PARAMETRIC SENSITIVITY ANALYSIS IN OPTIMAL CONTROL OF A REACTION DIFFUSION SYSTEM—PART I: SOLUTION DIFFERENTIABILITY

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Abstract. In this paper we consider a control-constrained optimal control problem governed by a system of semilinear parabolic reaction-diffusion equations. The optimal solutions are subject to perturbations of the dynamics and of the objective. We prove that local optimal solutions, as a function of the perturbation parameter, are Lipschitz continuous and directionally differentiable. We characterize the directional derivatives, also known as parametric sensitivities, as the solutions of auxiliary quadratic programming problems, i.e., linear-quadratic optimal control problems. Parametric sensitivities provide valuable information, e.g., in realtime optimal control environments.

Key words. optimal control, reaction-diffusion equations, control constraints, parameter perturbation, parametric sensitivity, generalized equation

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1. Introduction. Parametric sensitivity analysis for optimal control problems governed by partial differential equations (PDE) is concerned with the behavior of optimal solutions under perturbations of system data.

As an example, we consider the following reaction-diffusion optimal control problem: Let Ω denote a bounded domain in $\mathbb{R}^2$. For a finite terminal time $T > 0$, let Q be the time-space cylinder $\Omega \times (0,T)$ and let Σ be its lateral boundary $\partial\Omega \times (0,T)$.

Denoting by y_1 and y_2 the concentrations of two substances C_1 and C_2 involved in a reaction which obeys the law of mass action, and assuming a reaction of type $C_1 + C_2 \to C_3$ with the reverse direction neglected, we have the following reaction-diffusion system:

$$\frac{\partial y_1}{\partial t} = D_1 \Delta y_1 - k_1 y_1 y_2 \qquad \frac{\partial y_2}{\partial t} = D_2 \Delta y_2 - k_2 y_1 y_2 + u \quad \text{on } Q. \tag{1.1}$$

Here, D_i and k_i denote diffusion and reaction coefficients, respectively, and u is a distributed control function. In addition, we assume no-outflow conditions along the boundary of the domain

$$D_1 \frac{\partial y_1}{\partial n} = 0 \qquad D_2 \frac{\partial y_2}{\partial n} = 0 \quad \text{on } \Sigma \tag{1.2}$$

and prescribe some initial distribution of the concentrations:

$$y_1(\cdot,0) = y_{10} \qquad y_2(\cdot,0) = y_{20} \quad \text{on } \Omega. \tag{1.3}$$

We aim to minimize the distance of the terminal concentration to a desired one. Taking the control cost as a regularization term into account, our objective is

$$f(y,u) = \frac{\alpha_1}{2}\|y_1(\cdot,T) - y_{1T}\|^2_{\mathbb{L}^2(\Omega)} + \frac{\alpha_2}{2}\|y_2(\cdot,T) - y_{2T}\|^2_{\mathbb{L}^2(\Omega)} + \frac{\gamma}{2}\|u\|^2_{\mathbb{L}^2(Q)}. \tag{1.4}$$

We also impose control constraints

$$u_a \le u \le u_b \quad \text{a.e. on } Q, \tag{1.5}$$

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hence the optimal control problem under consideration is to

$$\text{Minimize (1.4) subject to (1.1)–(1.3) and (1.5).} \qquad (\text{RD}(p))$$

We allow for very general finite- or infinite-dimensional perturbations p of the system data, including perturbations of reaction and diffusion coefficients D_i and k_i, of parameters in the objective α_i and γ, and of initial concentrations y_{i0} as well as desired terminal states y_{iT}. All these perturbations can be summarized in a vector p. Given a nominal (unperturbed) value p_0, we answer the following questions:

(Q1) Under which conditions does there exist an implicitly defined (Lipschitz) continuous map $p \mapsto (\Sigma(p), \Xi(p), \Lambda(p))$ near p_0 (where Σ and Ξ denote the state and control, respectively, and Λ refers to the adjoint variable) such that $(\Sigma(p), \Xi(p), \Lambda(p))$ satisfies the first order necessary conditions of the perturbed problem (RD(p))?

(Q2) Under which conditions is the map $p \mapsto (\Sigma(p), \Xi(p), \Lambda(p))$ directionally differentiable at p_0?

(Q3) Given a direction $\overline{p}$, How can the directional derivative $D(\Sigma, \Xi, \Lambda)(p_0; \overline{p})$ be evaluated?

(Q4) Under which conditions is $(\Sigma(p), \Xi(p))$ not only a critical point but in fact a local optimal solution for all p near p_0?

Questions (Q1)–(Q4) address the stability of optimal solutions and thus the well-posedness of the optimal control problem (RD(p)). The directional derivative $D(\Sigma, \Xi, \Lambda)(p_0; \overline{p})$, also called the *parametric sensitivity derivative* or simply *parametric sensitivity*, is of particular interest in realtime applications, when the perturbation of system data $\overline{p}$ is known or can be measured or estimated: Having computed the parametric sensitivities beforehand (offline), a first order correction of the nominal solution is available at almost no numerical cost, using the Taylor formula

$$\Sigma(p_0 + \overline{p}) \approx \Sigma(p_0) + D\Sigma(p_0; \overline{p}) \tag{1.6}$$

and its analogues for the control and adjoint components.

The remainder of this paper is organized as follows: In Section 2, the optimal control problem (RD(p)) is restated in appropriate function spaces, and we prove some fundamental results about the state equation and the control problem.

The discussion of Lipschitz continuity of solutions $(\Sigma(p), \Xi(p), \Lambda(p))$ with respect to the parameter is based on the notion of strong regularity of the first order necessary (KKT) conditions for (RD(p)), as introduced in the pioneering work of Robinson [21]. The verification of strong regularity requires to establish that the solution of an auxiliary linear-quadratic control problem (AQP(δ)) depends Lipschitz-continuously on certain perturbations, which is confirmed in Section 3, Theorem 3.2. The proof makes use of a coercivity assumption (AC) for the Hessian of the Lagrangian, which in turn implies second order sufficiency, both for the nominal and perturbed problems. By Robinson's implicit function theorem, (Σ, Ξ, Λ) inherits the Lipschitz continuity from the solutions to the linear-quadratic auxiliary optimal control problems (AQP(δ)), Theorem 3.3.
Interestingly, strong regularity of the KKT conditions has other implications: It assures the well-posedness and convergence of the generalized Newton's method [1] and it is a prequisite in proving convergence of the discretized solution to the continuous solution as the mesh size tends to zero [16].

Section 4 covers the proof of directional differentiability. Using an extension to Robinson's implicit function theorem due to Dontchev [8], it is sufficient to prove that the solutions of the auxiliary problem (AQP(δ)) are directionally differentiable. This result is achieved in the main Theorem 4.1, and the derivative is characterized as the solution to yet another auxiliary linear-quadratic optimal control problem (DQP($\hat{\delta}$)).

In Section 5 we provide first and second order derivatives of the minimum value function which may be used for a second order prediction of the perturbed solution's objective value. As a by-product of our analysis, we obtain the marginal interpretation of the adjoint variable, i.e., that the adjoint variable gives the first order change in the value of the objective with respect to perturbations of the current state.

Tröltzsch [22] has proved the analogue of Theorem 3.2 for a linear-quadratic optimal control problem involving a scalar parabolic PDE, as opposed to a *system of PDEs*, and with respect to $\mathbb{L}^2$ and $\mathbb{L}^\infty$ norms. Malanowski and Tröltzsch [17] have extended this result to obtain $\mathbb{L}^\infty$-Lipschitz stability of solutions to optimal control problems with control constraints governed by a semilinear parabolic equation. Recently, Malanowski [15] has proved Bouligand differentiability of solutions for a class of semilinear parabolic equations. The present paper distinguishes itself from the latter one in that higher regularity of the state space is used here to overcome the well-known two-norm discrepancy issue relevant for the coercivity estimates [18]. This approach is useful not only for multiplicative nonlinearities as in the reaction-diffusion example, but for the broad class of nonlinearities which are differentiable with respect to the norm of $H^{2,1}(Q)$.

In the sequel, we shall frequently use the abbreviation $x = (y, u)$ for state/control pairs. Among the equivalent norms on a product space $X_1 \times X_2$, we use $\|(x_1, x_2)\|^2 = \|x_1\|^2 + \|x_2\|^2$. When no ambiguity arises, we write $\|x\|$ instead of $\|x\|_X$. Throughout the paper, c and $\tilde{c}$ denote positve constants, possibly with different meanings in different locations.

2. The Optimal Control Problem. We begin by defining appropriate function spaces for the optimal control problem (RD(p)): For the control component, we choose the usual $U = \mathbb{L}^2(Q)$ and let U_{ad} be the closed convex subset of admissible controls

$$U_{\text{ad}} = \{u \in \mathbb{L}^2(Q) : u_a(x,t) \le u(x,t) \le u_b(x,t) \text{ a.e. on } Q\} \subset \mathbb{L}^\infty(Q) \qquad (2.1)$$

with bounds $u_a \le u_b$ in $\mathbb{L}^\infty(Q)$. For the state space, we choose the anisotropic Sobolev space

$$Y = H^{2,1}(Q) = \{y \in \mathbb{L}^2(0,T;H^2(\Omega)) : y_t \in \mathbb{L}^2(0,T;\mathbb{L}^2(\Omega))\} \qquad (2.2)$$

which is a Hilbert space ([14], Chapter 4, Section 2.1) when endowed with the usual inner product which induces the norm

$$\|y\|_{H^{2,1}(Q)} = \left(\|y\|_{\mathbb{L}^2(0,T;H^2(\Omega))} + \|y_t\|_{\mathbb{L}^2(0,T;\mathbb{L}^2(\Omega))}\right)^{\frac{1}{2}}. \qquad (2.3)$$

Here, y_t denotes the distributional derivative of y with respect to the time variable. It is known ([13], Chapter 1, Theorem 3.1) that $H^{2,1}(Q)$ embeds into the space of continuous functions with values in $H^1(\Omega)$, $C([0,T];H^1(\Omega))$, and for $\Omega \subset \mathbb{R}^2$, it embeds compactly into $\mathbb{L}^p(Q)$ for $1 \le p < \infty$ [11, 12]. Moreover, for any $y \in H^{2,1}(Q)$, the Neumann boundary trace $\partial y/\partial n$ is an element of the interpolation space $H^{\frac{1}{2},\frac{1}{4}}(\Sigma)$ ([14], Chapter 4, Theorem 2.1). Thus for $y_i \in H^{2,1}(Q)$, we understand (1.1) in the sense of $\mathbb{L}^2(Q)$, while (1.2) and (1.3) are interpreted in the sense of traces on Σ and $\Omega \times \{0\}$, respectively.

Let us introduce the following basic assumptions which are taken to hold throughout the paper:

ASSUMPTION 2.1. *Let $\Omega \subset \mathbb{R}^2$ be a bounded domain with sufficiently smooth boundary. Let the diffusion coefficients D_i and the control weight γ be positive, and let the reaction coefficients k_i and the weight coefficients α_i be nonnegative. Assume moreover that the initial conditions y_{i0} are elements of $H^1(\Omega) \cap \mathbb{L}^\infty(\Omega)$ and that the lower bound u_a is nonnegative.*

The nonnegativity assumption for the lower control bound u_a corresponds to the fact that the reactants can not be withdrawn from the reaction domain.

