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SPARSE OPTIMAL CONTROL OF A PHASE FIELD TUMOR MODEL WITH MECHANICAL EFFECTS*

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Abstract. In this paper, we study an optimal control problem for a macroscopic mechanical tumor model based on the phase field approach. The model couples a Cahn–Hilliard-type equation to a system of linear elasticity and a reaction-diffusion equation for a nutrient concentration. By taking advantage of previous analytical well-posedness results established by the authors, we seek optimal controls in the form of a boundary nutrient supply as well as concentrations of cytotoxic and antiangiogenic drugs that minimize a cost functional involving mechanical stresses. Special attention is given to sparsity effects, where with the inclusion of convex nondifferentiable regularization terms to the cost functional, we can infer from the first-order optimality conditions that the optimal drug concentrations can vanish on certain time intervals.

Key words. sparse optimal control, tumor growth, Cahn–Hilliard equation, linear elasticity, mechanical effects, elliptic-parabolic system, optimality conditions

AMS subject classifications. 49J20, 49K20, 35K57, 74B05, 35Q92

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1. Introduction.

Mechanical stresses play a significant role in both enhancing and inhibiting the growth of tumors. The unregulated proliferation of tumor cells displaces nearby normal tissues, and in turn these tissues exert externally applied stress to resist tumor expansion. In various experimental studies (see [9, 25, 26, 44] and the references cited therein) high compressive stress has the effect of suppressing proliferation and can induce apoptosis (natural cell death) in tumor cells. However, in the case where the mechanical loads are not uniform, tumors can adapt by growing in directions of least stress. Moreover, deformations of the microenvironment brought about by these mechanical loads can alter the structure of nearby blood and lymphatic vessels, which are responsible for supplying the region with crucial nutrients, oxygen, therapeutic drugs, as well as drainage of excessive interstitial fluids containing waste products. The gradual reduction in blood flow turns the stressed region more hypoxic and more acidic; compounded with the reduction in nutrient levels, this further accelerates the invasive and metastatic potentials of the tumors cells. On the other hand, this also impairs the effectiveness of immune cells or therapeutic agents, as they are not able to reach certain tumor regions in sufficient quantities. With the use of mathematical modeling [29, 43], treatments aimed at alleviating stress seem

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to be a promising avenue that warrant further investigations and could be used in coordination with other anticancer therapies.

Recent progress in mathematical oncology has shown promising results in forecasting tumor growth and predictive simulations of treatments [1, 2, 32, 33, 34, 35]. Most models employ a continuum description involving partial differential equations to capture a multitude of biological and chemical mechanisms. Among those, we focus on the subclass of phase field tumor models [13, 23, 38, 45], where the corresponding numerical simulations (see, e.g., [14, 15, 17, 45, 46]) are able to replicate commonly observed morphologies exhibited by tumors and their vasculatures.

While there has been a surge of activity in the subsequent mathematical modeling and analysis of phase field tumor models (see [1, 11, 14, 15, 23, 38, 46] and the references cited therein), there seems to comparatively less focus on mechanical interactions in tumor growth within the subclass of phase field models aside from recent contributions [16, 22, 32, 33]; see also [3, 5, 19, 20] for results concerning the related Cahn–Larché system. In light of the significance of mechanical stress, for our study, we consider a simplification of the phase field model that was proposed and studied in the authors' previous work [22]. Consider a bounded domain $\Omega \subset \mathbb{R}^d$, $d \in \{2, 3\}$, with boundary $\Gamma := \partial\Omega$ that is either of $C^{1,1}$-regularity or is convex and is partitioned into two subregions Γ_D and Γ_N. For an arbitrary $T > 0$ (which can be interpreted as the length of the medical treatment), the following model posed in the space-time cylinder $\Omega \times (0, T)$ describes the evolution of a cellular mixture containing tumor and nontumor cells subject to various mechanisms involving a chemical species acting as nutrient and mechanical stresses:

