equivalently, of (6.27), is nonsingular if the *linear system*

$$\int_\Omega \sigma \operatorname{grad}\tilde{\phi}\cdot\operatorname{grad}\psi\,d\Omega + \int_{\Gamma_C} f'(\phi)\tilde{\phi}\psi\,d\Gamma + \frac{1}{\delta_0}\int_{\Gamma_A}\tilde{\lambda}\psi\,d\Gamma = \langle\tilde{\zeta},\psi\rangle \quad \forall\,\psi\in H^1(\Omega) \tag{6.39}$$

and

$$\int_\Omega \sigma \operatorname{grad}\tilde{\lambda}\cdot\operatorname{grad}\omega\,d\Omega + \int_{\Gamma_C} f''(\phi)\,\tilde{\phi}\,\lambda\,\omega\,d\Gamma + \int_{\Gamma_C} f'(\phi)\,\tilde{\lambda}\,\omega\,d\Gamma - \frac{1}{\epsilon_0}\int_\Omega\tilde{\phi}\,\omega\,d\Omega = \langle\tilde{\eta},\omega\rangle \quad \forall\,\omega\in H^1(\Omega) \tag{6.40}$$

has a unique solution $(\tilde{\phi},\tilde{\lambda})\in X$ for every $\tilde{\zeta},\tilde{\eta}\in H^1(\Omega)^*$.

An analogous definition holds for nonsingular solutions of the discrete optimality system (6.2)–(6.3), or equivalently, (6.28).

It is evident that (6.39)–(6.40) has a unique solution for large enough σ, e.g.,

$$\sigma > \max\left\{\frac{C}{\delta_0},\ \frac{C}{\epsilon_0},\ C\,\|\lambda\|_{L^4(\Gamma_C)}\,\|f''(\phi)\|_{L^4(\Gamma_C)}\right\}.$$

It is reasonable to assume that (6.39)–(6.40) has a unique solution generically with respect to σ, i.e., the optimal solutions are almost always nonsingular. Thus Theorem 6.1 and Proposition 6.3 lead to the following:

Theorem 6.4. *Assume* (ϕ, λ) *is a nonsingular solution of the optimality system* (5.2)–(5.3). *Assume that the finite element spaces* V^h *satisfy the condition* (6.1). *Then, there exists a* $\delta > 0$ *and* $h_0 > 0$ *such that for* $h \leq h_0$, *there exists a unique nonsingular solution* (ϕ^h, λ^h) *of the discrete optimality system* (6.2)–(6.3) *satisfying* $\|\phi^h - \phi\|_1 + \|\lambda^h - \lambda\|_1 \leq \delta$. *Moreover,*

$$\|\phi^h - \phi\|_1 + \|\lambda^h - \lambda\|_1 \to 0 \quad \textit{as } h \to 0\,. \tag{6.41}$$

If, in addition, the solution of the optimality system satisfies $(\phi, \lambda) \in H^{m+1}(\Omega) \times H^{m+1}(\Omega)$, *then there exists a constant* C, *independent of* h, *such that*

$$\|\phi - \phi^h\|_1 + \|\lambda - \lambda^h\|_1 \leq C h^m \left(\|\phi\|_{m+1} + \|\lambda\|_{m+1}\right). \tag{6.42}$$

A consequence of Theorems 6.4 is the following corollary that gives error estimates for the approximation of the controls.

Corollary 6.5. *Assume* (ϕ, λ) *is a nonsingular solution of the optimality system* (5.2)–(5.3). *Assume that the finite element spaces* V^h *satisfy the condition* (6.1). *Define the approximate control by*

$$u^h = -\frac{1}{\delta_0}\lambda^h \quad \text{on } \Gamma_{\mathrm{A}}\,.$$

Then

$$\|u^h - u\|_{1/2,\Gamma_{\mathrm{A}}} \to 0 \quad \text{as } h \to 0\,. \tag{6.43}$$

If, in addition, the solution of the optimality system satisfies $(\phi, \lambda) \in H^{m+1}(\Omega) \times H^{m+1}(\Omega)$, *then there exists a constant* C, *independent of* h, *such that for* $h \leq h_0$,

$$\|u^h - u\|_{1/2,\Gamma_{\mathrm{A}}} \leq \frac{C}{\delta_0} h^m \left(\|\phi\|_{m+1} + \|\lambda\|_{m+1}\right). \tag{6.44}$$

Proof. Recall that $u = -\frac{1}{\delta_0}\lambda$ on Γ_{A}; see (5.1). Then (6.43) and (6.44) follow trivially from (6.41)–(6.42) and the inequalities (see [1])

$$\|u - u^h\|_{1/2,\Gamma_{\mathrm{A}}} = \frac{1}{\delta_0}\|\lambda - \lambda^h\|_{1/2,\Gamma_{\mathrm{C}}} \leq \frac{1}{\delta_0}\|\lambda - \lambda^h\|_{1/2,\Gamma} \leq \frac{C}{\delta_0}\|\lambda - \lambda^h\|_1\,. \qquad \square$$