The main theorem about the semilinear state equation is the following:

THEOREM 2.2 (The state equation). *If $u \in \mathbb{L}^\infty(Q)$ is nonnegative, then the reaction-diffusion system* (1.1)–(1.3) *admits a unique solution* $(y_1, y_2) \in [H^{2,1}(Q)]^2$ *which is nonnegative and satisfies the a priori estimate*

$$\|y_1\|_{H^{2,1}(Q)} + \|y_2\|_{H^{2,1}(Q)} \le c\left((1 + \|y_{10}\|_{H^1(\Omega)})^2 + (1 + \|u\|_{\mathbb{L}^2(Q)} + \|y_{20}\|_{H^1(\Omega)})^2\right)$$

for some positive constant c.

Proof. We construct the solution from nested sequences of upper and lower solutions which converge monotonically, as suggested in Pao [20] for classical solutions. To this end, let $(\check{y}_1, \check{y}_2) = (0, 0)$ and let $(\hat{y}_1, \hat{y}_2)$ be the solution in $[H^{2,1}(Q)]^2$ (in virtue of Lemma 2.3 below) of

$$\frac{\partial \hat{y}_1}{\partial t} = D_1 \Delta \hat{y}_1 \qquad\qquad \frac{\partial \hat{y}_2}{\partial t} = D_2 \Delta \hat{y}_2 + u \quad \text{on } Q$$

with zero Neumann boundary conditions and y_{10} and y_{20} as initial conditions, respectively. By the weak maximum principle [2, 9], we have $\hat{y}_i \ge \check{y}_i$ and $\hat{y}_i \in \mathbb{L}^\infty(Q)$. We let

$$F_1(y_1, y_2) = k_1(\hat{y}_2 - y_2) y_1$$
$$F_2(y_1, y_2) = k_2(\hat{y}_1 - y_1) y_2 + u$$

and define linear differential operators

$$L_1 y = \frac{\partial y}{\partial t} - D_1 \Delta y + k_1 \hat{y}_2 y$$
$$L_2 y = \frac{\partial y}{\partial t} - D_2 \Delta y + k_2 \hat{y}_1 y.$$

Starting from the initial iterates $(\overline{y_1}^{(0)}, \underline{y_2}^{(0)}) = (\hat{y}_1, \check{y}_2)$ and $(\underline{y_1}^{(0)}, \overline{y_2}^{(0)}) = (\check{y}_1, \hat{y}_2)$, we construct the sequences (with $n \ge 0$)

$$L_1 \overline{y_1}^{(n+1)} = F_1(\overline{y_1}^{(n)}, \underline{y_2}^{(n)}) \qquad\qquad L_1 \underline{y_1}^{(n+1)} = F_1(\underline{y_1}^{(n)}, \overline{y_2}^{(n)})$$
$$L_2 \overline{y_2}^{(n+1)} = F_2(\overline{y_1}^{(n)}, \underline{y_2}^{(n)}) \qquad\qquad L_2 \underline{y_2}^{(n+1)} = F_2(\underline{y_1}^{(n)}, \overline{y_2}^{(n)})$$

with zero Neumann boundary conditions and y_{i0} as initial conditions. It follows again from the weak maximum principle and by induction that for all n,

$$\underline{y_1}^{(n)} \le \underline{y_1}^{(n+1)} \le \overline{y_1}^{(n+1)} \le \overline{y_1}^{(n)}$$
$$\underline{y_2}^{(n)} \le \underline{y_2}^{(n+1)} \le \overline{y_2}^{(n+1)} \le \overline{y_2}^{(n)}.$$

Thus the sequences $r_i = F_i(\overline{y_1}^{(n)}, \underline{y_2}^{(n)})$ and $s_i = F_i(\underline{y_1}^{(n)}, \overline{y_2}^{(n)})$ converge pointwise on Q and, by Lebesgue's Dominated Convergence Theorem, using bounds like

$$0 \le F_1(\overline{y_1}^{(n)}, \underline{y_2}^{(n)}) \le k_1 \hat{y}_2 \overline{y_1}^{(0)} + f_1,$$

they converge also in $\mathbb{L}^2(Q)$. By the a priori estimates from Lemma 2.3, the Cauchy property of r_i and s_i carries over to the sequences $\{\overline{y_i}^n\}$ and $\{\underline{y_i}^n\}$, which consequently converge to their limits $\overline{y_i}$ and $\underline{y_i}$ in the Hilbert space $H^{2,1}(Q)$. It follows easily that both pairs $(\underline{y_1}, \overline{y_2})$ and $(\overline{y_1}, \underline{y_2})$ satisfy the reaction-diffusion system (1.1)–(1.3). By construction, all components are nonnegative.

To establish uniqueness, let (y_1, y_2) and (z_1, z_2) be any two solutions of the reaction-diffusion system (1.1)–(1.3). Then their difference $w_i = y_i - z_i$ satisfies

$$\begin{aligned} \frac{\partial w_1}{\partial t} &= D_1 \Delta w_1 - k_1 z_2 w_1 - k_1 y_1 w_2 \quad \text{on } Q \\ \frac{\partial w_2}{\partial t} &= D_2 \Delta w_2 - k_2 z_2 w_1 - k_1 y_1 w_2 \quad \text{on } Q. \end{aligned}$$

plus homogeneous Neumann boundary conditions and zero initial conditions. Again by Lemma 2.3, $(w_1, w_2) = (0, 0)$ is the unique solution, thus y and z coincide.

As for the a priori estimate, we infer from (1.1) by Lemma 2.3:

$$\begin{aligned} \|y_1\|_{H^{2,1}(Q)} &\le c \left(k_1 \|y_1 y_2\|_{\mathbb{L}^2(Q)} + \|y_{10}\|_{H^1(\Omega)} \right) \\ \|y_2\|_{H^{2,1}(Q)} &\le c \left(k_2 \|y_1 y_2\|_{\mathbb{L}^2(Q)} + \|y_{20}\|_{H^1(\Omega)} + \|u\|_{\mathbb{L}^2(Q)} \right) \end{aligned} \tag{2.4}$$

and, by Hölder's and Young's inequality,

$$\|y_1 y_2\|_{\mathbb{L}^2(Q)} \le \frac{1}{2} \|y_1\|^2_{\mathbb{L}^4(Q)} + \frac{1}{2} \|y_2\|^2_{\mathbb{L}^4(Q)}. \tag{2.5}$$

For $\hat{y}_1$, as defined above, we have $0 \le y_1(x,t) \le \hat{y}_1(x,t)$ a.e. on Q, thus

$$\|y_1\|_{\mathbb{L}^4(Q)} \le \|\hat{y}_1\|_{\mathbb{L}^4(Q)} \le c \, \|\hat{y}_1\|_{H^{2,1}(Q)} \le \tilde{c} \, \|y_{10}\|_{H^1(Q)} \tag{2.6}$$

and similarly

$$\|y_2\|_{\mathbb{L}^4(Q)} \le \|\hat{y}_2\|_{\mathbb{L}^4(Q)} \le c \, \|\hat{y}_2\|_{H^{2,1}(Q)} \le \tilde{c} \, \|y_{20}\|_{H^1(Q)} + \tilde{c} \, \|u\|_{\mathbb{L}^2(Q)}. \tag{2.7}$$

Combining (2.4)–(2.7), the a priori estimate follows. ☐

LEMMA 2.3 (A linear system of PDEs). *Given coefficients $c_{ij} \in \mathbb{L}^2(0, T; \mathbb{L}^{1+\epsilon}(\Omega))$ with arbitrary $\epsilon > 0$ (in particular, with $c_{ij} \in H^{2,1}(Q)$), the linear system of PDEs*

$$\begin{aligned} \frac{\partial y_1}{\partial t} &= D_1 \Delta y_1 - c_{11} y_1 - c_{12} y_2 + f_1 && \text{on } Q \\ D_1 \frac{\partial y_1}{\partial n} &= g_1 && \text{on } \Sigma \\ y_1(\cdot, 0) &= h_1 && \text{on } \Omega \\ \frac{\partial y_2}{\partial t} &= D_2 \Delta y_2 - c_{21} y_1 - c_{22} y_2 + f_2 && \text{on } Q \\ D_2 \frac{\partial y_2}{\partial n} &= g_2 && \text{on } \Sigma \\ y_2(\cdot, 0) &= h_2 && \text{on } \Omega \end{aligned} \tag{2.8}$$

with data $f_i \in \mathbb{L}^2(Q)$, $g_i \in H^{\frac{1}{2},\frac{1}{4}}(\Sigma)$ *and* $h_i \in H^1(\Omega)$ *has a unique solution* $(y_1, y_2) \in [H^{2,1}(Q)]^2$ *which depends continuously on the data:*

$$\|y_1\|_{H^{2,1}(Q)} + \|y_2\|_{H^{2,1}(Q)} \le c \sum_{i=1}^{2} \left(\|f_i\|_{\mathbb{L}^2(Q)} + \|g_i\|_{H^{\frac{1}{2},\frac{1}{4}}(\Sigma)} + \|h_i\|_{H^1(\Omega)} \right). \quad (2.9)$$

Proof. We begin by showing the existence and uniqueness properties in the space $W(0,T)$: For fixed t, the linear operator $y \mapsto \langle A(t)y, \cdot \rangle$:

$$\begin{aligned} \langle A(t)\, y, v\rangle = D_1 \int_\Omega \nabla y_1(x)\, \nabla v_1(x)\, dx + \int_\Omega c_{11}(x,t)\, y_1(x)\, v_1(x)\, dx \\ + \int_\Omega c_{12}(x,t)\, y_2(x)\, v_1(x)\, dx + D_2 \int_\Omega \nabla y_2(x)\, \nabla v_2(x)\, dx \\ + \int_\Omega c_{21}(x,t)\, y_1(x)\, v_2(x)\, dx + \int_\Omega c_{22}(x,t)\, y_2(x)\, v_2(x)\, dx \end{aligned}$$

maps $[H^1(\Omega)]^2$ to its dual. It is straightforward, using the embedding of $H^1(\Omega)$ into $\mathbb{L}^p(\Omega)$ $(1 \le p < \infty)$, to verify the estimates

$$\begin{aligned} |\langle A(t)y, v\rangle| &\le c \max_{i,j} \|c_{ij}(\cdot,t)\|_{\mathbb{L}^{1+\epsilon}} \cdot \|y\|_{[H^1(\Omega)]^2} \cdot \|v\|_{[H^1(\Omega)]^2} \\ |\langle A(t)y, y\rangle| &\ge \beta \max_{i,j} \|c_{ij}(\cdot,t)\|_{\mathbb{L}^{1+\epsilon}} \cdot \|y\|^2_{[H^1(\Omega)]^2} + \beta_0 \max_{i,j} \|c_{ij}(\cdot,t)\|_{\mathbb{L}^{1+\epsilon}} \cdot \|y\|^2_{[\mathbb{L}^2(\Omega)]^2} \end{aligned}$$

with $\beta_0 \in \mathbb{R}$ and some positive constants c and β. Moreover, for the right hand side operator $F(t)$:

$$\langle F(t), y\rangle = \sum_{i=1}^{2} \langle f_i(\cdot,t), y_i\rangle + D_i \int_\Gamma g_i(x,t)\, y_i(x)\, dx$$

which maps $[H^{2,1}(Q)]^2$ to its dual, it follows similarly that

$$|\langle F(t), y\rangle| \le c \left(\|f(\cdot,t)\|_{[\mathbb{L}^2(\Omega)]^2} + \|g(\cdot,t)\|_{[\mathbb{L}^2(\Gamma)]^2} \right).$$

By a standard argument in the Gelfand triple setting ([5], p. 509), the existence and uniqueness of the weak solution in $[W(0,T)]^2$ follow. We can now interpret $\tilde{f}_i = -c_{i1}y_1 - c_{i2}y_2 + f_i$ in (2.8) as a source term for the usual heat equation. $\tilde{f}_i$ is easily seen to be in $\mathbb{L}^2(Q)$ as $W(0,T)$ embeds into any $\mathbb{L}^p(Q)$ $(1 \le p \le 4)$ ([7], p. 7). The $H^{2,1}(Q)$ regularity of the solution now follows from Lions and Magenes II [14], Chapter 4, Section 6.4. □

LEMMA 2.4 (Differentiability of the nonlinear term). *For* y_1 *and* y_2 *in* $H^{2,1}(Q)$, $\phi(y_1, y_2) = y_1 y_2 \in \mathbb{L}^2(Q)$ *is Fréchet differentiable, and the derivative is given by* $D\phi(y_1,y_2)(\overline{y_1}, \overline{y_2}) = y_2\overline{y_1} + y_1\overline{y_2}$.

