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Parametric Sensitivity Analysis for Optimal Boundary Control of a 3D Reaction-Diffusion System

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Abstract

A boundary optimal control problem for an instationary nonlinear reaction-diffusion equation system in three spatial dimensions is presented. The control is subject to pointwise control constraints and a penalized integral constraint. Under a coercivity condition on the Hessian of the Lagrange function, an optimal solution is shown to be a directionally differentiable function of perturbation parameters such as the reaction and diffusion constants or desired and initial states. The solution's derivative, termed parametric sensitivity, is characterized as the solution of an auxiliary linear-quadratic optimal control problem. A numerical example illustrates the utility of parametric sensitivities which allow a quantitative and qualitative perturbation analysis of optimal solutions.

Keywords: Optimal Control, Reaction-Diffusion Equations, Sensitivity Analysis.

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. The subject matter of the present paper is an optimal boundary control problem for a time-dependent coupled system of semilinear parabolic reaction-diffusion equations. The equations model a chemical or biological process where the species involved are subject to diffusion and reaction among each other. The goal in the optimal control problem is to drive the reaction-diffusion model from the given initial state as close as possible to a desired terminal state. However, the control has to be chosen within given upper and lower bounds which are motivated by physical or technological considerations.

In practical applications, it is unlikely that all parameters in the model are precisely known a priori. Therefore, we embed the optimal control problem into a family of problems, which depend on a parameter vector p. In our case, p can comprise physical parameters such as reaction and diffusion constants, but also desired terminal states, etc. In this paper we prove that under a coercivity condition on the Hessian of the Lagrange function, local solutions of the optimal control problem depend Lipschitz continuously and directionally differentiably on the parameter p. Moreover, we characterize the derivative as the solution of an additional linear-quadratic optimal control problem, known as the sensitivity problem. If these sensitivities are computed "offline", *i.e.*, along with the optimal solution of the nominal (unperturbed) problem belonging to the expected parameter value p_0, a first order Taylor approximation can give a real-time ("online") estimate of the perturbed solution.

Let us put the current paper into a wider perspective: Lipschitz dependence and differentiability properties of parameter-dependent optimal control problems for PDEs have been investigated in the recent papers [6, 11–14, 16, 18]. In particular, sensitivity results have been derived in [6] for a two-dimensional reaction-diffusion model with distributed control. In contrast, we consider here the more difficult situation in three spatial dimensions and with boundary control and present both theoretical and numerical results. Other numerical results can be found in [3, 7].

The main part of the paper is organized as follows: In Section 2, we introduce the reaction-diffusion system at hand and the corresponding optimal control problem. We also state its first order optimality conditions. Since this problem, without parameter dependence, has been thoroughly investigated in [9], we only briefly recall the main results. Section 3 is devoted to establishing the so-called *strong regularity property* for the optimality system. This necessitates the investigation of the *linearized* optimality system for which the solution is shown to be Lipschitz and differentiable with respect to perturbations. In Section 4, these properties for the linearized problem are shown to carry over to the original nonlinear optimality system, in virtue of a suitable implicit function theorem. Finally, we present some numerical results in Section 5 in order to further illustrate the concept of parametric sensitivities.

Necessarily all numerical results are based on a discretized version of our infinite-dimensional problem. Nevertheless we prefer to carry out the analysis in the continuous setting so that smoothness properties of the involved quantities become evident which could then be used for instance to determine rates of convergence under refinements of the discretization etc. In view of our problem involving a nonlinear time-dependent system of partial differential equations, its discretization yields a large scale nonlinear optimization problem, albeit with a special structure.

2 The Reaction-Diffusion Optimal Boundary Control Problem

Reaction-diffusion equations model chemical or biological processes where the species involved are subject to diffusion and reaction among each other. As an example, we consider the reaction $A + B \to C$ which obeys the law of mass action. To simplify the discussion, we assume that the backward reaction $C \to A + B$ is negligible and that the forward reaction proceeds with a constant (not temperature-dependent) rate. This leads to a coupled semilinear parabolic system for the respective concentrations (c_1, c_2, c_3) as follows:

$$\frac{\partial}{\partial t} c_1(t,x) = d_1 \Delta c_1(t,x) - k_1 c_1(t,x) c_2(t,x) \qquad \text{for all } (t,x) \in Q, \tag{1a}$$

$$\frac{\partial}{\partial t} c_2(t,x) = d_2 \Delta c_2(t,x) - k_2 c_1(t,x) c_2(t,x) \qquad \text{for all } (t,x) \in Q, \tag{1b}$$

$$\frac{\partial}{\partial t} c_3(t,x) = d_3 \Delta c_3(t,x) + k_3 c_1(t,x) c_2(t,x) \qquad \text{for all } (t,x) \in Q. \tag{1c}$$

The scalars d_i and k_i, $i = 1, \ldots, 3$, are the diffusion and reaction constants, respectively. Here and throughout, let $\Omega \subset \mathbb{R}^3$ denote the domain of reaction and let $Q = (0,T) \times \Omega$ be the time-space cylinder where $T > 0$ is the given final time. We suppose that the boundary $\Gamma = \partial\Omega$ is Lipschitz and can be decomposed into two disjoint parts $\Gamma = \Gamma_n \cup \Gamma_c$, where Γ_c denotes the control boundary. Moreover, we let $\Sigma_n = (0,T) \times \Gamma_n$ and $\Sigma_c = (0,T) \times \Gamma_c$. We impose the following Neumann boundary conditions:

$$d_1 \frac{\partial c_1}{\partial n}(t,x) = 0 \qquad \text{for all } (t,x) \in \Sigma, \tag{2a}$$

$$d_2 \frac{\partial c_2}{\partial n}(t,x) = u(t)\, \alpha(t,x) \qquad \text{for all } (t,x) \in \Sigma_c, \tag{2b}$$

$$d_2 \frac{\partial c_2}{\partial n}(t,x) = 0 \qquad \text{for all } (t,x) \in \Sigma_n, \tag{2c}$$

$$d_3 \frac{\partial c_3}{\partial n}(t,x) = 0 \qquad \text{for all } (t,x) \in \Sigma. \tag{2d}$$

Equation (2b) prescribes the boundary flux of the second substance B by means of a given shape function $\alpha(t,x) \geq 0$, modeling, *e.g.*, the location of a spray nozzle revolving with time around one of the surfaces of Ω, while $u(t)$ denotes the control intensity at time t which is to be determined. The remaining homogeneous Neumann boundary conditions simply correspond to a "no-outflow" condition of the substances through the boundary of the reaction vessel Ω.

In order to complete the description of the model, we impose initial conditions for all three substances involved, *i.e.*,

$$c_1(0,x) = c_{10}(x) \quad \text{for all } x \in \Omega, \tag{3a}$$
$$c_2(0,x) = c_{20}(x) \quad \text{for all } x \in \Omega, \tag{3b}$$
$$c_3(0,x) = c_{30}(x) \quad \text{for all } x \in \Omega. \tag{3c}$$

Our goal is to drive the reaction-diffusion model (1)–(3) from the given initial state near a desired terminal state. Hence, we introduce the cost functional

$$J_1(c_1,c_2,u) = \frac{1}{2}\int_\Omega \left(\beta_1\,|c_1(T)-c_{1T}|^2 + \beta_2\,|c_2(T)-c_{2T}|^2\right)\,\mathrm{d}x + \frac{\gamma}{2}\int_0^T |u-u_d|^2\,\mathrm{d}t.$$

Here and in the sequel, we will find it convenient to abbreviate the notation and write $c_1(T)$ instead of $c_1(T,\cdot)$ or omit the arguments altogether when no ambiguity arises.

In the cost functional, β_1, β_2 and γ are non-negative weights, c_{1T} and c_{2T} are the desired terminal states, and u_d is some desired (or expected) control. In order to shorten the notation, we have assumed that the objective J_1 does not depend on the product concentration c_3. This allows us to delete the product concentration c_3 from the equations altogether and consider only the system for (c_1, c_2). All results obtained can be extended to the three-component system in a straightforward way.