$$\varphi_t = \Delta\mu + U(\varphi, \sigma, \mathcal{E}(\boldsymbol{u})) \quad \text{in } Q := \Omega \times (0, T), \tag{1.1a}$$

$$\mu = -\Delta\varphi + \Psi'(\varphi) - \chi\sigma + \mathcal{W}_{,\varphi}(\varphi, \mathcal{E}(\boldsymbol{u})) \quad \text{in } Q, \tag{1.1b}$$

$$\mathcal{W}_{,\varphi}(\varphi, \mathcal{E}(\boldsymbol{u})) = -\mathcal{C}(\mathcal{E}(\boldsymbol{u}) - \bar{\mathcal{E}} - \varphi\mathcal{E}^*) : \mathcal{E}^* \tag{1.1c}$$

$$\beta\sigma_t = \Delta\sigma + S(\varphi, \sigma) \quad \text{in } Q, \tag{1.1d}$$

$$\mathbf{0} = \operatorname{div}(\mathcal{W}_{,\mathcal{E}}(\varphi, \mathcal{E}(\boldsymbol{u}))) \quad \text{in } Q, \tag{1.1e}$$

$$\mathcal{W}_{,\mathcal{E}}(\varphi, \mathcal{E}(\boldsymbol{u})) = \mathcal{C}(\mathcal{E}(\boldsymbol{u}) - \bar{\mathcal{E}} - \varphi\mathcal{E}^*) \tag{1.1f}$$

$$\varphi(0) = \varphi_0, \quad \sigma(0) = \sigma_0 \quad \text{in } \Omega, \tag{1.1g}$$

$$0 = \partial_{\boldsymbol{n}}\varphi = \partial_{\boldsymbol{n}}\mu, \quad \partial_{\boldsymbol{n}}\sigma + \kappa(\sigma - \sigma_B) = 0 \quad \text{on } \Sigma := \Gamma \times (0, T), \tag{1.1h}$$

$$\boldsymbol{u} = \mathbf{0} \quad \text{on } \Sigma_D := \Gamma_D \times (0, T), \tag{1.1i}$$

$$\mathcal{W}_{,\mathcal{E}}(\varphi, \mathcal{E}(\boldsymbol{u}))\boldsymbol{n} = \boldsymbol{g} \quad \text{on } \Sigma_N := \Gamma_N \times (0, T). \tag{1.1j}$$

We refer the reader to [22, 32, 33] for more background on the model and related topics while briefly describing the main components. In the above, the variable φ denotes a phase field parameter that serves to distinguish between the two different types of cellular material in the mixture, with tumor cells occupying the region $\{\varphi = 1\}$ and nontumor cells the region $\{\varphi = -1\}$. The subsystem (1.1a)–(1.1b) constitutes a Cahn–Hilliard-type equation, where μ is the associated chemical potential. Coupled to this is a reaction-diffusion equation (1.1d) for a nutrient σ, as well as a quasistatic linear elasticity system (1.1e) with displacement $\boldsymbol{u}$ and symmetric strain tensor $\mathcal{E}(\boldsymbol{u}) := \frac{1}{2}(\nabla\boldsymbol{u} + (\nabla\boldsymbol{u})^\top)$. We mention that there are certain cases where the nutrient evolves quasistatically, which is covered by the case $\beta = 0$. The terms $\mathcal{W}_{,\varphi}(\varphi, \mathcal{E}(\boldsymbol{u}))$ and $\mathcal{W}_{,\mathcal{E}}(\varphi, \mathcal{E}(\boldsymbol{u}))$ are partial derivatives of the elastic energy $\mathcal{W}(\varphi, \mathcal{E}(\boldsymbol{u}))$ with respect to its first and second arguments, respectively, and for this work, we consider the choice