Proof. The proof is a consequence of the estimate

$$\frac{\|h_1 h_2\|_{\mathbb{L}^2(Q)}}{\|h_1\|_{H^{2,1}(Q)} + \|h_2\|_{H^{2,1}(Q)}} \le \frac{\|h_1\|_{\mathbb{L}^4(Q)} \|h_2\|_{\mathbb{L}^4(Q)}}{\|h_1\|_{H^{2,1}(Q)} + \|h_2\|_{H^{2,1}(Q)}}$$

where the right hand side tends to zero as h_1, h_2 tend to zero in $H^{2,1}(Q)$ in view of the embedding $H^{2,1}(Q) \hookrightarrow \mathbb{L}^4(Q)$. □

LEMMA 2.5 (Properties of the solution operator). *Theorem* 2.2 *above gives rise to the definition of the solution operator* $S : \mathbb{L}^2(Q) \supset U_{\text{ad}} \to [H^{2,1}(Q)]^2$, *which is Fréchet* *differentiable, with the derivative at* u *in the direction of* $\overline{u}$ *given by the unique solution* $(\overline{y_1}, \overline{y_2})$ *of*

$$\begin{aligned} \frac{\partial \overline{y_1}}{\partial t} &= D_1 \Delta \overline{y_1} - k_1(y_2 \overline{y_1} + y_1 \overline{y_2}) & D_1 \frac{\partial \overline{y_1}}{\partial n} &= 0 & \overline{y_1}(\cdot, 0) &= 0 \\ \frac{\partial \overline{y_2}}{\partial t} &= D_2 \Delta \overline{y_2} - k_2(y_1 \overline{y_2} + y_2 \overline{y_1}) + \overline{u} & D_2 \frac{\partial \overline{y_2}}{\partial n} &= 0 & \overline{y_2}(\cdot, 0) &= 0, \end{aligned} \tag{2.10}$$

where $(y_1, y_2) = S(u)$.

Proof. The proof is an immediate consequence of the classical implicit function theorem in Banach spaces (e.g. Deimling [6], Theorem 15.1). □

THEOREM 2.6 (Existence of optimal solutions). *Let the desired terminal states* y_{1T}, y_{2T} *be elements of* $\mathbb{L}^2(\Omega)$. *Then there exists at least one global optimal solution of the optimal control problem* (RD(p)).

Proof. Since the objective f is bounded below by zero and the set of admissible control/state pairs M satisfying the state equation (1.1)–(1.3) is nonempty, there is a finite number $m := \inf f(M)$ and a sequence $\{(y_1^n, y_2^n, u^n)\} \subset M$ such that $f(y_1^n, y_2^n, u^n)$ converges to m. Since u^n is admissible, $\{u^n\}$ is bounded in $\mathbb{L}^2(Q)$, and by the a priori estimate from Theorem 2.2, $\{y_i^n\}$ is bounded in $H^{2,1}(Q)$. We can thus extract subsequences $u^n \rightharpoonup u$ weakly in $\mathbb{L}^2(Q)$ and $y_i^n \rightharpoonup y_i$ weakly in $H^{2,1}(Q)$ and, by compactness of the embedding, $y_i^n \to y_i$ strongly in $\mathbb{L}^4(Q)$.
To prove that (y_1, y_2, u) is feasible, we observe that for any $\phi \in \mathbb{L}^2(Q)^\star$,

$$\begin{aligned} |\langle \phi, y_1^n y_2^n - y_1 y_2 \rangle| &\le |\langle \phi, y_1^n (y_2^n - y_2) \rangle| + |\langle \phi, y_2 (y_1^n - y_1) \rangle| \\ &\le \|\phi\| \|y_1^n\|_{\mathbb{L}^4(Q)} \|y_2^n - y_2\|_{\mathbb{L}^4(Q)} + \|\phi\| \|y_2\|_{\mathbb{L}^4(Q)} \|y_1^n - y_1\|_{\mathbb{L}^4(Q)} \end{aligned}$$

which tends to zero, hence $y_1^n y_2^n \rightharpoonup y_1 y_2$ in $\mathbb{L}^2(Q)$. By definition of the norm on $H^{2,1}(Q)$, $\partial y_1^n / \partial t - D_1 \Delta y_1^n + k_1 y_1^n y_2^n \rightharpoonup \partial y_1/\partial t - D_1 \Delta y_1 + k_1 y_1 y_2$ in $\mathbb{L}^2(Q)$ holds, the left hand side being identically zero. Choosing ϕ equal to the Riesz representation of $\partial y_1/\partial t - D_1 \Delta y_1 + k_1 y_1 y_2$ shows that the convergence is also strong in $\mathbb{L}^2(Q)$. Similar arguments apply for the second part of (1.1) and for the boundary and initial conditions (1.2)–(1.3). Taking into account that U_{ad} is closed and convex, it is weakly closed, thus (y_1, y_2, u) is admissible and satisfies the state equation.
By weak lower semicontinuity of the objective, it follows that $f(y_1, y_2, u) = m$ holds. □

Before turning to the first order necessary conditions, let us briefly discuss the adjoint equation:

THEOREM 2.7 (Adjoint equation). *Let the desired terminal states* y_{1T}, y_{2T} *be elements of* $H^1(\Omega)$, *and let* y_1, y_2 *be any elements of* $H^{2,1}(Q)$. *Then the linear adjoint equation*

$$\begin{aligned} -\frac{\partial \lambda_1}{\partial t} &= D_1 \Delta \lambda_1 - y_2(k_1 \lambda_1 + k_2 \lambda_2) && \text{on } Q \\ D_1 \frac{\partial \lambda_1}{\partial n} &= 0 && \text{on } \Sigma \\ \lambda_1(\cdot, T) &= -\alpha_1 (y_1(\cdot, T) - y_{1T}) && \text{on } \Omega \\ -\frac{\partial \lambda_2}{\partial t} &= D_2 \Delta \lambda_2 - y_1(k_1 \lambda_1 + k_2 \lambda_2) && \text{on } Q \\ D_2 \frac{\partial \lambda_2}{\partial n} &= 0 && \text{on } \Sigma \end{aligned} \tag{2.11}$$

$$\lambda_2(\cdot,T) = -\alpha_2(y_2(\cdot,T) - y_{2T}) \qquad \text{on } \Omega.$$

has a unique solution in $[H^{2,1}(Q)]^2$*, which satisfies the a priori estimate*

$$\|\lambda_1\|_{H^{2,1}(Q)} + \|\lambda_2\|_{H^{2,1}(Q)} \le c\left(\alpha_1\|y_1(\cdot,T) - y_{1T}\|_{H^1(\Omega)} + \alpha_2\|y_2(\cdot,T) - y_{2T}\|_{H^1(\Omega)}\right)$$

for some positive constant c.

Proof. The adjoint equation is a PDE of type (2.8), only running backwards in time. □

Local optimal solutions for (RD(p)) satisfy the following first order necessary (KKT) conditions:

THEOREM 2.8 (First order necessary conditions). *Let the desired terminal states* y_{1T}, y_{2T} *be elements of* $H^1(\Omega)$*. Let* (y,u) *be a local optimal solution of problem* (RD(p))*, and let* (λ_1,λ_2) *be the unique solution in* $[H^{2,1}(Q)]^2$ *of the linear adjoint equation* (2.11)*. Then* (y,u,λ) *satisfies the variational inequality*

$$0 \le \int_Q (\gamma u - \lambda_2)(\overline{u} - u)\,dx\,dt \qquad \text{for all } \overline{u} \in U_{\text{ad}}. \tag{2.12}$$

Proof. Let us define the reduced objective

$$\mathbb{L}^2(Q) \ni u \mapsto \tilde{f}(u) = f(S(u),u) \in \mathbb{R}. \tag{2.13}$$

For u being a local optimizer for problem (RD(p)), it is necessary that $0 \le D\tilde{f}(u;\overline{u}-u)$ holds for all $\overline{u} \in U_{\text{ad}}$. One easily concludes from the chain rule that

$$D\tilde{f}(u;\overline{u}-u) = \sum_{i=1}^{2} \alpha_i \int_Q (S_{iT}(u) - y_{1T}) DS_{iT}(u;\overline{u}-u) + \gamma \int_Q u(\overline{u}-u), \tag{2.14}$$

where S_{iT} is the solution operator S followed by the linear and continuous action of taking the terminal value of the ith solution component. Multiplying the first equation in (2.11) by $\overline{y_1}$ (the solution of (2.10)), integration over Q, performing integration by parts and substituting the boundary conditions for λ_1 and $\overline{y_1}$, one finds that

$$\alpha_1 \int_\Omega (y_1(\cdot,T) - y_{1T})\,\overline{y_1}(\cdot,T) = \int_Q k_1 y_1 \overline{y_2}\lambda_1 - k_2 y_2 \overline{y_1}\lambda_2,$$

which matches the first term in (2.14). A similar procedure, starting from the equation for λ_2, shows that

$$\alpha_2 \int_\Omega (y_2(\cdot,T) - y_{2T})\,\overline{y_2}(\cdot,T) = \int_Q k_2 y_2\,\overline{y_1}\lambda_2 - k_1 y_1 \overline{y_2}\,\lambda_1 - (\overline{u}-u)\lambda_2,$$

which concludes the proof. □

For future reference, let us denote by $e : [H^{2,1}(Q)]^2 \times \mathbb{L}^2(Q) \to [\mathbb{L}^2(Q) \times H^{\frac{1}{2},\frac{1}{4}}(\Sigma) \times H^1(\Omega)]^2$ the collection of the left hand sides of the state equations (1.1)–(1.3) when written in the form $e(y_1,y_2,u;p) = 0$. In addition, we define the Lagrangian of problem (RD(p)) as

$$\begin{aligned} L(y,u,\lambda;p) &= f(y,u;p) + \int_Q \left(\frac{\partial y_1}{\partial t} - D_1\Delta y_1 + k_1 y_1 y_2\right)\lambda_1 + \int_\Sigma D_1 \frac{\partial y_1}{\partial n}\lambda_1 \\ &+ \int_\Omega (y_1(\cdot,0) - y_{10})\,\lambda_1(\cdot,0) + \int_Q \left(\frac{\partial y_2}{\partial t} - D_2\Delta y_2 + k_2 y_1 y_2 - u\right)\lambda_2 + \int_\Sigma D_2 \frac{\partial y_2}{\partial n}\lambda_2 \\ &+ \int_\Omega (y_2(\cdot,0) - y_{20})\,\lambda_2(\cdot,0). \end{aligned} \tag{2.15}$$

Motivated by the variational inequality (2.12), we also define the control constraint multiplier

$$\mu = -(\gamma u - \lambda_2) = -L_u(y, u, \lambda; p). \tag{2.16}$$

It is rather standard to prove that if u and λ satisfy the variational inequality (2.12), then $\mu < 0$ on some subset $\underline{Q}$ implies that $u = u_a$ there, etc.