The control $u : [0,T] \to \mathbb{R}$ is subject to pointwise box constraints $u_a(t) \leq u(t) \leq u_b(t)$. It is reasonable to assume that $u_a(t) \geq 0$, which together with $\alpha(t,x) \geq 0$ implies that the second (controlled) substance B can not be withdrawn through the boundary. The presence of an upper limit u_b is motivated by technological reasons. In addition to the pointwise constraint, it may be desirable to limit the total amount of substance B added during the process, *i.e.*, to impose a constraint like

$$\int_0^T u(t)\,\mathrm{d}t \leq u_c.$$

In the current investigation, we do not enforce this inequality directly but instead we add a penalization term

$$J_2(u) = \frac{1}{\varepsilon}\max\left\{0, \int_0^T u(t)\,\mathrm{d}t - u_c\right\}^3$$

to the objective, which then assumes the final form

$$J(c_1, c_2, u) = J_1(c_1, c_2, u) + J_2(u). \tag{4}$$

Our optimal control problem can now be stated as problem (**P**)

$$\begin{aligned} \text{Minimize} \quad J(c_1, c_2, u) \quad \text{s.t.} \quad & \text{(1a)–(1b), (2a)–(2c) and (3a)–(3b)} \\ \text{and} \quad & u_a(t) \le u(t) \le u_b(t) \quad \text{hold.} \end{aligned} \tag{P}$$

2.1 State Equation and Optimality System

The results in this section draw from the investigations carried out in [9] and are stated here for convenience and without proof. Our problem (**P**) can be posed in the setting

$$\begin{aligned} u \in U &= L^2(0, T) \\ (c_1, c_2) \in Y &= W(0, T) \times W(0, T). \end{aligned}$$

That is, we consider the state equation (1a)–(1b), (2a)–(2c) and (3a)–(3b) in its weak form, see Remark 2.4 and Section 2.2 for details. Here and throughout, $L^2(0, T)$ denotes the usual Sobolev space [1] of square-integrable functions on the interval $(0, T)$ and the Hilbert space $W(0, T)$ is defined as

$$W(0, T) = \big\{\varphi \in L^2(0, T; H^1(\Omega)) : \frac{\partial}{\partial t}\varphi \in L^2(0, T; H^1(\Omega)')\big\}.$$

containing functions of different regularity in space and time. Here, $H^1(\Omega)$ is again the usual Sobolev space and $H^1(\Omega)'$ is its dual. At this point we note for later reference the compact embedding [17, Chapter 3, Theorem 2.1]

$$W(0, T) \hookrightarrow\hookrightarrow L^2(0, T; H^s(\Omega)) \quad \text{for any } 1/2 < s < 1 \tag{5}$$

involving the fractional-order space $H^s(\Omega)$. For convenience of notation, we define the admissible set

$$U_{\text{ad}} = \{u \in U \ : \ u_a(t) \le u(t) \le u_b(t)\}.$$

Let us summarize the fundamental results about the state equation and problem (**P**). We begin with the following assumption which is needed throughout the paper:

Assumption 2.1 *(a) Let $\Omega \subset \mathbb{R}^3$ be a bounded open domain with Lipschitz continuous boundary $\Gamma = \partial\Omega$, which is partitioned into the control part Γ_c and the remainder Γ_n. Let d_i and k_i, $i = 1, 2$ be positive constants, and assume that $\alpha \in L^\infty(0, T; L^2(\Gamma_c))$ is non-negative. The initial conditions c_{i0}, $i = 1, 2$ are supposed to be in $L^2(\Omega)$. $T > 0$ is the given final time of the process.*

(b) *For the control problem, we assume desired terminal states* $c_{iT} \in L^2(\Omega)$, $i = 1, 2$, *and desired control* $u_d \in L^2(0, T)$ *to be given. Moreover, let* β_1, β_2 *be non-negative and* γ *be positive. Finally, we assume that the penalization parameter* ε *is positive and that* $u_c \in \mathbb{R}$ *and* u_a *and* u_b *are in* $L^\infty(0, T)$ *such that* $\int_0^T u_a(t)\,\mathrm{d}t \le u_c$.

Theorem 2.2 *Under Assumption 2.1(a), the state equation (1a)–(1b), (2a)–(2c) and (3a)–(3b) has a unique weak solution* $(c_1, c_2) \in W(0, T) \times W(0, T)$ *for any given* $u \in L^2(0, T)$. *The solution satisfies the a priori estimate*

$$\|c_1\|_{W(0,T)} + \|c_2\|_{W(0,T)} \le C\left(1 + \|c_{10}\|_{L^2(\Omega)} + \|c_{20}\|_{L^2(\Omega)} + \|u\|_{L^2(0,T)}\right)$$

with some constant $C > 0$.

In order to state the system of first order necessary optimality conditions, we introduce the active sets

$$\begin{aligned} A_-(u) &= \{t \in [0, T] \ : \ u(t) = u_a(t)\} \\ A_+(u) &= \{t \in [0, T] \ : \ u(t) = u_b(t)\} \end{aligned}$$

for any given control $u \in U_{\mathrm{ad}}$.

Theorem 2.3 *Under Assumption 2.1, the optimal control problem (*$\mathbf{P}$*) possesses at least one global solution in* $Y \times U_{\mathrm{ad}}$. *If* $(c_1, c_2, u) \in Y \times U_{\mathrm{ad}}$ *is a local solution, then there exists a unique adjoint variable* $(\lambda_1, \lambda_2) \in Y$ *satisfying*

$$\begin{aligned} -\frac{\partial}{\partial t}\lambda_1 - d_1\Delta\lambda_1 &= -k_1 c_2 \lambda_1 - k_2 c_2 \lambda_2 && \text{in } Q, && \text{(6a)} \\ -\frac{\partial}{\partial t}\lambda_2 - d_2\Delta\lambda_2 &= -k_1 c_1 \lambda_1 - k_2 c_1 \lambda_2 && \text{in } Q, && \text{(6b)} \\ d_1\frac{\partial \lambda_1}{\partial n} &= 0 && \text{on } \Sigma, && \text{(6c)} \\ d_2\frac{\partial \lambda_2}{\partial n} &= 0 && \text{on } \Sigma, && \text{(6d)} \\ \lambda_1(T) &= -\beta_1(c_1(T) - c_{1T}) && \text{in } \Omega, && \text{(6e)} \\ \lambda_2(T) &= -\beta_2(c_2(T) - c_{2T}) && \text{in } \Omega && \text{(6f)} \end{aligned}$$

in the weak sense, and a unique Lagrange multiplier $\xi \in L^2(0, T)$ *such that the optimality condition*

$$\gamma(u(t) - u_d(t)) + \frac{3}{\varepsilon}\max\left\{0, \int_0^T u(t)\,\mathrm{d}t - u_c\right\}^2 - \int_{\Gamma_c} \alpha(t, x)\,\lambda_2(t, x)\,\mathrm{d}x + \xi(t) = 0 \quad (7)$$

holds for almost all $t \in [0, T]$, *together with the complementarity condition*

$$\xi|_{A_-(u)} \le 0, \quad \xi|_{A_+(u)} \ge 0. \quad (8)$$

Remark 2.4 *The partial differential equations throughout this paper are always meant in their weak form. In case of the state and adjoint equations (1)–(3) and (6), respectively, the weak forms are precisely stated in Section 2.2 below, see the definition of F. However, we prefer to write the equations in their strong form to make them easier understandable.*

Solutions to the optimality system (6)–(8), including the state equation, can be found numerically by employing, *e.g.*, semismooth Newton or primal-dual active set methods, see [8, 10, 19] and [2, 9], respectively.

In the sequel, we will often find it convenient to use the abbreviations $y = (c_1, c_2)$ for the vector of state variables, $x = (y, u)$ for state/control pairs, and $\lambda = (\lambda_1, \lambda_2)$ for the vector of adjoint states. In passing, we define the Lagrangian associated to our problem (**P**),

$$\begin{aligned}\mathcal{L}(x, \lambda) = J(x) + \int_0^T \Big\{ \langle \frac{\partial}{\partial t} c_1, \lambda_1 \rangle + d_1 \int_\Omega \nabla c_1 \nabla \lambda_1 \, \mathrm{d}x + \int_\Omega k_1 c_1 c_2 \lambda_1 \, \mathrm{d}x \Big\} \, \mathrm{d}t \\ + \int_0^T \Big\{ \langle \frac{\partial}{\partial t} c_2, \lambda_2 \rangle + d_2 \int_\Omega \nabla c_2 \nabla \lambda_2 \, \mathrm{d}x + \int_\Omega k_2 c_1 c_2 \lambda_2 \, \mathrm{d}x - d_2 \int_{\partial\Omega} \alpha \, u \, \lambda_2 \, \mathrm{d}x \Big\} \, \mathrm{d}t \\ + \int_\Omega (c_1(0) - c_{10}) \, \lambda_1(0) \, \mathrm{d}x + \int_\Omega (c_2(0) - c_{20}) \, \lambda_2(0) \, \mathrm{d}x \end{aligned} \tag{9}$$

for any $x = (c_1, c_2, u) \in Y \times U$ and $\lambda = (\lambda_1, \lambda_2) \in Y$. The bracket $\langle u, v \rangle$ denotes the duality between $u \in H^1(\Omega)'$ and $v \in H^1(\Omega)$. The Lagrangian is twice continuously differentiable, and its Hessian with respect to the state and control variables is readily seen to be

$$\begin{aligned}\mathcal{L}_{xx}(x, \lambda)(\overline{x}, \overline{x}) = \beta_1 \|\overline{c}_1(T)\|^2_{L^2(\Omega)} + \beta_2 \|\overline{c}_2(T)\|^2_{L^2(\Omega)} + \gamma \|\overline{u}\|^2_{L^2(0,T)} \\ + \frac{6}{\varepsilon} \max \Big\{ 0, \int_0^T u(t) \, \mathrm{d}t - u_c \Big\} \Big(\int_0^T \overline{u}(t) \, \mathrm{d}t \Big)^2 + 2 \int_Q (k_1 \lambda_1 + k_2 \lambda_2) \, \overline{c}_1 \overline{c}_2 \, \mathrm{d}x \, \mathrm{d}t. \end{aligned} \tag{10}$$