Now we wish to apply Theorem 6.2 to derive $L^2(\Gamma_{\mathrm{C}})$-error estimates for the approximations of u. To this end, we assume the domain Ω is convex and for each given $\epsilon \in (0, 1/4)$, we introduce spaces

$$H = H^{1/2+\epsilon}(\Omega) \times H^{1/2+\epsilon}(\Omega) \qquad \text{and} \qquad W = H^{3/2+\epsilon}(\Omega) \times H^{3/2+\epsilon}(\Omega)\,.$$

Note that $X \subset H$ with a compact imbedding so that (6.18) implies

$$\|(T - T^h)\|_{\mathscr{L}(Y;H)} \to 0 \quad \text{as } h \to 0\,.$$

Again using finite element approximation results in [6] we have that if Ω is convex and $T(\zeta,\eta,\theta) \in H^{m+1}(\Omega) \times H^{m+1}(\Omega)$, then

$$\|(T - T^h)(\zeta,\eta,\theta)\|_H \le Ch^{m-\epsilon+1/2} \|T(\zeta,\eta,\theta)\|_{H^{m+1}(\Omega)\times H^{m+1}(\Omega)} \,.$$

Proposition 6.6. *For each* $(\phi,\lambda) \in W$, *the operator* $G'(\phi,\lambda) : X \to Y$ *defined by* (6.33)–(6.35) *can be extended as a linear operator of* $\mathscr{L}(H;Y)$. *Furthermore, the mapping* $w \to G'(w)$ *is continuous from* W *onto* $\mathscr{L}(H;Y)$.

Proof. Note that $W \subset L^\infty(\Omega) \times L^\infty(\Omega)$ and $H^{1/2+\epsilon}(\Omega)|_\Gamma \subset L^2(\Gamma)$ with continuous imbeddings. For each $(\phi,\lambda) \in W$, we can easily verify from (6.33)–(6.35) that

$$\begin{aligned} &\|G'(\phi,\lambda)(\tilde\psi,\tilde\omega)\|_Y \\ &\quad \le A(\phi)\,\{\|\tilde\omega\|_{0,\Gamma_{\rm A}} + \|\tilde\psi\|_{0,\Gamma_{\rm C}} + \|\tilde\psi\|_0 + \|\tilde\omega\|_{0,\Gamma_{\rm C}}\} \\ &\quad \le C_T\, A(\phi)\,\{\|\tilde\omega\|_{1/2+\epsilon} + \|\tilde\psi\|_{1/2+\epsilon}\} \quad \forall\, (\tilde\psi,\tilde\omega) \in H \,, \end{aligned}$$

where

$$A(\phi) = C \max\left\{ \frac{1}{\delta_0},\ \frac{1}{\epsilon_0},\ \max_{|\mathbf{x}|\le\|\phi\|_{3/2+\epsilon}} (|f'(\mathbf{x})| + \alpha),\ \max_{|\mathbf{x}|\le\|\phi\|_{3/2+\epsilon}} (|f''(\mathbf{x})|\, \|\lambda\|_{3/2+\epsilon}) \right\}$$

and C_T is a constant such that $\|\psi\|_{0,\Gamma} \le C_T \|\psi\|_{1/2+\epsilon}$ for all $\psi \in H^{1/2+\epsilon}(\Omega)$. The desired results follow easily from this estimate. □

If (ϕ,λ) is a nonsingular solution of (5.2)–(5.3), using the denseness of $H^1(\Omega)$ in $H^{1/2+\epsilon}(\Omega)$ and regularity theories for (6.39)–(6.40), we infer that (6.12) holds.

Thus we have verified all the requirements in Theorem 6.2 so that we can draw the following conclusion:

Theorem 6.7. *Assume* Ω *is convex and* (ϕ,λ) *is a nonsingular solution of the optimality system* (5.2)–(5.3). *Assume that the finite element spaces* V^h *satisfy the condition* (6.1). *Then, there exists a* $\delta > 0$ *and* $h_0 > 0$ *such that for* $h \le h_0$, *there exists a unique nonsigular solution* (ϕ^h,λ^h) *of the discrete optimality system* (6.2)–(6.3) *satisfying* $\|\phi^h - \phi\|_1 + \|\lambda^h - \lambda\|_1 \le \delta$. *If, in addition, the solution of the optimality system satisfies* $(\phi,\lambda) \in H^{m+1}(\Omega) \times H^{m+1}(\Omega)$, *then there exists a constant* C, *independent of* h, *such that*

$$\|\phi - \phi^h\|_{\epsilon+1/2} + \|\lambda - \lambda^h\|_{\epsilon+1/2} \le Ch^{m-\epsilon+1/2}\left(\|\phi\|_{m+1} + \|\lambda\|_{m+1}\right) . \tag{6.45}$$

A consequence of Theorem 6.7 is the following corollary that gives the $L^2(\Gamma_{\rm A})$-error estimates for the the approximation of the controls.