3. Strong Regularity and Lipschitz Continuity of Solutions. It is the concern of the present section to establish the Lipschitz continuity with respect to a general parameter p of critical points for the optimal control problem (RD(p)). The proof relies on a coercivity assumption (AC) on the Hessian of the Lagrangian which in turn implies second order sufficiency, i.e., under (AC), critical points are in fact local optimal solutions. To be specific, we let

$$p = (D_1, D_2, k_1, k_2, \alpha_1, \alpha_2, \gamma, y_{10}, y_{20}, y_{1T}, y_{2T})^\top \in \mathbb{R}^7 \times [H^1(\Omega)]^4 \tag{3.1}$$

be the vector of perturbation parameters. Other parameters like the Neumann boundary values could also be included but have been omitted to improve readability.

For $u \in \mathbb{L}^2(Q)$, let

$$N_2(u) = \begin{cases} \{\phi \in \mathbb{L}^2(Q) : \int_Q \phi\,(\overline{u} - u) \le 0 \text{ for all } \overline{u} \in U_{\text{ad}}\} & \text{if } u \in U_{\text{ad}} \\ \emptyset & \text{if } u \notin U_{\text{ad}} \end{cases} \tag{3.2}$$

denote the normal cone at u with respect to U_{ad}. With the set-valued operator $N(u) = (\{0\}, N_2(u), \{0\}) : \mathbb{L}^2(Q) \to 2^Z$, the first order necessary conditions, consisting of the adjoint equation (2.11), optimality condition (2.12) and the state equation (1.1)–(1.3), can be written as a generalized equation

$$0 \in F(y, u, \lambda; p) + N(u) \tag{3.3}$$

with the target space Z, defined as

$$Z = [\mathbb{L}^2(Q) \times H^{\frac{1}{2},\frac{1}{4}}(\Sigma) \times H^1(\Omega)]^2 \times \mathbb{L}^2(Q) \times [\mathbb{L}^2(Q) \times H^{\frac{1}{2},\frac{1}{4}}(\Sigma) \times H^1(\Omega)]^2, \tag{3.4}$$

and

$$F(y, u, \lambda; p) = \begin{pmatrix} -\partial\lambda_1/\partial t - D_1 \Delta\lambda_1 + y_2(k_1\lambda_1 + k_2\lambda_2) \\ D_1 \partial\lambda_1/\partial n \\ \lambda_1(\cdot, T) + \alpha_1(y_1(\cdot, T) - y_{1T}) \\ -\partial\lambda_2/\partial t - D_2 \Delta\lambda_2 + y_1(k_1\lambda_1 + k_2\lambda_2) \\ D_2 \partial\lambda_2/\partial n \\ \lambda_2(\cdot, T) + \alpha_2(y_2(\cdot, T) - y_{2T}) \\ \gamma u - \lambda_2 \\ \partial y_1/\partial t - D_1 \Delta y_1 + k_1 y_1 y_2 \\ D_1 \partial y_1/\partial n \\ y_1(\cdot, 0) - y_{10} \\ \partial y_2/\partial t - D_2 \Delta y_2 + k_2 y_1 y_2 - u \\ D_2 \partial y_2/\partial n \\ y_2(\cdot, 0) - y_{20} \end{pmatrix}. \tag{3.5}$$

Instead of proving the Lipschitz continuity of solutions $(y, u, \lambda) = (\Sigma(p), \Xi(p), \Lambda(p))$ for (3.3) directly, we use Robinson's implicit function theorem for strongly regular generalized equations [21], which has the benefit that one needs to examine solutions to a linearized version of (3.3) only.

For the remainder of the paper, let us denote by p_0 a fixed reference or nominal value of the parameter p, and let (y_0, u_0, λ_0) satisfy the first order necessary conditions and thus (3.3) for this value p_0. The components of p_0 are still denoted as in (3.1), without an additional index.

We recall that (3.3) is said to be strongly regular at the nominal critical point $(y_0, u_0, \lambda_0; p_0)$ if there exist $\epsilon > 0$ and $\eta > 0$ such that for any $\delta \in Z$ with $\|\delta\|_Z < \epsilon$, the linearized generalized equation (where F' denotes the Fréchet derivative of F with respect to (y, u, λ))

$$\delta \in F(y_0, u_0, \lambda_0; p_0) + F'(y_0, u_0, \lambda_0; p_0) \begin{pmatrix} y - y_0 \\ u - u_0 \\ \lambda - \lambda_0 \end{pmatrix} + N(u) \tag{3.6}$$

has a solution $(y, u, \lambda) = (\sigma(\delta), \xi(\delta), \lambda(\delta))$ which is unique in the η-neighborhood of (y_0, u_0, λ_0), and which depends Lipschitz-continuously on δ, i.e., for some $L > 0$,

$$\|\sigma(\delta) - \sigma(\delta')\|_{[H^{2,1}(Q)]^2} + \|\xi(\delta) - \xi(\delta')\|_{\mathbb{L}^2(Q)} + \|\lambda(\delta) - \lambda(\delta')\|_{[H^{2,1}(Q)]^2} \le L\,\|\delta - \delta'\|_Z.$$

Note that for $\delta = 0$, the nominal critical point (y_0, u_0, λ_0) satisfies both the nonlinear (3.3) and the linearized generalized equation (3.6).
In the absence of control constraints, $N(u)$ collapses to the singleton $\{0\}$, and the strong regularity of (3.3) is nothing else than bounded invertibility of F' at the nominal critical point, as is required by the classical implicit function theorem in Banach spaces (e.g. Deimling [6], Theorem 15.1).

In the case of (RD(p)), the linearized generalized equation (3.6) with perturbation $\delta = (\delta_1, \ldots, \delta_{13})^\top$ reads:

$$\begin{aligned}
-\frac{\partial}{\partial t}\lambda_1 - D_1\Delta\lambda_1 + k_1 y_2^0 \lambda_1 + k_2 y_2^0 \lambda_2 + k_1 \lambda_1^0 y_2 + k_2 \lambda_2^0 y_2 &= k_1 y_2^0 \lambda_1^0 + k_2 y_2^0 \lambda_2^0 + \delta_1 \\
D_1 \frac{\partial}{\partial n}\lambda_1 &= \delta_2 \\
\lambda_1(\cdot, T) &= -\alpha_1 (y_1(\cdot, T) - y_{1T}) + \delta_3 \\
-\frac{\partial}{\partial t}\lambda_2 - D_2\Delta\lambda_2 + k_2 y_1^0 \lambda_2 + k_1 y_1^0 \lambda_1 + k_2 \lambda_2^0 y_1 + k_1 \lambda_1^0 y_1 &= k_2 y_1^0 \lambda_2^0 + k_1 y_1^0 \lambda_1^0 + \delta_4 \\
D_2 \frac{\partial}{\partial n}\lambda_2 &= \delta_5 \\
\lambda_2(\cdot, T) &= -\alpha_2 (y_2(\cdot, T) - y_{2T}) + \delta_6
\end{aligned} \tag{3.7}$$

$$\int_Q (\gamma u - \lambda_2 - \delta_7)\,(\overline{u} - u) \ge 0 \quad \text{for all } \overline{u} \in U_{\text{ad}} \tag{3.8}$$

$$\begin{aligned}
\frac{\partial}{\partial t} y_1 - D_1 \Delta y_1 + k_1 y_2^0 y_1 + k_1 y_1^0 y_2 &= k_1 y_1^0 y_2^0 + \delta_8 \\
D_1 \frac{\partial}{\partial n} y_1 &= \delta_9 \\
y_1(\cdot, 0) &= y_{10} + \delta_{10}
\end{aligned}$$

$$\begin{aligned}\frac{\partial}{\partial t}y_2 - D_2\Delta y_2 + k_2 y_2^0 y_1 + k_2 y_1^0 y_2 - u &= k_2 y_1^0 y_2^0 + \delta_{11}\\ D_2\frac{\partial}{\partial n}y_2 &= \delta_{12}\\ y_2(\cdot,0) &= y_{20} + \delta_{13}.\end{aligned} \tag{3.9}$$

To prove strong regularity of the KKT conditions (3.3), it is particularly helpful that we can interpret (3.7)–(3.9) as the first order necessary conditions of the following auxiliary linear-quadratic optimal control problem (AQP(δ)), whose verification is straightforward and therefore omitted:

$$\begin{aligned}&\text{Minimize}\quad \frac{\alpha_1}{2}\|y_1(\cdot,T)-y_{1T}\|^2_{\mathbb{L}^2(\Omega)} + \frac{\alpha_2}{2}\|y_2(\cdot,T)-y_{2T}\|^2_{\mathbb{L}^2(\Omega)} + \frac{\gamma}{2}\|u\|^2_{\mathbb{L}^2(Q)}\\ &+\int_Q (k_1\lambda_1^0 + k_2\lambda_2^0)\,y_1 y_2 - \int_Q (k_1\lambda_1^0 + k_2\lambda_2^0)(y_2^0 y_1 + y_1^0 y_2)\\ &-\int_Q \delta_1 y_1 - \int_\Sigma \delta_2 y_1 - \int_\Omega \delta_3 y_1(\cdot,T) - \int_Q \delta_4 y_2 - \int_\Sigma \delta_5 y_2 - \int_\Omega \delta_6 y_2(\cdot,T)\\ &-\int_Q \delta_7 u\end{aligned} \tag{AQP(δ)}$$

subject to the linear state equation (3.9) and the constraint $u \in U_{\text{ad}}$.