The Hessian is a bounded bilinear form, *i.e.*, there exists a constant $C > 0$ such that

$$\mathcal{L}_{xx}(x, \lambda)(\overline{x}_1, \overline{x}_2) \le C \, \|\overline{x}_1\|_{Y \times U} \|\overline{x}_2\|_{Y \times U}$$

holds for all $(\overline{x}_1, \overline{x}_2) \in [Y \times U]^2$.

2.2 Parameter Dependence

As announced in the introduction, we consider problem (**P**) in dependence on a vector of parameters p and emphasize this by writing (**P**(p)). It is our goal to investigate the behavior of locally optimal solutions of (**P**(p)), or solutions of the optimality system (6)–(8) for that matter, as p deviates from its given nominal value p^*. In practice, the parameter vector p can be thought of as problem data which may be subject to perturbation or uncertainty. The nominal value p^* is then simply the expected value of the data. Our main result (Theorem 4.1) states that under a coercivity condition on the Hessian (10) of the Lagrange function, the solution of the optimality system belonging to ($\mathbf{P}(p)$) depends directionally differentiably on p. The derivatives are called parametric sensitivities since they yield the sensitivities of their underlying quantities with respect to perturbations in the parameter. Our analysis can be used to predict the solution at p near the nominal value p^* using a Taylor expansion. This can be exploited to devise a solution algorithm for ($\mathbf{P}(p)$) with real-time capabilities, provided that the nominal solution to ($\mathbf{P}(p^*)$) along with the sensitivities are computed beforehand ("offline"). In addition, the sensitivities allow a qualitative perturbation analysis of optimal solutions.

In our current problem, we take

$$\begin{aligned} p = (d_1, d_2, k_1, k_2, \beta_1, \beta_2, \gamma, u_c, \varepsilon, c_{10}, c_{20}, c_{1T}, c_{2T}, u_d) \\ \in \mathbb{R}^9 \times L^2(\Omega)^4 \times L^2(0,T) =: Q \end{aligned} \tag{11}$$

as the vector of perturbation parameters. Note that p belongs to an infinite-dimensional Hilbert space and that, besides containing physical parameters such as the reaction and diffusion constants k_i and d_i, it comprises non-physical data such as the penalization parameter ε.

In order to carry out our analysis, it is convenient to rewrite the optimality system (6)–(8) plus the state equation as a generalized equation, involving a set-valued operator. We notice that the complementarity condition (8) together with (7) is equivalent to the variational inequality

$$\int_0^T \xi(t)(\overline{u}(t) - u(t))\,\mathrm{d}t \le 0 \quad \forall \overline{u} \in U_{\mathrm{ad}}. \tag{12}$$

This can also be expressed as $\xi \in N(u)$ where

$$N(u) = \{v \in L^2(0,T) : \int_0^T v\,(\overline{u} - u)\,\mathrm{d}t \le 0 \text{ for all } \overline{u} \in U_{\mathrm{ad}}\}$$

if $u \in U_{\mathrm{ad}}$, and $N(u) = \emptyset$ if $u \notin U_{\mathrm{ad}}$. This set-valued operator is known as the dual cone of U_{ad} at u (after identification of $L^2(0,T)$ with its dual). To rewrite the remaining components of the optimality system into operator form, we introduce

$$F : W(0,T) \times L^2(0,T) \times W(0,T) \times Q \to Z$$

with the target space Z given by

$$Z = L^2(0,T;H^1(\Omega)')^2 \times L^2(\Omega)^2 \times L^2(0,T) \times L^2(0,T;H^1(\Omega)')^2 \times L^2(\Omega)^2.$$

The components of F are given next. Wherever it appears, ϕ denotes an arbitrary function in $L^2(0,T;H^1(\Omega))$. For reasons of brevity, we introduce $K = k_1\lambda_1 + k_2\lambda_2$.

$$\begin{aligned}
F_1(y,u,\lambda,p)(\phi) &= \int_0^T \left\{ \langle -\frac{\partial}{\partial t}\lambda_1, \phi\rangle + d_1 \int_\Omega \nabla\lambda_1 \cdot \nabla\phi \,\mathrm{d}x + \int_\Omega K c_2\, \phi \,\mathrm{d}x \right\} \mathrm{d}t \\
F_2(y,u,\lambda,p)(\phi) &= \int_0^T \left\{ \langle -\frac{\partial}{\partial t}\lambda_2, \phi\rangle + d_2 \int_\Omega \nabla\lambda_2 \cdot \nabla\phi \,\mathrm{d}x + \int_\Omega K c_1\, \phi \,\mathrm{d}x \right\} \mathrm{d}t \\
F_3(y,u,\lambda,p) &= \lambda_1(T) + \beta_1(c_1(T) - c_{1T}) \\
F_4(y,u,\lambda,p) &= \lambda_2(T) + \beta_2(c_2(T) - c_{2T}) \\
F_5(y,u,\lambda,p) &= \gamma(u-u_d) + \frac{3}{\varepsilon}\max\left\{0, \int_0^T u(t)\,\mathrm{d}t - u_c\right\}^2 - \int_{\Gamma_c} \alpha\,\lambda_2 \,\mathrm{d}x \\
F_6(y,u,\lambda,p)(\phi) &= \int_0^T \left\{ \langle \frac{\partial}{\partial t}c_1, \phi\rangle + d_1 \int_\Omega \nabla c_1 \cdot \nabla\phi \,\mathrm{d}x + \int_\Omega k_1 c_1 c_2\, \phi \,\mathrm{d}x \right\} \mathrm{d}t \\
F_7(y,u,\lambda,p)(\phi) &= \int_0^T \left\{ \langle \frac{\partial}{\partial t}c_2, \phi\rangle + d_2 \int_\Omega \nabla c_2 \cdot \nabla\phi \,\mathrm{d}x + \int_\Omega k_2 c_1 c_2\, \phi \,\mathrm{d}x \right\} \mathrm{d}t \\
&\quad - \int_\Sigma \alpha\, u\, \phi \,\mathrm{d}x\,\mathrm{d}t \\
F_8(y,u,\lambda,p) &= c_1(0) - c_{10} \\
F_9(y,u,\lambda,p) &= c_2(0) - c_{20}.
\end{aligned}$$

At this point it is not difficult to see that the optimality system (6)–(8), including the state equation (1a)–(1b), (2a)–(2c) and (3a)–(3b), is equivalent to the generalized equation

$$0 \in F(y,u,\lambda,p) + \mathcal{N}(u) \tag{13}$$

where we have set $\mathcal{N}(u) = (0,0,0,0,N(u),0,0,0,0)^\top \subset Z$. In the next section, we will investigate the following linearization around a given solution (y^*,u^*,λ^*) of (13) and for the given parameter p^*. This linearization depends on a new parameter $\delta \in Z$:

$$\delta \in F(y^*,u^*,\lambda^*,p^*) + F'(y^*,u^*,\lambda^*,p^*) \begin{pmatrix} y-y^* \\ u-u^* \\ \lambda-\lambda^* \end{pmatrix} + \mathcal{N}(u). \tag{14}$$

Herein F' denotes the Fréchet derivative of F with respect to (y,u,λ). Note that F is the gradient of the Lagrangian $\mathcal{L}$ and F' is its Hessian whose "upper-left block" was already mentioned in (10).