$$\mathcal{W}(\varphi, \mathcal{E}(\boldsymbol{u})) = \frac{1}{2}(\mathcal{E}(\boldsymbol{u}) - \bar{\mathcal{E}} - \varphi\mathcal{E}^*) : \mathcal{C}(\mathcal{E}(\boldsymbol{u}) - \bar{\mathcal{E}} - \varphi\mathcal{E}^*),$$

where $\mathcal{C}$ is a constant, symmetric, and positive definite elasticity tensor satisfying the usual symmetry conditions and the phase-dependent stress-free strain $\bar{\mathcal{E}}(\varphi)$ under Vegard's law is given by the linear ansatz $\bar{\mathcal{E}}(\varphi) = \bar{\mathcal{E}} + \varphi\mathcal{E}^*$ with constant symmetric second-order tensors $\bar{\mathcal{E}}$ and $\mathcal{E}^*$. Furthermore, in (1.1b) the directed movement of cells by chemotaxis is captured by the term $-\chi\sigma$, with $\chi \geq 0$ playing the role of chemotactic sensitivity [23], while the term $\Psi'(\varphi)$ is the derivative of a double-well potential $\Psi(\varphi)$ with equal minima at $\varphi = \pm 1$. In our setting this term plays the role of cellular adhesion that leads to the development of regions of tumor and nontumor cells well separated by interfacial layers described by the set $\{-1 < \varphi < 1\}$.

For boundary conditions, we subdivide the boundary Γ into the partition

$$\Gamma = \overline{\Gamma_D} \cup \overline{\Gamma_N} \quad \text{such that} \quad \Gamma_D \cap \Gamma_N = \emptyset.$$

Both portions are assumed to be relatively open and to have positive Hausdorff measures, and on the portion Γ_D, representing a rigid structure of the tumor environment such as bone, the displacement $\boldsymbol{u}$ is set to be zero, and on the complement portion Γ_N, the normal component of the stress tensor $\mathcal{W}_{,\mathcal{E}}$ is equal to some given load $\boldsymbol{g}$ provided by a fixed source. Meanwhile, (1.1h) highlights that the cellular diffusive flux $\partial_{\boldsymbol{n}}\mu$ is zero across the boundary, and for $\kappa > 0$ the nutrient flux $\partial_{\boldsymbol{n}}\sigma$ is proportional to the difference between a nutrient source σ_B from nearby capillaries and the nutrient level at the boundary. The case of a zero nutrient diffusive flux is covered by the choice $\kappa = 0$.

Finally, the source term $U(\varphi, \sigma, \mathcal{E}(\boldsymbol{u}))$ in (1.1a) captures cellular growth that can be influenced by nutrient concentration and mechanical stress. The example we will use is

$$U(\varphi, \sigma, \mathcal{E}(\boldsymbol{u})) = \lambda_p \sigma f(\varphi) g(\mathcal{W}_{,\mathcal{E}}(\varphi, \mathcal{E}(\boldsymbol{u}))) - (\lambda_a + m(t))k(\varphi),$$

where $\lambda_p \geq 0$, $\lambda_a \geq 0$ are constant proliferation and apoptosis (cell death) rates and f, g, and k are Lipschitz and bounded functions. For instance, we can model the proliferation and apoptosis of only the tumor cells by prescribing the conditions $f(1) = k(1) = 1$, $f(-1) = k(-1) = 0$; see, e.g., [23], where one example is $f(\varphi) = k(\varphi) = \frac{1}{2}(1 + \varphi)$ for $\varphi \in [-1, 1]$. Meanwhile, to account for the effect of reduced proliferation due to the increase in mechanical stress [4, 9, 25, 44], we may consider as a motivating example the function $g : \mathbb{R}^{d\times d} \to \mathbb{R}$ defined as

$$g(\boldsymbol{A}) = \frac{1}{\sqrt{1 + |\boldsymbol{A}|^2}} \text{ for } \boldsymbol{A} \in \mathbb{R}^{d\times d}, \tag{1.2}$$