The following coercivity estimate is essential in proving both uniqueness and Lipschitz dependence of the solutions to (AQP(δ)):

$$\begin{aligned}&\frac{1}{2}L_{xx}(y_0,u_0,\lambda_0;p_0)(x,x)\\ &\quad= \frac{\alpha_1}{2}\|y_1(\cdot,T)\|^2_{\mathbb{L}^2(\Omega)} + \frac{\alpha_2}{2}\|y_2(\cdot,T)\|^2_{\mathbb{L}^2(\Omega)} + \frac{\gamma}{2}\|u\|^2_{\mathbb{L}^2(Q)} + \int_Q (k_1\lambda_1^0 + k_2\lambda_2^0)\,y_1 y_2\\ &\quad\geq \rho\left(\|y_1\|^2_{H^{2,1}(Q)} + \|y_2\|^2_{H^{2,1}(Q)} + \|u\|^2_{\mathbb{L}^2(Q)}\right)\end{aligned} \tag{AC}$$

for some $\rho > 0$ and for all $(y,u) \in [H^{2,1}(Q)]^2 \times \mathbb{L}^2(Q)$ which satisfy

$$\begin{aligned}\frac{\partial}{\partial t}y_1 - D_1\Delta y_1 + k_1 y_2^0 y_1 + k_1 y_1^0 y_2 &= 0 \text{ in } Q\\ D_1\frac{\partial}{\partial n}y_1 &= 0 \text{ on } \Sigma\\ y_1(\cdot,0) &= 0 \text{ on } \Omega\\ \frac{\partial}{\partial t}y_2 - D_2\Delta y_2 + k_2 y_2^0 y_1 + k_2 y_1^0 y_2 &= u \text{ in } Q\\ D_2\frac{\partial}{\partial n}y_2 &= 0 \text{ on } \Sigma\\ y_2(\cdot,0) &= 0 \text{ on } \Omega.\end{aligned} \tag{3.10}$$

and $u(x,t) = 0$ where $a(x,t) = b(x,t)$.

Remark 3.1 (Smallness of the adjoint). *The coercivity condition* (AC) *is satisfied whenever* $\|k_1\lambda_1^0 + k_2\lambda_2^0\|_{\mathbb{L}^2(Q)}$ *is sufficiently small, since we can estimate*

$$\int_Q (k_1\lambda_1^0 + k_2\lambda_2^0)\,y_1 y_2 \geq -\|k_1\lambda_1^0 + k_2\lambda_2^0\|_{\mathbb{L}^2(Q)} \cdot \|y_1\|_{\mathbb{L}^4(Q)} \cdot \|y_2\|_{\mathbb{L}^4(Q)}$$

$$\geq -c\,\|k_1\lambda_1^0 + k_2\lambda_2^0\|_{\mathbb{L}^2(Q)} \cdot \|u\|^2_{\mathbb{L}^2(Q)}$$

in view of the embedding $H^{2,1}(Q) \hookrightarrow \mathbb{L}^4(Q)$ *and the a priori estimate* (2.9).
In particular, again by a priori estimate (2.9) *applied to the adjoint equation, the smallness condition is satisfied if* $\alpha_1\|y_1^0(\cdot,T) - y_{1T}\|_{H^1(\Omega)}$ *and* $\alpha_2\|y_2^0(\cdot,T) - y_{2T}\|_{H^1(\Omega)}$ *are sufficiently small.*

THEOREM 3.2 (Lipschitz stability of (σ, ξ, λ)). *Suppose that the coercivity assumption* (AC) *holds. Then for any perturbation* $\delta \in Z$, $(\mathrm{AQP}(\delta))$ *has a globally unique solution, denoted by* $(\sigma(\delta), \xi(\delta), \lambda(\delta))$, *which depends Lipschitz-continuously on* δ:

$$\begin{aligned}&\|\sigma(\delta) - \sigma(\delta')\|_{[H^{2,1}(Q)]^2} + \|\xi(\delta) - \xi(\delta')\|_{\mathbb{L}^2(Q)} + \|\lambda(\delta) - \lambda(\delta')\|_{[H^{2,1}(Q)]^2} \\ &\leq L\,\|\delta - \delta'\|_Z.\end{aligned} \tag{3.11}$$

In particular, the KKT conditions (3.3) *for* $(\mathrm{RD}(p))$ *are strongly regular at the nominal critical point* $(y_0, u_0, \lambda_0; p_0)$.

Proof. The existence and uniqueness of solutions to $(\mathrm{AQP}(\delta))$ are obvious conclusions in view of the objective being convex and weakly lower semicontinuous, and in view of the set of admissible (y, u) being convex, closed and bounded [3], Chapter 2, Theorem 1.2.
Let δ and δ' be any two perturbations from Z, and let (y, u, λ) and (y', u', λ') refer to the solutions of $(\mathrm{AQP}(\delta))$ and $(\mathrm{AQP}(\delta'))$, respectively. We abbreviate all differences in the sequel according to the pattern $\underline{\delta} = \delta - \delta'$. Then $\underline{y}$ satisfies

$$\begin{aligned}\frac{\partial}{\partial t}\underline{y_1} - D_1\Delta\underline{y_1} + k_1 y_2^0\underline{y_1} + k_1 y_1^0\underline{y_2} &= \underline{\delta_8} \text{ on } Q\\ D_1\frac{\partial}{\partial n}\underline{y_1} &= \underline{\delta_9} \text{ on } \Sigma\\ \underline{y_1}(\cdot,0) &= \underline{\delta_{10}} \text{ on } \Omega\\ \frac{\partial}{\partial t}\underline{y_2} - D_2\Delta\underline{y_2} + k_2 y_2^0\underline{y_1} + k_2 y_1^0\underline{y_2} - \underline{u} &= \underline{\delta_{11}} \text{ on } Q\\ D_2\frac{\partial}{\partial n}\underline{y_2} &= \underline{\delta_{12}} \text{ on } \Sigma\\ \underline{y_2}(\cdot,0) &= \underline{\delta_{13}} \text{ on } \Omega.\end{aligned} \tag{3.12}$$

Multiplying the first equation in (3.12) by $\underline{\lambda_1}$, adding the fourth equation multiplied by $\underline{\lambda_2}$, and plugging in the adjoint equation (3.7) for $\underline{\lambda_1}$ and $\underline{\lambda_2}$ yields

$$\begin{aligned}&\int_Q \underline{\delta_1}\,\underline{y_1} + \underline{\delta_4}\,\underline{y_2} - 2(k_1\lambda_1^0 + k_2\lambda_2^0)\,\underline{y_1}\,\underline{y_2} + \int_Q -\underline{\delta_8}\,\underline{\lambda_1} - \underline{\delta_{11}}\,\underline{\lambda_2} + \int_Q -\underline{\lambda_2}\,\underline{u}\\ &\quad + \int_\Sigma \underline{\delta_2}\,\underline{y_1} + \underline{\delta_5}\,\underline{y_2} + \int_\Sigma -\underline{\delta_9}\,\underline{\lambda_1} - \underline{\delta_{12}}\,\underline{\lambda_2}\\ &\quad + \int_\Omega \Big[-\alpha_1\,\underline{y_1}(\cdot,T) + \underline{\delta_3}\Big]\,\underline{y_1}(\cdot,T) + \int_\Omega \Big[-\alpha_2\,\underline{y_2}(\cdot,T) + \underline{\delta_6}\Big]\,\underline{y_2}(\cdot,T)\\ &\quad + \int_\Omega -\underline{\delta_{10}}\,\underline{\lambda_1}(\cdot,0) - \underline{\delta_{13}}\,\underline{\lambda_2}(\cdot,0)\\ &= 0.\end{aligned} \tag{3.13}$$

From the variational inequality, choosing $\overline{u} = u$ or $\overline{u} = u'$, respectively, it follows that

$$\int_Q \Big(-\gamma\, \underline{\overline{u}} + \underline{\overline{\lambda_2}} + \underline{\overline{\delta_7}}\Big)\, \underline{\overline{u}} \geq 0. \tag{3.14}$$

Let us denote by $q(y,u)$ the quadratic functional $\frac{1}{2}L_{xx}(y_0,u_0,\lambda_0;p_0)(x,x)$, i.e.,

$$q(y,u) = \frac{\alpha_1}{2}\|y_1(\cdot,T)\|^2_{\mathbb{L}^2(Q)} + \frac{\alpha_2}{2}\|y_2(\cdot,T)\|^2_{\mathbb{L}^2(Q)} + \int_Q (k_1\lambda_1^0 + k_2\lambda_2^0)y_1y_2 + \frac{\gamma}{2}\|u\|^2_{\mathbb{L}^2(Q)}.$$

Solving (3.13) for $\int_Q \underline{\overline{\lambda_2}}\,\underline{\overline{u}}$ and plugging into (3.14), then using Hölder's inequality, it follows that

$$\begin{aligned}
2q(\underline{\overline{y}},\underline{\overline{u}}) &\leq \int_Q \underline{\overline{\delta_1}}\,\underline{\overline{y_1}} + \underline{\overline{\delta_4}}\,\underline{\overline{y_2}} + \int_\Sigma \underline{\overline{\delta_2}}\,\underline{\overline{y_1}} + \underline{\overline{\delta_5}}\,\underline{\overline{y_2}} \\
&\quad + \int_\Omega \underline{\overline{\delta_3}}\,\underline{\overline{y_1}}(\cdot,T) + \underline{\overline{\delta_6}}\,\underline{\overline{y_2}}(\cdot,T) + \int_Q \underline{\overline{\delta_7}}\,\underline{\overline{u}} \\
&\quad + \int_Q - \underline{\overline{\delta_8}}\,\underline{\overline{\lambda_1}} - \underline{\overline{\delta_{11}}}\,\underline{\overline{\lambda_2}} + \int_\Sigma - \underline{\overline{\delta_9}}\,\underline{\overline{\lambda_1}} - \underline{\overline{\delta_{12}}}\,\underline{\overline{\lambda_2}} \\
&\quad + \int_\Omega - \underline{\overline{\delta_{10}}}\,\underline{\overline{\lambda_1}}(\cdot,0) - \underline{\overline{\delta_{13}}}\,\underline{\overline{\lambda_2}}(\cdot,0) \\
&\leq c\|\underline{\overline{y}}\|_{[H^{2,1}(Q)]^2}\Big(\|\underline{\overline{\delta_1}}\|_{\mathbb{L}^2(Q)} + \|\underline{\overline{\delta_2}}\|_{H^{\frac{1}{2},\frac{1}{4}}(\Sigma)} + \|\underline{\overline{\delta_3}}\|_{H^1(\Omega)} \\
&\quad + \|\underline{\overline{\delta_4}}\|_{\mathbb{L}^2(Q)} + \|\underline{\overline{\delta_5}}\|_{H^{\frac{1}{2},\frac{1}{4}}(\Sigma)} + \|\underline{\overline{\delta_6}}\|_{H^1(\Omega)}\Big) \\
&\quad + \|\underline{\overline{u}}\|_{\mathbb{L}^2(Q)} \cdot \|\underline{\overline{\delta_7}}\|_{\mathbb{L}^2(Q)} \\
&\quad + c\|\underline{\overline{\lambda}}\|_{[H^{2,1}(Q)]^2}\Big(\|\underline{\overline{\delta_8}}\|_{\mathbb{L}^2(Q)} + \|\underline{\overline{\delta_9}}\|_{H^{\frac{1}{2},\frac{1}{4}}(\Sigma)} + \|\underline{\overline{\delta_{10}}}\|_{H^1(\Omega)} \\
&\quad + \|\underline{\overline{\delta_{11}}}\|_{\mathbb{L}^2(Q)} + \|\underline{\overline{\delta_{12}}}\|_{H^{\frac{1}{2},\frac{1}{4}}(\Sigma)} + \|\underline{\overline{\delta_{13}}}\|_{H^1(\Omega)}\Big).
\end{aligned} \tag{3.15}$$