3 Properties of the Linearized Problem

In order to become more familiar with the linearized generalized equation (14), we write it in its strong form, assuming smooth perturbations $\delta = (\delta_1, \ldots, \delta_5)$. For better readability, the given parameter p^* is still denoted as in (11), without additional * in every component. We obtain from the linearizations of F_1 through F_4:

$$-\frac{\partial}{\partial t}\lambda_1 - d_1\Delta\lambda_1 + K\,c_2^* + K^* c_2 = K^* c_2^* + \delta_1 \quad \text{in } Q, \tag{15a}$$

$$-\frac{\partial}{\partial t}\lambda_2 - d_2\Delta\lambda_2 + K\,c_1^* + K^* c_1 = K^* c_1^* + \delta_2 \quad \text{in } Q, \tag{15b}$$

$$d_1\frac{\partial\lambda_1}{\partial n} = \delta_1|_\Sigma \quad \text{on } \Sigma, \tag{15c}$$

$$d_2\frac{\partial\lambda_2}{\partial n} = \delta_2|_\Sigma \quad \text{on } \Sigma, \tag{15d}$$

$$\lambda_1(T) = -\beta_1(c_1(T) - c_{1T}) + \delta_3 \quad \text{in } \Omega, \tag{15e}$$

$$\lambda_2(T) = -\beta_2(c_2(T) - c_{2T}) + \delta_4 \quad \text{in } \Omega, \tag{15f}$$

where we have abbreviated $K = k_1\lambda_1 + k_2\lambda_2$ and $K^* = k_1\lambda_1^* + k_2\lambda_2^*$. From the components F_6 through F_9 we obtain a linearized state equation:

$$\frac{\partial}{\partial t}c_1 - d_1\Delta c_1 + k_1c_1c_2^* + k_1c_1^*c_2 = k_1c_1^*c_2^* + \delta_6 \quad \text{in } Q, \tag{16a}$$

$$\frac{\partial}{\partial t}c_2 - d_2\Delta c_2 + k_2c_1c_2^* + k_2c_1^*c_2 = k_2c_1^*c_2^* + \delta_7 \quad \text{in } Q, \tag{16b}$$

$$d_1\frac{\partial c_1}{\partial n} = \delta_6|_\Sigma \quad \text{on } \Sigma, \tag{16c}$$

$$d_2\frac{\partial c_2}{\partial n} = \alpha\,u + \delta_7|_\Sigma \quad \text{on } \Sigma, \tag{16d}$$

$$c_1(0) = c_{10} + \delta_8 \quad \text{in } \Omega, \tag{16e}$$

$$c_2(0) = c_{20} + \delta_9 \quad \text{in } \Omega. \tag{16f}$$

Finally, the component F_5 becomes the variational inequality

$$\int_0^T \xi(t)(\overline{u}(t) - u(t))\,\mathrm{d}t \le 0 \quad \forall \overline{u} \in U_{\mathrm{ad}} \tag{17}$$

where in analogy to the original problem, $\xi \in L^2(0,T)$ is defined through

$$\gamma(u - u_d) + \frac{3}{\varepsilon}\max\Big\{0, \int_0^T u^*(t)\,\mathrm{d}t - u_c\Big\}^2 - \int_{\Gamma_c}\alpha\,\lambda_2\,\mathrm{d}x - \delta_5$$
$$+ \frac{6}{\varepsilon}\max\Big\{0, \int_0^T u^*(t)\,\mathrm{d}t - u_c\Big\}\int_0^T (u(t) - u^*(t))\,\mathrm{d}t + \xi(t) = 0. \tag{18}$$

In turn, the system (15)–(18) is easily recognized as the optimality system for an auxiliary linear quadratic optimization problem, which we term ($\mathbf{AQP}(\delta)$):

$$
\begin{aligned}
\text{Minimize } & \frac{1}{2}\mathcal{L}_{xx}(x^*,\lambda^*)(x,x) - \beta_1 \int_\Omega c_{1T}\, c_1(T)\,\mathrm{d}x - \beta_2 \int_\Omega c_{2T}\, c_2(T)\,\mathrm{d}x \\
& + \frac{3}{\varepsilon} \max\Big\{0, \int_0^T u^*(t)\,\mathrm{d}t - u_c\Big\}^2 \int_0^T u(t)\,\mathrm{d}t \\
& - \frac{6}{\varepsilon} \max\Big\{0, \int_0^T u^*(t)\,\mathrm{d}t - u_c\Big\} \Big(\int_0^T u^*(t)\,\mathrm{d}t\Big)\Big(\int_0^T u(t)\,\mathrm{d}t\Big) \\
& - \gamma \int_0^T u_d\, u\,\mathrm{d}t - \int_Q (k_1\lambda_1^* + k_2\lambda_2^*)(c_1^* c_2 + c_1 c_2^*)\,\mathrm{d}x\,\mathrm{d}t \\
& - \langle \delta_1, c_1\rangle - \langle \delta_2, c_2\rangle - \int_\Omega \delta_3 c_1(T) - \int_\Omega \delta_4 c_2(T) - \int_0^T \delta_5 u\,\mathrm{d}t \qquad (19)
\end{aligned}
$$

subject to the linearized state equation (16) above and $u \in U_{\mathrm{ad}}$. The bracket $\langle \delta_1, c_1\rangle$ here denotes the duality between $L^2(0,T;H^1(\Omega))$ and its dual $L^2(0,T;H^1(\Omega)')$. In order for ($\mathbf{AQP}(\delta)$) to have a strictly convex objective and thus to have a unique solution, we require the following assumption:

Assumption 3.1 (Coercivity Condition)
We assume that there exists $\rho > 0$ such that

$$\mathcal{L}_{xx}(x^*,\lambda^*)(x,x) \geq \rho\, \|x\|^2_{Y\times U}$$

holds for all $x = (c_1, c_2, u) \in Y \times U$ which satisfy the linearized state equation (16) in weak form, with all right hand sides except the term $\alpha\, u$ replaced by zero.

Sufficient conditions for Assumption 3.1 to hold are given in [9, Theorem 3.15]. We now prove our first result for the auxiliary problem ($\mathbf{AQP}(\delta)$):

Proposition 3.1 (Lipschitz Stability for the Linearized Problem)
Under Assumption 2.1, holding for the parameter p^*, and Assumption 3.1, ($\mathbf{AQP}(\delta)$) has a unique solution which depends Lipschitz continuously on the parameter $\delta \in Z$. That is, there exists $L > 0$ such that for all $\hat\delta, \check\delta \in Z$ with corresponding solutions $(\hat x, \hat\lambda)$ and $(\check x, \check\lambda)$,

$$
\begin{aligned}
& \|\hat c_1 - \check c_1\|_{W(0,T)} + \|\hat c_2 - \check c_2\|_{W(0,T)} + \|\hat u - \check u\|_{L^2(0,T)} \\
& \qquad + \|\hat\lambda_1 - \check\lambda_1\|_{W(0,T)} + \|\hat\lambda_2 - \check\lambda_2\|_{W(0,T)} \leq L\, \|\hat\delta - \check\delta\|_Z
\end{aligned}
$$

hold.

Proof. The proof follows the technique of [18] and is therefore kept relatively short here. Throughout, we denote by capital letters the differences we wish to estimate, *i.e.*, $C_1 = \hat{c}_1 - \check{c}_1$, etc. To improve readability, we omit the differentials $\mathrm{d}x$ and $\mathrm{d}t$ in integrals whenever possible. We begin by testing the weak form of the adjoint equation (15) by C_1 and C_2, and testing the weak form of the state equation (16) by Λ_1 and Λ_2, using integration by parts with respect to time and plugging in the initial and terminal conditions from (15) and (16). One obtains

$$\begin{aligned}\beta_1\|C_1(T)\|^2 + \beta_2\|C_2\|^2 + 2\int_Q K^* C_1\, C_2 + \int_\Sigma \alpha\, U\Lambda \\ = -\langle C_1, \Delta_1\rangle - \langle C_2, \Delta_2\rangle + \int_\Omega C_1(T)\Delta_3 + \int_\Omega C_2(T)\Delta_4 - \langle \Lambda_1, \Delta_6\rangle - \langle \Lambda_2, \Delta_7\rangle \\ - \int_\Omega \Lambda_1(0)\Delta_8 - \int_\Omega \Lambda_2(0)\Delta_9. \quad (20)\end{aligned}$$

From the variational inequality (17), using $\overline{u} = \hat{u}$ or $\overline{u} = \check{u}$ as test functions, we get

$$-\int_\Sigma \alpha\, U\Lambda_2 \leq -\gamma\,\|U\|^2 + \int_0^T U\Delta_5 - \frac{6}{\varepsilon}\max\left\{0, \int_0^T u^*(t)\,\mathrm{d}t - u_c\right\}\left(\int_0^T U\right)^2. \quad (21)$$