Corollary 6.8. *Assume* Ω *is convex and* (ϕ,λ) *is a nonsingular solution of the optimality system* (5.2)–(5.3). *Assume that the finite element spaces* V^h *satisfy the condition* (6.1). *Define the approximate control by*

$$u^h = -\frac{1}{\delta_0}\lambda^h \quad \text{on } \Gamma_{\mathrm{A}}\,.$$

If the solution of the optimality system satisfies $(\phi, \lambda) \in H^{m+1}(\Omega) \times H^{m+1}(\Omega)$, *then for each* $\epsilon \in (0, 1/4)$ *there exists a constant* C*, independent of* h*, such that for* $h \le h_0$,

$$\|u^h - u\|_{0,\Gamma_{\mathrm{A}}} \le \frac{C}{\delta_0} h^{m-\epsilon+1/2}\big(\|\phi\|_{m+1} + \|\lambda\|_{m+1}\big)\,. \tag{6.46}$$

Proof. Recall that $u = -\frac{1}{\delta_0}\lambda$ on Γ_{A}; see (5.1). Then (6.46) follows trivially from (6.45) and the trace theorems (see [1])

$$\|u - u^h\|_{0,\Gamma_{\mathrm{A}}} = \frac{1}{\delta_0}\|\lambda - \lambda^h\|_{0,\Gamma_{\mathrm{C}}} \le \frac{1}{\delta_0}\|\lambda - \lambda^h\|_{0,\Gamma} \le \frac{C}{\delta_0}\|\lambda - \lambda^h\|_{\epsilon+1/2}\,. \qquad \square$$

Acknowledgements. The authors thank Dr. W. Sun for useful discussions related to this article. The authors also thank anonymous referees for their many useful comments that simplified and improved the proofs of several results; in particular, the current proof of Theorem 2.2 is suggested by an anonymous referee.

References

1. Adams, R. (1975): Sobolev Spaces. Academic Press, New York
2. Amaya, K., Aoki, S. (1992): Optimum design of cathodic protection system by 3-D BEM. Boundary Element Technology **VII**, 375–388
3. Babuška, I., Aziz, A. (1972): Survey lectures on the mathematical foundations of the finite element method. In: Aziz, A. (ed.) The Mathematical Foundations of the Finite Element Method with Applications to Partial Differential Equations. Academic, New York
4. Bockris, J.O.M., Reddy, A.K.M. (1974): Modern Electrochemistry. Plenum Press, New York
5. Brezzi, F., Rappaz, J., Raviart, P.-A. (1980): Finite-dimensional approximation of nonlinear problems. Part I: Branches of nonsingular solutions. Numer. Math. **36**, 1
6. Ciarlet, P. (1978): The Finite Element Method for Elliptic Problems. North-Holland, Amsterdam
7. Crouzeix, M., Rappaz, J. (1989): On Numerical Approximation in Bifurcation Theory. Masson, Paris
8. Girault, V., Raviart, P.-A. (1986): Finite Element Methods for Navier-Stokes Equations. Springer, Berlin
9. Gossez, J.P. (1974): Nonlinear elliptic boundary value problems for equations with rapidly or slowly increasing coefficients. Trans. Amer. Math. Soc. **190**, 163–205
10. Grisvard, P. (1966): Commutativité de deux foncteurs d'interpolation et applications. J. Math. Pures Appl. **45**, 143–290
11. Grisvard, P. (1985): Elliptic Problems on Nonsmooth Domains. Pitman, Boston
12. Hess, P. (1973): A strongly nonlinear elliptic boundary value problem. J. Math. Anal. Appl. **43**, 241–249
13. Hess, P. (1973): On nonlinear mappings of monotone type with respect to two Banach spaces. J. Math. Pures Appl. **52**, 13–26
14. Hou, L.S., Sun, W. (1994): Numerical methods for optimal control of impressed cathodic protection systems. Int. J. Numer. Meth. Engrg. **37**, 2779–2796
15. Hou, L.S., Sun, W.: Optimal positioning of anodes for cathodic protection. To appear
16. Kačur, J. (1973): On boundedness of the weak solution for some class of quasilinear partial differential equations. Čas. Pěst. Mat. **98**, 43–55

17. J. Nečas, (1967): Les Méthodes Directes en Théorie des Équations Elliptiques. Academia, Prague
18. Peetre, J. (1966): Espaces d'interpolation et théorème de Soboleff. Ann. Inst. Fourier (Grenoble **16**), 279–317
19. Tikhomorov, V. (1982): Fundamental Principles of the Theory of Extremal Problems. Wiley, Chichester
20. Zamani. N.G., Chuang, J.M. (1987): Optimal control of current in a cathodic protection system: a numerical investigation. Optimal Control Appl. & Meth. **8**, 339–350
21. Zamani, N.G., Porter, J.F., Mufti, A.A. (1986): A survey of computational efforts in the field of corrosion engineering. Int. J. Numer. Meth. Eng. **23**, 1295–1311