The difference $\underline{\overline{y}}$ can be decomposed as $y - y' = z + w$ where z satisfies (3.12) with all $\underline{\overline{\delta_i}}$ replaced by zero, while w satisfies (3.12) with $\underline{\overline{u}}$ replaced by zero. In the following estimate, we use the coercivity assumption (AC), along with the estimates $\|z\|^2 \geq \|y-y'\|^2 - 2\|y-y'\|\|w\| + \|w\|^2$ and $\|z\| \leq \|y-y'\| + \|w\|$. Abbreviating $K = \|k_1\lambda_1^0 + k_2\lambda_2^0\|_{\mathbb{L}^2(Q)}$, we find that

$$\begin{aligned}
q(y-y',\underline{\overline{u}}) &= q(z,\underline{\overline{u}}) + \alpha_1\int_\Omega z_1(\cdot,T)w_1(\cdot,T) + \alpha_2\int_\Omega z_2(\cdot,T)w_2(\cdot,T) \\
&\quad + \frac{\alpha_1}{2}\int_\Omega [w_1(\cdot,T)]^2 + \frac{\alpha_2}{2}\int_\Omega [w_2(\cdot,T)]^2 + \int_Q (k_1\lambda_1^0 + k_2\lambda_2^0)(w_1z_2 + z_1w_2 + w_1w_2) \\
&\geq \rho\left(\|z\|^2_{[H^{2,1}(Q)]^2} + \|\underline{\overline{u}}\|^2_{\mathbb{L}^2(Q)}\right) \\
&\quad - \alpha_1\|z_1(\cdot,T)\|_{\mathbb{L}^2(\Omega)}\cdot\|w_1(\cdot,T)\|_{\mathbb{L}^2(\Omega)} - \alpha_2\|z_2(\cdot,T)\|_{\mathbb{L}^2(\Omega)}\cdot\|w_2(\cdot,T)\|_{\mathbb{L}^2(\Omega)} \\
&\quad - K\Big(\|w_1\|_{\mathbb{L}^4(Q)}\cdot\|z_2\|_{\mathbb{L}^4(Q)} + \|z_1\|_{\mathbb{L}^4(Q)}\cdot\|w_2\|_{\mathbb{L}^4(Q)} + \|w_1\|_{\mathbb{L}^4(Q)}\cdot\|w_2\|_{\mathbb{L}^4(Q)}\Big) \\
&\geq \rho\left(\|\underline{\overline{y}}\|^2_{[H^{2,1}(Q)]^2} - 2\|\underline{\overline{y}}\|_{[H^{2,1}(Q)]^2}\cdot\|w\|_{[H^{2,1}(Q)]^2} + \|w\|^2_{[H^{2,1}(Q)]^2} + \|\underline{\overline{u}}\|^2_{\mathbb{L}^2(Q)}\right) \\
&\quad - c\alpha_1\|z_1\|_{H^{2,1}(Q)}\cdot\|w_1\|_{H^{2,1}(Q)} - c\alpha_2\|z_2\|_{H^{2,1}(Q)}\cdot\|w_2\|_{H^{2,1}(Q)}
\end{aligned}$$

$$
\begin{aligned}
&- cK\Big(\|w_1\|_{H^{2,1}(Q)} \cdot \|z_2\|_{H^{2,1}(Q)} + \|z_1\|_{H^{2,1}(Q)} \cdot \|w_2\|_{H^{2,1}(Q)} \\
&\quad + \|w_1\|_{H^{2,1}(Q)} \cdot \|w_2\|_{H^{2,1}(Q)}\Big) \\
\geq\ & \rho \left(\|\underline{y}\|^2_{[H^{2,1}(Q)]^2} - 2\|\underline{y}\|_{[H^{2,1}(Q)]^2} \cdot \|w\|_{[H^{2,1}(Q)]^2} + \|\underline{u}\|^2_{\mathbb{L}^2(Q)}\right) \\
&- c\alpha_1 \left(\|\underline{y_1}\|_{H^{2,1}(Q)} \cdot \|w_1\|_{H^{2,1}(Q)} + \|w_1\|^2_{H^{2,1}(Q)}\right) \\
&- c\alpha_2 \left(\|\underline{y_2}\|_{H^{2,1}(Q)} \cdot \|w_2\|_{H^{2,1}(Q)} + \|w_2\|^2_{H^{2,1}(Q)}\right) \\
&- cK\Big(\|w_1\|_{H^{2,1}(Q)} \cdot \|\underline{y_2}\|_{H^{2,1}(Q)} \\
&\quad + \|\underline{y_1}\|_{H^{2,1}(Q)} \cdot \|w_2\|_{H^{2,1}(Q)} + 3\|w_1\|_{H^{2,1}(Q)} \cdot \|w_2\|_{H^{2,1}(Q)}\Big),
\end{aligned} \tag{3.16}
$$

Combining (3.15) and (3.16) gives

$$
\begin{aligned}
&\rho \left(\|\underline{y}\|^2_{[H^{2,1}(Q)]^2} + \|\underline{u}\|^2_{\mathbb{L}^2(Q)}\right) \\
&\qquad \leq 2\rho\, \|\underline{y}\|_{[H^{2,1}(Q)]^2} \cdot \|w\|_{[H^{2,1}(Q)]^2} \\
&\qquad\quad + c\alpha_1 \left(\|\underline{y_1}\|_{H^{2,1}(Q)} \cdot \|w_1\|_{H^{2,1}(Q)} + \|w_1\|^2_{H^{2,1}(Q)}\right) \\
&\qquad\quad + c\alpha_2 \left(\|\underline{y_2}\|_{H^{2,1}(Q)} \cdot \|w_2\|_{H^{2,1}(Q)} + \|w_2\|^2_{H^{2,1}(Q)}\right) \\
&\qquad\quad + cK\Big(\|w_1\|_{H^{2,1}(Q)} \cdot \|\underline{y_2}\|_{H^{2,1}(Q)} + \|\underline{y_1}\|_{H^{2,1}(Q)} \cdot \|w_2\|_{H^{2,1}(Q)} \\
&\qquad\quad\ + 3\|w_1\|_{H^{2,1}(Q)} \cdot \|w_2\|_{H^{2,1}(Q)}\Big) \\
&\qquad\quad + \frac{1}{2} c\, \|\underline{y}\|_{H^{2,1}(Q)} \sum_{i=1}^{6} \|\underline{\delta_i}\| + \frac{1}{2}\|\underline{u}\|_{\mathbb{L}^2(Q)} \cdot \|\underline{\delta_7}\|_{\mathbb{L}^2(Q)} \\
&\qquad\quad + \frac{1}{2} c\, \|\underline{\lambda}\|_{H^{2,1}(Q)} \sum_{i=8}^{13} \|\underline{\delta_i}\|.
\end{aligned} \tag{3.17}
$$

In (3.17), we estimate $\|w\| \leq c \sum_{i=8}^{13} \|\underline{\delta_i}\|$ for all terms involving $\|w_i\|^2$ or $\|w_i\|\|w_j\|$; we estimate $\|\underline{y_i}\|\|w_j\| \leq \epsilon\|\underline{y_i}\|^2 + \|w_j\|^2/\epsilon$ (by Young's inequality) for all terms involving $\|\underline{y_i}\|\|w_j\|$; we use Young's inequality for all terms involving $\|\underline{y}\|\|\underline{\delta_i}\|$ and $\|\underline{u}\|\|\underline{\delta_7}\|$; we use the a priori estimate $\|\underline{\lambda}\| \leq c \left(\sum_{i=1}^{6} \|\underline{\delta_i}\| + \|\underline{y}\|\right)$ for $\|\underline{\lambda}\| \sum_{i=8}^{13} \|\underline{\delta_i}\|$; and rearrange terms, to obtain

$$
\|\underline{y}\| + \|\underline{u}\| + \|\underline{\lambda}\| \leq c \sum_{i=1}^{13} \|\underline{\delta_i}\|,
$$

which proves the claim. ∎

By Robinson's implicit function theorem, the Lipschitz continuity of (σ, ξ, λ) implies the same property for the critical points of the Karush-Kuhn-Tucker system (3.3):

THEOREM 3.3 (Lipschitz stability of (Σ, Ξ, Λ)). *Suppose that the coercivity assumption* (AC) *holds. Assume that there exists $\nu > 0$ and $\epsilon > 0$ such that for all p_1,*

p_2 *from the normed linear space of parameters such that* $\|p_i - p_0\| < \epsilon$, *we have*

$$\|F(y_0, u_0, \lambda_0; p_1) - F(y_0, u_0, \lambda_0; p_2)\|_Z \le \nu \|p_1 - p_2\|, \tag{3.18}$$

then there exist ϵ' *and* $\eta > 0$ *and a Lipschitz continuous map* $p \mapsto (\Sigma(p), \Xi(p), \Lambda(p))$ *such that for all* $\|p - p_0\| < \epsilon'$, $(\Sigma(p), \Xi(p), \Lambda(p))$ *is a solution to* (3.3) *which is unique in the* η*-neighborhood of* (y_0, u_0, λ_0), *and* $(\Sigma(p_0), \Xi(p_0), \Lambda(p_0)) = (y_0, u_0, \lambda_0)$. *Moreover, due to the coercivity assumption, the critical points* $(\Sigma(p), \Xi(p), \Lambda(p))$ *satisfy second order sufficient conditions and are indeed local optimal solutions to* (RD(p)).

Proof. The first assertion follows directly from Robinson [21], Theorem 2.1 and Corollary 2.2. We observe that the coercivity assumption (AC) implies that the second order sufficient conditions [19] hold. By Theorem 3.5, the second order sufficient conditions hold not only for the nominal solution (y_0, u_0, λ_0), but in a neighborhood of this solution. Consequently, choosing ϵ' sufficiently small, $(\Sigma(p), \Xi(p), \Lambda(p))$ is a locally unique optimal solution. ∎

REMARK 3.4. *Assumption* (3.18) *holds for a broad range of parameter perturbations of the KKT system* (3.3), *including the perturbations specified in* (3.1).

THEOREM 3.5 (Stability of second order sufficient conditions). *The coercivity assumption* (AC) *implies that a second order sufficient condition holds at the nominal solution* $(y_0, u_0, \lambda_0; p_0)$. *Under the requisites of Theorem* 3.3, *assumption* (AC) *still holds with a number* $0 < \rho' < \rho$ *if* (y_1^0, y_2^0) *is replaced by* $\Sigma(p)$, *and if the parameter vector* p_0 *is replaced by* p. *In particular, the perturbed solution* $(\Sigma(p), \Xi(p), \Lambda(p))$ *also satisfies second order sufficient conditions and it is thus a locally unique solution for* (RD(p)).