Unless otherwise stated, all norms are the natural norms for the respective terms. Adding the inequality (21) to (20) above and collecting terms yields

$$\begin{aligned}&\mathcal{L}_{xx}(x^*, \lambda^*)((C_1, C_2, U), (C_1, C_2, U)) \\ &\quad\leq -\langle C_1, \Delta_1\rangle - \langle C_2, \Delta_2\rangle + \int_\Omega C_1(T)\Delta_3 + \int_\Omega C_2(T)\Delta_4 + \int_0^T U\Delta_5 \\ &\qquad - \langle \Lambda_1, \Delta_6\rangle - \langle \Lambda_2, \Delta_7\rangle - \int_\Omega \Lambda_1(0)\Delta_8 - \int_\Omega \Lambda_2(0)\Delta_9 \\ &\quad\leq \kappa\,(1 + c^2)\big(\|C_1\|^2 + \|C_2\|^2 + \|\Lambda_1\|^2 + \|\Lambda_2\|^2\big) + \kappa\,\|U\|^2 + \frac{1}{4\kappa}\sum_{i=1}^{9}\|\Delta_i\|^2 \quad (22)\end{aligned}$$

where the last inequality has been obtained using Hölder's inequality, the embedding $W(0,T) \hookrightarrow C([0,T]; L^2(\Omega))$ and Young's inequality in the form $ab \leq \kappa a^2 + b^2/(4\kappa)$. The number $\kappa > 0$ denotes a sufficiently small constant which will be determined later at our convenience. Here and throughout, generic constants are denoted by c. They may take different values in different locations.
In order to make use of the Coercivity Assumption 3.1, we decompose $C_i = z_i + w_i$, $i = 1, 2$ and consider their respective equations, see (16). The z components account for the control influence while the w components arise from the perturbation differences

$\Delta_1, \ldots, \Delta_4$. We have on Q, Σ and Ω, respectively,

$$
\begin{aligned}
\frac{\partial}{\partial t} z_1 - d_1 \Delta z_1 + k_1 z_1 c_2^* + k_1 c_1^* z_2 &= 0 & \frac{\partial}{\partial t} w_1 - d_1 \Delta w_1 + k_1 w_1 c_2^* + k_1 c_1^* w_2 &= \Delta_6 \\
\frac{\partial}{\partial t} z_2 - d_2 \Delta z_2 + k_2 z_1 c_2^* + k_2 c_1^* z_2 &= 0 & \frac{\partial}{\partial t} w_2 - d_2 \Delta w_2 + k_2 w_1 c_2^* + k_2 c_1^* w_2 &= \Delta_7 \\
d_1 \frac{\partial z_1}{\partial n} &= 0 & d_1 \frac{\partial w_1}{\partial n} &= \Delta_6|_\Sigma \\
d_2 \frac{\partial z_2}{\partial n} &= \alpha\, U & d_2 \frac{\partial w_2}{\partial n} &= \Delta_7|_\Sigma \\
z_1(0) &= 0 & w_1(0) &= \Delta_8 \\
z_2(0) &= 0 & w_2(0) &= \Delta_9.
\end{aligned}
$$

Note that for (z_1, z_2, U), the Coercivity Assumption 3.1 applies and that standard a priori estimates yield $\|z_1\| + \|z_2\| \le c\|U\|$ and $\|w_1\| + \|w_2\| \le c(\|\Delta_6\| + \|\Delta_7\| + \|\Delta_8\| + \|\Delta_9\|)$. Using the generic estimates $\|z_i\|^2 \ge \|C_i\|^2 - 2\|C_i\|\|w_i\| + \|w_i\|^2$ and $\|z_i\| \le \|C_i\| + \|w_i\|$, the embedding $W(0,T) \hookrightarrow C([0,T]; L^2(\Omega))$ and the coercivity assumption, we obtain

$$
\begin{aligned}
\mathcal{L}_{xx}(x^*, \lambda^*)((C_1, C_2, U), (C_1, C_2, U)) &= \mathcal{L}_{xx}(x^*, \lambda^*)((z_1, z_2, U), (z_1, z_2, U)) \\
&\quad + \beta_1 \int_\Omega z_1(T) w_1(T) + \beta_2 \int_\Omega z_2(T) w_2(T) + \frac{\beta_1}{2}\|w_1(T)\|^2 + \frac{\beta}{2}\|w_2(T)\|^2 \\
&\quad + \int_Q K^*(w_1 z_2 + z_1 w_2 + w_1 w_2) \\
&\ge \rho\left(\|C_1\|^2 + \|C_2\|^2 + \|U\|^2\right) - 2\rho\big(\|C_1\|\|w_1\| + \|C_2\|\|w_2\|\big) \\
&\quad - \beta_1 c\,\|w_1\|\big(\|C_1\| + \|w_1\|\big) - \beta_2 c\,\|w_2\|\big(\|C_2\| + \|w_2\|\big) \\
&\quad - c\,\|K^*\|_{L^2(Q)}\big(\|w_1\|\|C_2\| + \|C_1\|\|w_2\| + 3\|w_1\|\|w_2\|\big). \qquad (23)
\end{aligned}
$$

For the last term, we have employed Hölder's inequality and the embedding $W(0,T) \hookrightarrow L^4(Q)$, see [4, p. 7]. Combining the inequalities (22) and (23) yields

$$
\begin{aligned}
\rho\left(\|C_1\|^2 + \|C_2\|^2 + \|U\|^2\right) &\le 2\rho\big(\|C_1\|\|w_1\| + \|C_2\|\|w_2\|\big) + \beta_1 c\,\|w_1\|\big(\|C_1\| + \|w_1\|\big) \\
&+ \beta_2 c\,\|w_2\|\big(\|C_2\| + \|w_2\|\big) + c\,\|K^*\|_{L^2(\Omega)}\big(\|w_1\|\|C_2\| + \|C_1\|\|w_2\| + 3\|w_1\|\|w_2\|\big) \\
&+ \frac{1}{8\kappa}\sum_{i=1}^{9}\|\Delta_i\|^2 + \frac{\kappa}{2}(1+c^2)\big(\|C_1\|^2 + \|C_2\|^2 + \|\Lambda_1\|^2 + \|\Lambda_2\|^2\big) + \frac{\kappa}{2}\|U\|^2 \qquad (24)
\end{aligned}
$$

and the last two terms can be absorbed in the left hand side when choosing $\kappa > 0$ sufficiently small and observing that Λ_1 and Λ_2 depend continuously on the data C_1 and C_2. By the a priori estimate stated above, w_i, $i = 1, 2$, can be estimated against the data $\Delta_7, \ldots, \Delta_9$. Using again Young's inequality on the terms $\|C_i\|\|w_j\|$ and absorbing the quantities of type $\kappa\|C_i\|^2$ into the left hand side, we obtain the Lipschitz dependence of (C_1, C_2, U) on $\Delta_1, \ldots, \Delta_9$. Invoking once more the continuous dependence of Λ_i on (C_1, C_2), Lipschitz stability is seen to hold also for the adjoint variable. $\square$

If (x^*, λ^*) is a solution to the optimality system (6)–(8) and state equation, then the previous theorem implies that the generalized equation (13) is strongly regular at this solution, compare [15]. Before showing that the Coercivity Assumption 3.1 implies also directional differentiability of the solution of $(\mathbf{AQP}(\delta))$ in dependence on δ, we introduce the *strongly active subsets* for the solution (y^*, u^*, λ^*) with multiplier ξ^* given by (7),

$$\begin{aligned} A^0_-(u^*) &= \{t \in [0,T] \ : \ \xi^*(t) < 0\} \\ A^0_+(u^*) &= \{t \in [0,T] \ : \ \xi^*(t) > 0\} \end{aligned}$$

Note that necessarily $u^* = u_a$ on $A^0_-(u^*)$ and $u^* = u_b$ on $A^0_+(u^*)$ hold in view of the variational inequality (12). Based on the notion of strongly active sets, we define $\widehat{U}_{\text{ad}}$, the set of admissible control variations:

$$u \in \widehat{U}_{\text{ad}} \Leftrightarrow u \in L^2(0,T) \text{ and } \begin{cases} u = 0 & \text{on } A^0_-(u^*) \cup A^0_+(u^*) \\ u \geq 0 & \text{on } A_-(u^*) \\ u \leq 0 & \text{on } A_+(u^*). \end{cases}$$

This definition reflects the fact that if the solution u^* associated to the parameter value p^* is equal to the lower bound u_a at some point $t \in [0,T]$, we can approach it only from above (and vice versa for the upper bound). In addition, if the control constraint is strongly active at some point, *i.e.*, if it has a nonzero multiplier ξ^* there, the variation is zero.

Proposition 3.2 (Differentiability for the Linearized Problem)
Under Assumptions 2.1 and 3.1, the unique solution to $(\mathbf{AQP}(\delta))$ *depends directionally differentiably on the parameter* $\delta \in Z$. *The directional derivative in the direction of* $\hat{\delta} \in Z$ *is given by the solution of the auxiliary linear quadratic problem* $(\mathbf{DQP}(\hat{\delta}))$,

$$\textit{Minimize } \frac{1}{2}\mathcal{L}_{xx}(x^*, \lambda^*)(x,x) - \langle \hat{\delta}_1, c_1 \rangle - \langle \hat{\delta}_2, c_2 \rangle - \int_\Omega \hat{\delta}_3 c_1(T) - \int_\Omega \hat{\delta}_4 c_2(T) - \int_0^T \hat{\delta}_5 u \, \mathrm{d}t$$

subject to $u \in \widehat{U}_{\rm ad}$ and the linearized state equation

$$
\begin{aligned}
\frac{\partial}{\partial t} c_1 - d_1 \Delta c_1 + k_1 c_1 c_2^* + k_1 c_1^* c_2 &= \hat{\delta}_6 && \text{in } Q && \text{(25a)}\\
\frac{\partial}{\partial t} c_2 - d_2 \Delta c_2 + k_2 c_1 c_2^* + k_2 c_1^* c_2 &= \hat{\delta}_7 && \text{in } Q && \text{(25b)}\\
d_1 \frac{\partial c_1}{\partial n} &= \hat{\delta}_6|_\Sigma && \text{on } \Sigma && \text{(25c)}\\
d_2 \frac{\partial c_2}{\partial n} &= \alpha\, u + \hat{\delta}_7|_\Sigma && \text{on } \Sigma, && \text{(25d)}\\
c_1(0) &= \hat{\delta}_8 && \text{in } \Omega && \text{(25e)}\\
c_2(0) &= \hat{\delta}_9 && \text{in } \Omega. && \text{(25f)}
\end{aligned}
$$

Proof. Let $\hat{\delta} \in Z$ be any given direction of perturbation and let $\{\tau_n\}$ be a sequence of real numbers such that $\tau_n \searrow 0$. We set $\delta_n = \tau_n \hat{\delta}$ and denote the solution of $(\mathbf{AQP}(\delta_n))$ by $(c_1^n, c_2^n, u^n, \lambda_1^n, \lambda_2^n)$. Note that $(c_1^*, c_2^*, u^*, \lambda_1^*, \lambda_2^*)$ is the solution of $(\mathbf{AQP}(0))$. Then, by virtue of Proposition 3.1, we have

$$
\left\| \frac{c_1^n - c_1^*}{\tau_n} \right\| + \left\| \frac{c_2^n - c_2^*}{\tau_n} \right\| + \left\| \frac{u_n - u^*}{\tau_n} \right\| + \left\| \frac{\lambda_1^n - \lambda_1^*}{\tau_n} \right\| + \left\| \frac{\lambda_2^n - \lambda_2^*}{\tau_n} \right\| \le L\, \|\hat{\delta}\| \quad (26)
$$

in the norms of $W(0,T)$, $L^2(0,T)$, and Z, respectively, and with some Lipschitz constant $L > 0$. We can thus extract weakly convergent subsequences (still denoted by index n) and use the compact embedding of $W(0,T)$ into $L^2(Q)$ to obtain

$$
\frac{u^n - u^*}{\tau_n} \rightharpoonup \tilde{u} \quad \text{in } L^2(0,T) \qquad (27)
$$

$$
\frac{c_1^n - c_1^*}{\tau_n} \rightharpoonup \hat{c}_1 \quad \text{in } W(0,T) \quad \text{and} \quad \to \hat{c}_1 \quad \text{in } L^2(Q) \qquad (28)
$$

and similarly for the remaining components. Taking yet another subsequence, all components except the control are seen also to converge pointwise almost everywhere in Q. From here, we only sketch the remainder of the proof since it closely parallels the ones given in [6, 12]. In addition to the arguments given there, our analysis relies on the strong convergence (and thus pointwise convergence almost everywhere on $[0,T]$ of a subsequence) of

$$
\int_{\Gamma_c} \alpha\, \frac{\lambda_2^n - \lambda_2^*}{\tau^n} \to \int_{\Gamma_c} \alpha\, \hat{\lambda}_2 \quad \text{in } L^2(0,T) \qquad (29)
$$

which follows from the compact embedding of $W(0,T)$ into $L^2(0,T; H^s(\Omega))$ for $1/2 < s < 1$ (see (5)) and the continuity of the trace operator $H^s(\Omega) \to L^2(\Gamma_c)$. One expresses u^n as the pointwise projection of $u^n + \xi^n/\gamma$ onto the admissible set $U_{\rm ad}$

with ξ^n given by (18) evaluated at (u^n, λ_2^n). Using (27) and (29), one shows that $(u^n - u^*)/\tau^n$ possesses a pointwise convergent subsequence (still denoted by index n). Distinguishing cases, one finds the pointwise limit $\hat{u}$ of $(u^n - u^*)/\tau^n$ to be the pointwise projection of $\lim_{n\to\infty}(u^n + \xi^n/\gamma)$ onto the new admissible set $\widehat{U}_{\mathrm{ad}}$. Using a suitable upper bound in Lebesgue's Dominated Convergence Theorem, one shows that $\hat{u}$ is also the limit in the sense of $L^2(0,T)$ and thus $\hat{u} = \tilde{u}$ must hold. It remains to show that the limit $(\hat{c}_1, \hat{c}_2, \hat{u}, \hat{\lambda}_1, \hat{\lambda}_2)$ satisfy the first order optimality system for $(\mathbf{DQP}(\hat{\delta}))$ (which is routine) and that the limits actually hold in their strong senses in $W(0,T)$ (which follows from standard a priori estimates). Since we could have started with a subsequence of τ^n in the first place and since the limit $(\hat{c}_1, \hat{c}_2, \hat{u}, \hat{\lambda}_1, \hat{\lambda}_2)$ must always be the same in view of the Coercivity Assumption 3.1, the convergence extends to the whole sequence. ∎

4 Properties of the Nonlinear Problem

In the current section, we shall prove that the solutions to the original nonlinear generalized equation (13) depend on p in the same way as the solutions to the linearized generalized equation (14) depend on δ. To this end, we invoke an implicit function theorem for generalized equations. Throughout this section, let again p^* be a given nominal (or unperturbed or expected) value of the parameter vector

$$\begin{aligned} p = (d_1, d_2, k_1, k_2, \beta_1, \beta_2, \gamma, u_c, \varepsilon, c_{10}, c_{20}, c_{1T}, c_{2T}, u_d) \\ \in \mathbb{R}^9 \times L^2(\Omega)^4 \times L^2(0,T) =: Q \end{aligned}$$

satisfying Assumption 2.1. Moreover, let $(x^*, \lambda^*) = (c_1^*, c_2^*, u^*, \lambda_1^*, \lambda_2^*)$ be a solution of the first order necessary conditions (6)–(8) plus the state equation, or, in other words, of the generalized equation (13).

Theorem 4.1 (Lipschitz Continuity and Directional Differentiability) *Under Assumptions 2.1 and 3.1, there exists a neighborhood $\mathcal{B}(p^*) \subset Q$ of p^* and a neighborhood $\mathcal{B}(y^*, u^*, \lambda^*) \subset Y \times U \times Y$ and a Lipschitz continuous function*

$$\mathcal{B}(p^*) \ni p \mapsto (y_p, u_p, \lambda_p) \in \mathcal{B}(y^*, u^*, \lambda^*)$$

such that (y_p, u_p, λ_p) solves the optimality system (6)–(8) plus the state equation for parameter p and such that it is the only critical point in $\mathcal{B}(y^*, u^*, \lambda^*)$. Moreover, the map $p \mapsto (y_p, u_p, \lambda_p)$ is directionally differentiable, and its derivative in the direction $\hat{p} \in Q$ is given by the unique solution of $(\mathbf{DQP}(\hat{\delta}))$, in the direction of $\hat{\delta} = -F_p(y^*, u^*, \lambda^*, p^*)\,\hat{p}$.