Proof. For second order sufficient conditions to hold, it suffices to choose $u \in r(U_{\text{ad}} - u_0)$ with some $r > 0$, see Maurer and Zowe [19], Theorem 5.6, which is superseded by assumption (AC). For now, let ϵ' be chosen according to Theorem 3.3, possibly to be adjusted later, and let $\|p - p_0\| < \epsilon'$. It follows easily that

$$|L_{xx}(\Sigma(p), \Xi(p), \Lambda(p); p)(\overline{x}, \overline{x}) - L_{xx}(y_0, u_0, \lambda_0; p_0)(\overline{x}, \overline{x})| \le c_1 \epsilon' \|\overline{x}\|_X^2 \tag{3.19}$$

for arbitrary $\overline{x} \in X$. The norm on $X = [H^{2,1}(Q)]^2 \times \mathbb{L}^2(Q)$ is the usual norm of the product space.
Now let $\overline{\overline{y}}$ satisfy the linear PDE (3.10) given with (AC), where (y_1^0, y_2^0) has been replaced by $\Sigma(p)$, p_0 has been replaced by p, and where the arbitrary $\overline{\overline{u}} \in \mathbb{L}^2(Q)$ serves as control, $\overline{\overline{u}} = 0$ where $a(x,t) = b(x,t)$. In other words, $(\overline{\overline{y}}, \overline{\overline{u}}) \in K(p)$, where $K(p)$ is the linear space

$$K(p) = \ker e_x(\Sigma(p), \Xi(p); p) \cap \{(y, u) : u = 0 \text{ where } u_a = u_b\}.$$

If we define $\overline{y}$ to satisfy (3.10) with control $\overline{\overline{u}}$—in other words, $(\overline{y}, \overline{\overline{u}}) \in K(p_0)$—, then their difference $\overline{\overline{y}} - \overline{y}$ also satisfies a linear PDE, and it follows from the a priori estimates in Lemma 2.3 that

$$\|\overline{\overline{y}} - \overline{y}\|_{[H^{2,1}(Q)]^2} \le c_2 \epsilon' \|\overline{\overline{y}}\|_{[H^{2,1}(Q)]^2} \tag{3.20}$$

holds. Using the triangle inequality, we obtain from (3.20)

$$\|\overline{\overline{y}} - \overline{y}\|_{[H^{2,1}(Q)]^2} \le \frac{c_2 \epsilon'}{1 - c_2 \epsilon'} \|\overline{y}\|_{[H^{2,1}(Q)]^2}.$$

We have thus proved that for any $\overline{\overline{x}} = (\overline{\overline{y}}, \overline{\overline{u}}) \in K(p)$, there exists $\overline{x} = (\overline{y}, \overline{\overline{u}}) \in K(p_0)$ such that their difference satisfies

$$\|\overline{\overline{x}} - \overline{x}\|_X \le \frac{c_2 \epsilon'}{1 - c_2 \epsilon'} \|\overline{x}\|_X. \tag{3.21}$$

Using the standard estimate from Maurer and Zowe [19], Lemma 5.5, possibly making ϵ' smaller, it follows from (3.21) that

$$L_{xx}(y_0, u_0, \lambda_0; p_0)(\overline{\overline{x}}, \overline{\overline{x}}) \geq \rho' \|\overline{\overline{x}}\|_X^2 \tag{3.22}$$

holds with some $\rho' > 0$.
Combining (3.19) and (3.22) finally yields

$$\begin{aligned} L_{xx}(\Sigma(p), \Xi(p), \Lambda(p); p)(\overline{\overline{x}}, \overline{\overline{x}}) &\geq L_{xx}(y_0, u_0, \lambda_0; p_0)(\overline{\overline{x}}, \overline{\overline{x}}) - c_1 \epsilon' \|\overline{\overline{x}}\|_X^2 \\ &\geq (\rho_0 - c_1 \epsilon') \|\overline{\overline{x}}\|_X^2 \end{aligned}$$

with some $\rho' > 0$, which concludes the proof. □

REMARK 3.6. *By the choice of $H^{2,1}(Q)$ for the state space, in which the state equation's nonlinearity is differentiable, the two-norm discrepancy for the second order sufficient conditions has been avoided here.*

Before we turn to the differentiability properties of the solutions, we mention an obvious corollory concerning the control constraint multiplier μ:

COROLLARY 3.7. *Under the requisites of Theorem 3.3, the control constraint multiplier introduced in (2.16) is a Lipschitz continuous function of p for $\|p - p_0\| < \epsilon'$:*

$$\mu = M(p) = -(\gamma \Xi(p) - \Lambda_2(p)) = -L_u(\Sigma(p), \Xi(p), \Lambda(p); p).$$

4. Directional Differentiability of Solutions.

In extension of the Lipschitz stability results from the previous section, we prove that under the same coercivity assumption (AC), the local optimal solutions $(\Sigma(p), \Xi(p), \Lambda(p))$ are directionally differentiable. Moreover, we characterize the directional differentials in terms of the solutions of another linear-quadratic optimal control problem.

Let us introduce the following definitions of the subsets of Q where the nominal control u_0 is active and strongly active, respectively:

$$\begin{aligned} \underline{Q} &= \{(x,t) \in Q : u_0(x,t) = u_a(x,t)\} & \overline{Q} &= \{(x,t) \in Q : u_0(x,t) = u_b(x,t)\} \\ \underline{Q}^0 &= \{(x,t) \in \underline{Q} : \mu_0(x,t) > 0\} & \overline{Q}^0 &= \{(x,t) \in \overline{Q} : \mu_0(x,t) < 0\} \end{aligned}$$

where $\mu_0 = -(\gamma u_0 - \lambda_2^0)$ denotes the constraint multiplier belonging to the constraint $u_0 \in U_{\text{ad}}$. Moreover, we denote by $\hat{U}_{\text{ad}}$ the set of admissible control variations:

$$u \in \hat{U}_{\text{ad}} \Leftrightarrow \begin{cases} u = 0 & \text{on } \underline{Q}^0 \cup \overline{Q}^0 \\ u \geq 0 & \text{on } \underline{Q} \\ u \leq 0 & \text{on } \underline{Q} \end{cases}$$

which reflects the fact that if the nominal control u_0 is equal to the lower bound u_a, we can approach it only from above and vice versa. In addition, if the control constraint is strongly active, the variation is zero there.

THEOREM 4.1 (Directional differentiability of (σ, ξ, λ)). *Suppose that the coercivity assumption* (AC) *holds. Then for any given direction $\hat{\delta} \in Z$, the map $\delta \mapsto (\sigma(\delta), \xi(\delta), \lambda(\delta))$ is directionally differentiable at $\delta = 0$, and the differential $D(\sigma, \xi, \lambda)(0; \hat{\delta})$ is given by the unique solution and adjoint state in* $[H^{2,1}(Q)]^2 \times \mathbb{L}^2(Q) \times$

$[H^{2,1}(Q)]^2$ *of the auxiliary linear-quadratic optimal control problem*

$$\begin{aligned}
&\text{Minimize} \quad \frac{\alpha_1}{2}\|y_1(\cdot,T)\|^2_{\mathbb{L}^2(\Omega)} + \frac{\alpha_2}{2}\|y_2(\cdot,T)\|^2_{\mathbb{L}^2(\Omega)} + \frac{\gamma}{2}\|u\|^2_{\mathbb{L}^2(Q)} \\
&+ \int_Q (k_1\lambda_1^0 + k_2\lambda_2^0)\, y_1 y_2 \\
&- \int_Q \hat\delta_1 y_1 - \int_\Sigma \hat\delta_2 y_1 - \int_\Omega \hat\delta_3 y_1(\cdot,T) - \int_Q \hat\delta_4 y_2 - \int_\Sigma \hat\delta_5 y_2 - \int_\Omega \hat\delta_6 y_2(\cdot,T) \\
&- \int_Q \hat\delta_7 u \qquad\qquad (\mathrm{DQP}(\hat\delta))
\end{aligned}$$

subject to $u \in \hat U_{\mathrm{ad}}$ and

$$\begin{aligned}
\frac{\partial}{\partial t}y_1 - D_1\Delta y_1 + k_1 y_2^0 y_1 + k_1 y_1^0 y_2 &= \hat\delta_8 \\
D_1\frac{\partial}{\partial n}y_1 &= \hat\delta_9 \\
y_1(\cdot,0) &= \hat\delta_{10} \\
\frac{\partial}{\partial t}y_2 - D_2\Delta y_2 + k_2 y_2^0 y_1 + k_2 y_1^0 y_2 &= u + \hat\delta_{11} \\
D_2\frac{\partial}{\partial n}y_2 &= \hat\delta_{12} \\
y_2(\cdot,0) &= \hat\delta_{13}.
\end{aligned} \tag{4.1}$$

Proof. Let $\hat\delta \in Z$ be any direction, and let $\tau^n \searrow 0$ and $\delta^n = \tau^n\hat\delta$. In virtue of Theorem 3.2, we have

$$\left\|\frac{y^n - y_0}{\tau^n}\right\|_{[H^{2,1}(Q)]^2} \le L\,\|\hat\delta\| \qquad \left\|\frac{\lambda^n - \lambda_0}{\tau^n}\right\|_{[H^{2,1}(Q)]^2} \le L\,\|\hat\delta\|$$

where $y^n = \sigma(\delta^n)$ etc. Since $H^{2,1}(Q)$ is a Hilbert space, there exists a subsequence, still denoted by index n, such that $(y^n - y_0)/\tau^n$ converges weakly to some element $\hat y \in [H^{2,1}(Q)]^2$, and by compactness of the embedding, the convergence is strong in $[\mathbb{L}^2(Q)]^2$. Moreover, we can extract another subsequence such that the convergence is also pointwise, and the same argument applies to $(\lambda^n - \lambda_0)/\tau^n$. From the variational inequality (3.8) it follows that $u^n = P_{U_{\mathrm{ad}}}((\lambda_2^n + \delta_7^n)/\gamma)$ where $P_{U_{\mathrm{ad}}}$ denotes the pointwise projection onto the admissible set U_{ad}. By distinguishing the subsets of Q where the nominal control u_0 is either inactive, active or strongly active, it is straightforward to verify that the pointwise limit $\hat u = \lim_{n\to\infty}(u^n - u_0)/\tau^n$ satisfies

$$\hat u = P_{\hat U_{\mathrm{ad}}}\left((\hat\lambda_2 + \hat\delta_7)/\gamma\right) \tag{4.2}$$

and is thus an element of $\mathbb{L}^2(Q)$.
Moreover, by Lebesgue's Dominated Convergence Theorem, since we have the pointwise estimate

$$\left|\frac{u^n - u_0}{\tau^n} - \hat u\right| \le g^n = \frac{1}{\gamma}\left(\left|\frac{\lambda_2^n - \lambda_2^0}{\tau^n}\right| + \left|\frac{\delta_7^n}{\tau^n}\right|\right) + \frac{1}{\gamma}\left(|\hat\lambda_2| + |\hat\delta_7|\right),$$

and g^n converges pointwise and in $\mathbb{L}^2(Q)$ to $2(|\hat\lambda_2| + |\hat\delta_7|)/\gamma$, we find that $(u^n - u_0)/\tau^n$ converges to $\hat u$ also in $\mathbb{L}^2(Q)$.