Proof. The proof is based on the implicit function theorem for generalized equations from [5, 15]. It relies on the strong regularity property, which was shown in

Proposition 3.1. It remains to verify that F is Lipschitz in p near p^*, uniformly in a neighborhood of (y^*, u^*, λ^*), and that F is differentiable with respect to p, which is straightforward. The formula for its derivative is given in the remark below. □

Remark 4.2 *In order to compute the parametric sensitivities of the nominal solution* $(c_1^*, c_2^*, u^*, \lambda_1^*, \lambda_2^*)$ *for* ($\mathbf{P}(p^*)$) *in a perturbation direction* $\hat{p}$, *we need to solve the linear-quadratic problem* ($\mathbf{DQP}(\hat{\delta})$) *with*

$$\begin{aligned}
\hat{\delta} &= -F_p(y^*, u^*, \lambda^*, p^*)\,\hat{p} \\
&= -\Big(\hat{d}_1 \int_Q \nabla\lambda_1^* \cdot \nabla \cdot + \int_Q (\hat{k}_1\lambda_1^* + \hat{k}_2\lambda_2^*)c_2^* \cdot, \hat{d}_2 \int_Q \nabla\lambda_2^* \cdot \nabla \cdot + \int_Q (\hat{k}_1\lambda_1^* + \hat{k}_2\lambda_2^*)c_1^* \cdot, \\
&\qquad \hat{\beta}_1(c_1^*(T) - c_{1T}^*) - \beta_1^*\hat{c}_{1T}, \hat{\beta}_2(c_2^*(T) - c_{2T}^*) - \beta_2^*\hat{c}_{2T}, \\
&\hat{\gamma}(u^* - u_d^*) - \gamma^*\hat{u}_d - \frac{3\hat{\varepsilon}}{(\varepsilon^*)^2}\max\left\{0, \int_0^T u^*(t)\,\mathrm{d}t - u_c^*\right\}^2 - \frac{6}{\varepsilon^*}\max\left\{0, \int_0^T u^*(t)\,\mathrm{d}t - u_c^*\right\}\hat{u}_c, \\
&\qquad \hat{d}_1 \int_Q \nabla c_1^* \cdot \nabla \cdot + \int_Q \hat{k}_1 c_1^* c_2^* \cdot, \hat{d}_2 \int_Q \nabla c_2^* \cdot \nabla \cdot + \int_Q \hat{k}_2 c_1^* c_2^* \cdot, -\hat{c}_{10}, -\hat{c}_{20}\Big).
\end{aligned}$$

We close this section by remarking that the parametric sensitivities allow to compute a second-order expansion of the value of the objective, see [6,12] for details. In addition, the Coercivity Assumption 3.1 implies that second order sufficient conditions hold at the nominal and also at the perturbed solutions, so that points satisfying the first order necessary conditions are indeed strict local optimizers.

5 Numerical Results

In this section, we present some numerical results and show evidence that the parametric sensitivities yield valuable information which is useful in making qualitative and quantitative estimates of the solution under perturbations. In our example, the three-dimensional geometry of the problem is given by the annular cylinder between the planes $z = 0$ and $z = 0.5$ with inner radius 0.4 and outer radius 1.0 whose rotational axis is the z-axis (Figure 1). The control boundary Γ_c is the upper annulus, and we use the control shape function

$$\alpha(t, x) = \exp\left(-5\left[(x_1 - 0.7\cos(2\pi t))^2 + (x_2 - 0.7\sin(2\pi t))^2\right]\right).$$

which corresponds to a nozzle circling for $t \in [0, 1]$ once around in counter-clockwise direction at a radius of 0.7. For fixed t, α is a function which decays exponentially with the square of the distance from the current location of the nozzle. The problem was discretized using the finite element method on a mesh consisting of 1797 points and 7519 tetrahedra. The 'triangulation' of the domain Ω by tetrahedra is also shown

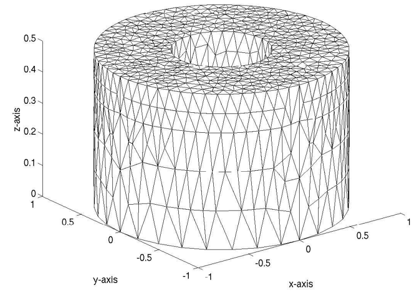

Figure 1: Domain $\Omega \subset \mathbb{R}^3$ and its triangulation with tetrahedra

in Figure 1. In the time direction, the interval $[0, T]$ was uniformly divided into 100 parts. By controlling the second substance B, we wish to steer the concentration of the first substance A to zero at terminal time $T = 1$, *i.e.*, we choose

$$\beta_1^* = 1 \qquad \beta_2^* = 0 \qquad c_{1T}^* \equiv 0$$

The control cost parameter is $\gamma^* = 10^{-2}$ and the control bounds are chosen as

$$u_a \equiv 1 \qquad u_b \equiv 5.$$

The chemical reaction is governed by equations (1)–(3) with parameters

$$d_1^* = 0.15 \qquad d_2^* = 0.20 \qquad k_1^* = 1.0 \qquad k_2^* = 1.0.$$

As initial concentrations, we use

$$c_{10}^* \equiv 1.0 \qquad c_{20}^* \equiv 0.0.$$

The discrete optimal solution without the contribution from the penalized integral constraint J_2 (corresponding to $\varepsilon = \infty$) yields

$$\int_0^T u^*(t)\,\mathrm{d}t = 4.2401, \qquad J_1(c_1^*, c_2^*, u^*) = 0.2413.$$

In order for this constraint to become relevant, we choose $u_c^* = 3.5$ and enforce it using the penalization parameter $\varepsilon^* = 1$. Details on the numerical implementation are given in [8,9]. For the discretization described above, we obtain a problem size of approximately 726 000 variables, including the adjoint states, which takes a couple of minutes to solve on a standard desktop PC.

In Figures 3–4 (left columns) and Figure 2 (left), we show the individual components of the optimal solution. We note that the optimal control lies on the upper bound in the first part of the time interval, then in the interior of the admissible interval $[1, 5]$ and finally on the lower bound. From Figure 3 (left) we infer that as time

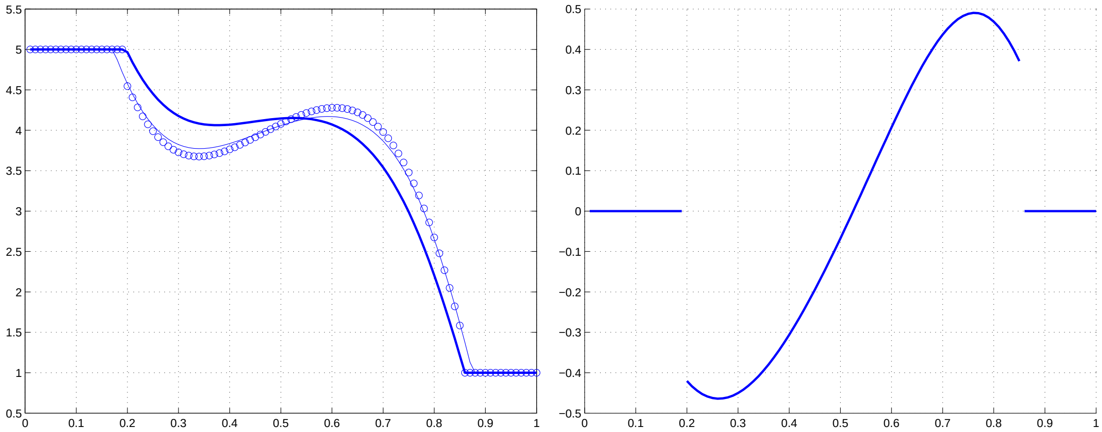

Figure 2: Left: Optimal control u^* (thick solid), true perturbed control u_p (thin solid) and predicted control (circles). Right: Parametric sensitivity du_{p^*}/dp in the direction of $p - p^*$.

advances, substance A decays and approaches the desired value of zero to the extent permitted by the control cost parameter γ and the control bounds. Figure 4 (left) nicely shows the influence of the revolving control nozzle on the upper surface of the annular cylinder, adding amounts of substance B over time which then diffuse towards the interior of the reaction vessel and react with substance A.

In order to illustrate the sensitivity calculus, we perturb the reaction constants k_1^* and k_2^* by 50%, taking

$$k_1 = 1.5 \qquad k_2 = 1.5$$

as their new values. With the reaction now proceeding faster, one presumes that the desired goal of consuming substance A within the given time interval will be achieved to a higher degree, which will in fact be confirmed below from sensitivity information. Figure 2 (left) shows, next to the nominal control, the solution obtained by a first order Taylor approximation using the sensitivity of the control variable, *i.e.*,

$$u_p \approx u_{p^*} + \frac{d}{dp} u_{p^*} (p - p^*).$$

To allow a comparison, the true perturbed solution is also depicted, which of course required the repeated solution of the nonlinear optimal control problem ($\mathbf{P}(p)$). It is remarkable how well the perturbed solution can be predicted in face of a 50% perturbation using the sensitivity information, without recomputing the solution to the nonlinear problem. We observe that the perturbed control is lower than the nominal one in the first part of the time interval, later to become higher. This behavior can not easily be predicted without any sensitivity information at hand. Besides, a qualitative analysis of the state sensitivities reveals more interesting information. We

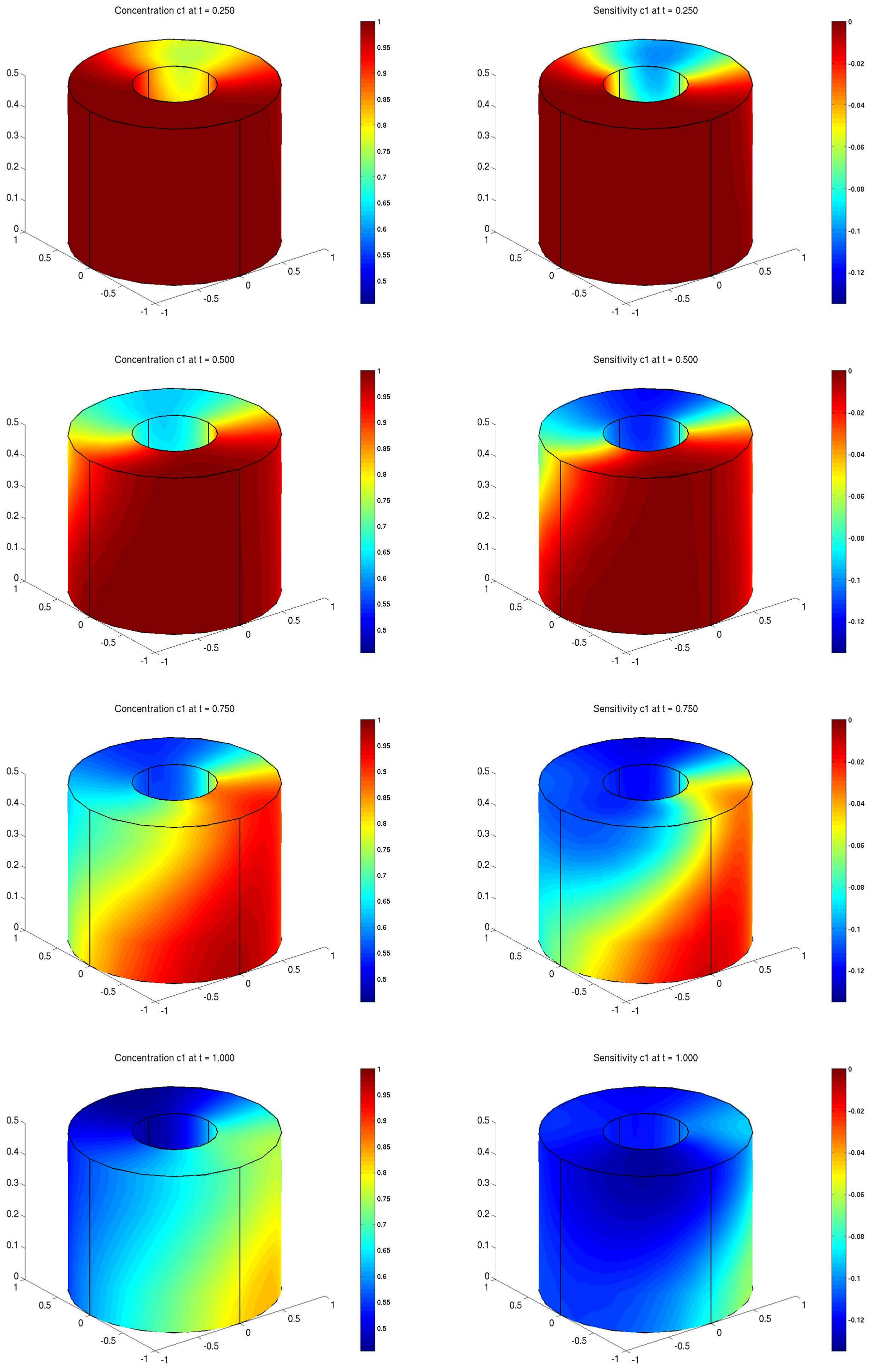

Figure 3: Concentrations of substance A (left) and its sensitivity (right) at times $t = 0.25$, $t = 0.50$, $t = 0.75$, and $t = 1.00$.

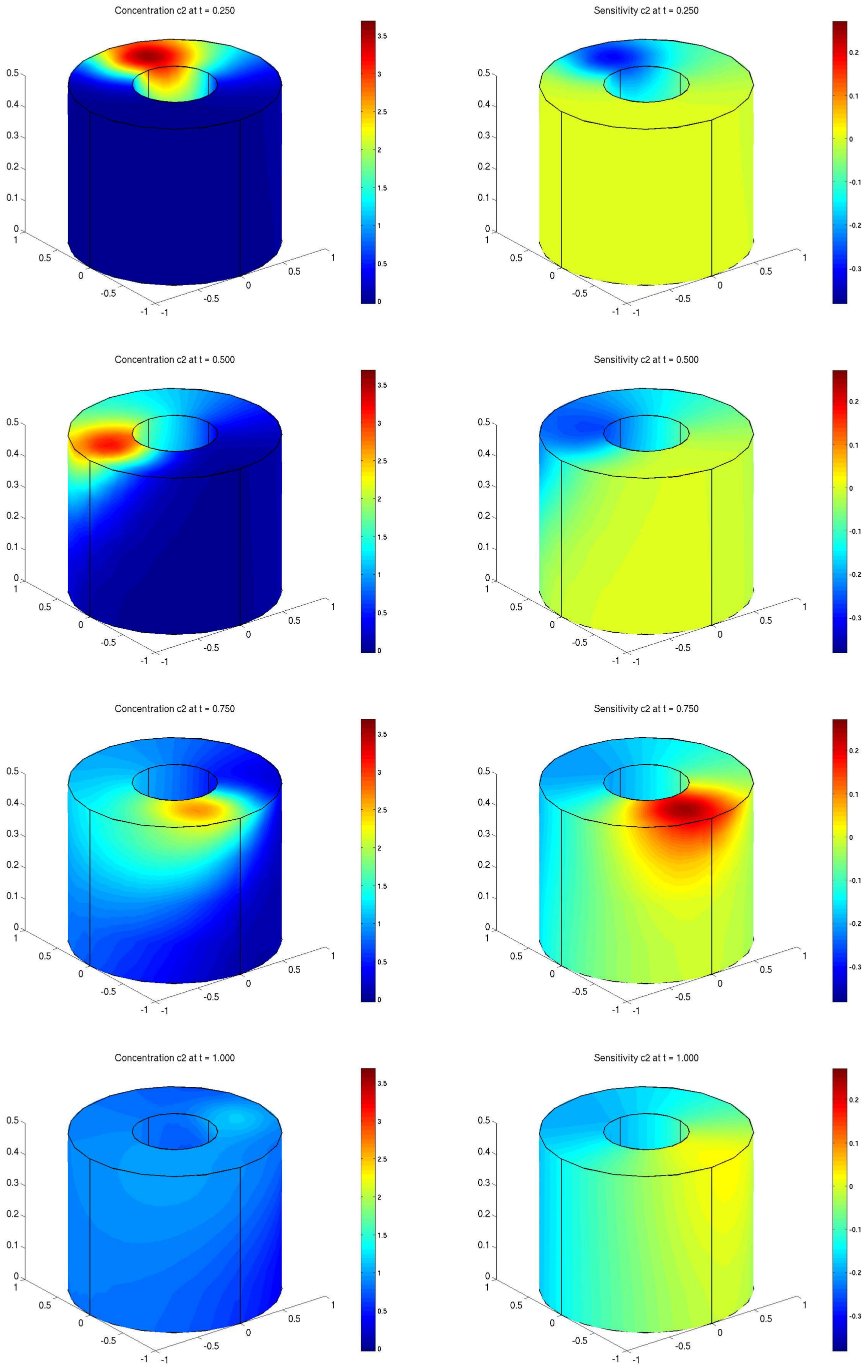

Figure 4: Concentrations of substance B (left) and its sensitivity (right) at times $t = 0.25$, $t = 0.50$, $t = 0.75$, and $t = 1.00$.

have argued above that with the reaction proceeding faster, the control goal can more easily be reached. This can be inferred from Figure 3 (right column), showing that the sensitivity derivatives of the first substance are negative throughout, *i.e.*, the perturbed solution comes closer in a pointwise sense to the desired zero terminal state (to first order). The sensitivities for the second state component (see Figure 4, right column) nicely reflect the expected behavior inferred from the control sensitivities, see Figure 2 (right). As the perturbed control is initially lower than the unperturbed one after leaving the upper bound, the sensitivity of the second substance is below zero there. Later, it becomes positive, as does the sensitivity for the control variable.

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