Like in Theorem 2.6, using the weak convergence, one proves that the limit $(\hat{y}, \hat{u})$ satisfies the state equation (4.1), and that the limit $\hat{\lambda}$ satisfies the adjoint equation corresponding to (DQP($\hat{\delta}$)). The difference quotient $(y^n - y_0)/\tau^n - \hat{y}$ satisfies the state equation (4.1) with all $\hat{\delta}$ replaced by zeros and u replaced by $(u^n - u_0)/\tau^n - \hat{u}$. A similar calculation can be done for the adjoint equation. As the solution depends continuously on the right hand side data (Lemma (2.8)), which converges to zero, it follows from the a priori estimate that in fact

$$\frac{y^n - y_0}{\tau^n} \to \hat{y} \quad \text{in } [H^{2,1}(Q)]^2 \qquad\qquad \frac{\lambda^n - \lambda_0}{\tau^n} \to \hat{\lambda} \quad \text{in } [H^{2,1}(Q)]^2.$$

The whole argument remains valid if in the beginning, we start with an arbitrary subsequence of τ^n. Since in view of the coercivity assumption (AC), the limit $(\hat{y}, \hat{u}, \hat{\lambda})$ is the unique solution of (DQP($\hat{\delta}$)), the convergence extends to the whole sequence, and the proof is complete. □

Just like in the case of Lipschitz continuity, the solutions to the nonlinear KKT conditions (3.3) inherit the property of directional differentiability from the solutions of the linearized generalized equation (3.6):

THEOREM 4.2 (Directional differentiability of (Σ, Ξ, Λ)). *Suppose that the coercivity assumption* (AC) *holds. Assume that the Lipschitz condition* (3.18) *holds and that in addition,* $F(y_0, u_0, \lambda_0; p)$ *is Fréchet differentiable with respect to* p *at* p_0*. Then the map* $p \mapsto (\Sigma(p), \Xi(p), \Lambda(p))$ *is directionally differentiable at* p_0*, and the differential* $D(\Sigma, \Xi, \Lambda)(0; \overline{p})$ *is given by the chain rule*

$$D(\Sigma, \Xi, \Lambda)(p_0; \overline{p}) = D(\sigma, \xi, \lambda)(0; -F_p(y_0, u_0, \lambda_0; p_0)\,\overline{p}), \tag{4.3}$$

i.e., by the solution of (DQP($\hat{\delta}$)) *with* $\hat{\delta} = -F_p(y_0, u_0, \lambda_0; p_0)\,\overline{p}$.

Proof. The theorem follows from Dontchev [8], Theorem 2.4, observing that $g(y, u, \lambda) = F(y_0, u_0, \lambda_0; p_0) + F'(y_0, u_0, \lambda_0; p_0)(y - y_0, u - u_0, \lambda - \lambda_0)$ strongly approximates F in (y, u, λ) at (y_0, u_0, λ_0) in the sense of [8]. □

REMARK 4.3. *For Theorem* 4.2 *to hold it is sufficient that* $F(y_0, u_0, \lambda_0; p)$ *be directionally differentiable with respect to* p *at* p_0*. For the perturbations listed in* (3.1)*, however, Fréchet differentiability holds.*

In analogy to Corollary 3.7, we obtain directional differentiability of the control constraint multiplier:

COROLLARY 4.4. *Under the requisites of Theorem* 4.2*, the control constraint multiplier* $\mu = M(p)$ *is also directionally differentiable at* p_0 *with*

$$DM(p_0; \overline{p}) = -(\overline{\gamma} u_0 + \gamma_0 D\Xi(p_0; \overline{p}) - D\Lambda_2(p_0; \overline{p})).$$

At this point it becomes evident that the map $\delta \mapsto (\sigma(\delta), \xi(\delta), \lambda(\delta))$ can not in general be Fréchet differentiable since its directional derivative is not linear: If (y, u, λ) is the directional derivative of (σ, ξ, λ) in the direction of $\hat{\delta}$, then $-u$ may not be in $\hat{U}_{\text{ad}}$, thus $-(y, u, \lambda)$ may not be the derivative in the direction of $-\hat{\delta}$. Linearity is only observed if $\hat{U}_{\text{ad}}$ is a linear space, i.e., if strict complementarity holds at the nominal solution (that is, if $\underline{Q} = \underline{Q}^0$ and $\overline{Q} = \overline{Q}^0$ hold up to sets of measure zero). Consequently, the directional derivative of $p \mapsto (\Sigma(p), \Xi(p), \Lambda(p))$ will only be linear in the case of strict complementarity.

5. Taylor expansion of the objective value and examples. The minimum value function

$$\Phi(p) = f(\Sigma(p), \Xi(p), \Lambda(p); p) = L(\Sigma(p), \Xi(p), \Lambda(p); p)$$

yields the objective value along the local optimal solutions as p ranges over a neighborhood of the nominal p_0. Using the differentiability properties of the state, control and adjoint functions, one can construct first and second order derivatives of the minimum value function. To improve readability, let us denote by L^0 the evaluation of the Lagrangian at the nominal arguments $(y_0, u_0, \lambda_0; p_0)$. In addition, let us denote by $\overline{y}$ and $\hat{y}$ the directional derivatives of the nominal state in the directions of $\overline{p}$ and $\hat{p}$, respectively, i.e., $\overline{y} = D\Sigma(p_0; \overline{p})$, and similarly for the control and adjoint variables.

THEOREM 5.1. *Under the requisites of Theorem 4.2, the minimum value function Φ is Fréchet differentiable at p_0 with*

$$D\Phi(p_0; \overline{p}) = L_p(y_0, u_0, \lambda_0; p_0)\overline{p}. \tag{5.1}$$

Its second order directional derivatives also exist and are given by

$$D^2\Phi(p_0; \overline{p}, \hat{p}) = [\overline{y} \;\; \overline{u} \;\; \overline{p}] \begin{bmatrix} L^0_{yy} & L^0_{yu} & L^0_{yp} \\ L^0_{uy} & L^0_{uu} & L^0_{up} \\ L^0_{py} & L^0_{pu} & L^0_{pp} \end{bmatrix} \begin{bmatrix} \hat{y} \\ \hat{u} \\ \hat{p} \end{bmatrix}. \tag{5.2}$$

Proof. From the classical chain rule, it follows that

$$D\Phi(p_0; \overline{p}) = L^0_y \overline{y} + L^0_u \overline{u} + L^0_\lambda \overline{\lambda} + L^0_p \overline{p}.$$

By the optimality condition for the nominal problem, the first and third terms vanish. Since $\mu_0 = -L^0_u$ and $\overline{u} = 0$ where $\mu_0 \neq 0$ by definition of $\hat{U}_{\text{ad}}$, the second term is also seen to be zero, thus (5.1) holds.
Differentiating $L_p(\Sigma(p), \Xi(p), \Lambda(p); p)$ totally with respect to p, in the direction of $\hat{p}$, yields by the classical chain rule the second directional differential of the minimum value function:

$$D^2\Phi(p_0; \overline{p}, \hat{p}) = [\overline{y} \;\; \overline{u} \;\; \overline{\lambda} \;\; \overline{p}] \begin{bmatrix} L^0_{yy} & L^0_{yu} & L^0_{y\lambda} & L^0_{yp} \\ L^0_{uy} & L^0_{uu} & L^0_{u\lambda} & L^0_{up} \\ L^0_{\lambda y} & L^0_{\lambda u} & L^0_{\lambda\lambda} & L^0_{\lambda p} \\ L^0_{py} & L^0_{pu} & L^0_{p\lambda} & L^0_{pp} \end{bmatrix} \begin{bmatrix} \hat{y} \\ \hat{u} \\ \hat{\lambda} \\ \hat{p} \end{bmatrix},$$

which is easily seen to be the same as (5.2) as L^0_λ and $L^0_{\lambda\lambda}$ vanish. ☐

To be specific, let

$$\overline{p} = (\overline{D_1}, \overline{D_2}, \overline{k_1}, \overline{k_2}, \overline{\alpha_1}, \overline{\alpha_2}, \overline{\gamma}, \overline{y_{10}}, \overline{y_{20}}, \overline{y_{1T}}, \overline{y_{2T}})^\top$$

be any given parameter direction. Then the first order directional derivative of Φ is

$$\begin{aligned} D\Phi(p_0; \overline{p}) &= L_p(y_0, u_0, \lambda_0; p_0)\overline{p} \\ &= \frac{\overline{\alpha_1}}{2}\|y_1(\cdot, T) - y_{1T}\|^2_{\mathbb{L}^2(Q)} - \alpha_1 \int_\Omega (y^0_1(\cdot, T) - y_{1T})\overline{y_{1T}} \\ &+ \frac{\overline{\alpha_2}}{2}\|y_2(\cdot, T) - y_{2T}\|^2_{\mathbb{L}^2(Q)} - \alpha_2 \int_\Omega (y^0_2(\cdot, T) - y_{2T})\overline{y_{2T}} + \frac{\overline{\gamma}}{2}\|u_0\|^2_{\mathbb{L}^2(Q)} \\ &+ \int_Q (-\overline{D_1}\Delta y^0_1 + \overline{k_1} y^0_1 y^0_2)\lambda^0_1 - \int_\Omega \overline{y_{10}}\lambda^0_1(\cdot, 0) \\ &+ \int_Q (-\overline{D_2}\Delta y^0_2 + \overline{k_2} y^0_1 y^0_2)\lambda^0_2 - \int_\Omega \overline{y_{20}}\lambda^0_2(\cdot, 0). \end{aligned}$$

In particular, we have verified the well-known marginal interpretation of the adjoint variable [4]: When only the initial conditions y_{i0} are perturbed, then the adjoint variable at $t = 0$ gives the (negative) first order change of the minimum value function:

$$D\Phi(p_0; \overline{p}) = -\int_\Omega \overline{y_{10}} \lambda_1^0(\cdot, 0) - \int_\Omega \overline{y_{20}} \lambda_2^0(\cdot, 0).$$

The second order differential can be easily computed explicitly for our example, but we omit the lengthy term here for brevity.

6. Conclusion. In this paper, we have examined optimal solutions for a control-constrained optimal control problem governed by a system of semilinear parabolic reaction-diffusion equations. These solutions depend on an infinite-dimensional parameter p which models perturbations of the dynamics in terms of reaction and diffusion coefficients, initial conditions, and of some quantities in the objective function. Under a natural coercivity assumption, which implies that second order sufficient conditions are satisfied at the nominal and the perturbed solutions, we have found that the optimal solutions depend Lipschitz-continuously on the parameter, and that their directional derivative exists. The directional derivative, also called the parametric sensitivity of the optimal solution, has been characterized as the unique solution of an additional linear-quadratic optimal control problem. Hence, these parametric sensitivities are computable at the relatively low numerical cost equivalent to one additional QP step. This sensitivity information offers one approach towards realtime optimal control of time-dependent partial differential equations. Since the sensitivities can be computed beforehand (offline) along with the nominal solution, the Taylor expansions $\Sigma(p_0 + \overline{p}) \approx y_0 + D\Sigma(p_0; \overline{p})$ etc. can be evaluated at negligible numerical cost to give an estimate of the perturbed solution. The directional derivative of the control constraint multiplier μ shows where a control constraint tends to become active, more strongly active, or inactive. Altogether, the parametric sensitivities yield qualitative and quantitative information about the first order change of the nominal solution.

For a practical algorithm for the computation of the sensitivities, based on a primal-dual active set SQP strategy, along with numerical results, we point to [9] and the follow-up paper [10].

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