where $|\boldsymbol{A}|$ is the Frobenius norm of the matrix $\boldsymbol{A}$, so that as the magnitude of the stress $\mathcal{W}_{,\mathcal{E}}(\varphi, \mathcal{E}(\boldsymbol{u}))$ increases, the effects of the proliferation term $\lambda_p \sigma f(\varphi) g(\mathcal{W}_{,\mathcal{E}}(\varphi, \mathcal{E}(\boldsymbol{u})))$ become less significant. This is different from the choice considered in [22], as the derivation of optimal conditions in our present contribution requires a differentiable g. What is not present in the previous work [22] is the coefficient $m(t)$, and when paired with $k(\varphi)$, we use the product $m(t)k(\varphi)$ to model a cytotoxic drug–induced decrease in tumor proliferation. A motivating example for $m(t)$ from [11] is

$$m(t) = \sum_{i=1}^{n} d_c e^{-\frac{t - T_i}{\tau}} H(t - T_i), \tag{1.3}$$

with drug dosage d_c and drug delivery times T_i for $i = 1, \dots, n$, where n is the number of chemotherapy cycles, τ denoting the mean lifetime of the drug, and H is the Heaviside function. After the ith infusion, the effect of the drug decreases exponentially until the next infusion at time T_{i+1}. For drugs with sufficiently short mean lifetime τ or with large enough infusion gap $T_i - T_{i-1}$, there are certain time intervals where the coefficient m is close to zero.

Similarly, the source term $S(\varphi, \sigma)$ in (1.1d) accounts for nutrient consumption and transport to and from external capillaries. The example we will use is of the form

$$S(\varphi, \sigma) = -h(\varphi)(\lambda_c \sigma - s(t)) + B(\sigma_c - \sigma)$$

with constant consumption rate $\lambda_c \geq 0$, capillary supply rate $B \geq 0$, capillary nutrient concentration σ_c, and a Lipschitz, bounded function h. For instance, we can model nutrient consumption only by the tumor cells by prescribing the conditions $h(1) = 1$ and $h(-1) = 0$, with one example being $h(\varphi) = \frac{1}{2}(1 + \varphi)$ for $\varphi \in [-1, 1]$. A new element absent from [22] is the coefficient $s(t)$, which models the reduction in nutrient supply caused by antiangiogenic therapy, and in [11] a similar form to (1.3) is proposed for $s(t)$, meaning that under suitable conditions, the coefficient $s(t)$ takes values close to zero for certain time intervals.

It is common to prescribe cytotoxic drugs in chemotherapy that serve to disrupt the cellular division process and promote apoptosis, but tumors can overcome these effects by developing drug resistance or by generating new vasculatures through angiogenesis to obtain nutrients that compensate any loss of mass from chemotherapy. Therefore, in certain situations, it is of interest to combine two or more different therapies so that their joint effect can account for more mechanisms that allow tumors to avoid complete elimination and have an overall larger positive impact on the treatment than the individual monotherapies. Unfortunately, the results of various experimental and clinical studies (see [36] and the references cited therein) have not produced clear guidelines on how to proceed with combined therapies, in part due to the multitude of drugs presently available and patient-specific interactions of multiple drugs. Hence, mathematicians and physicians have turn toward the framework of optimal control to infer protocols, dosages, and timings that maximize tumor reduction and minimize harmful side effects [27, 30, 31, 37, 39]. To contribute to this effort, we study an optimal control problem with the model (1.1) as the state system, and as controls, we work with the boundary nutrient supply $w_1 = \sigma_B$, the cytotoxic coefficient $w_2 = m(t)$, and the antiangiogentic coefficient $w_3 = s(t)$. The cost functional we consider is

$$\begin{aligned} J(\varphi, \boldsymbol{u}, w_1, w_2, w_3) := {} & \frac{\alpha_\Omega}{2} \|\varphi(T) - \varphi_\Omega\|^2_{L^2(\Omega)} + \frac{\alpha_Q}{2} \|\varphi - \varphi_Q\|^2_{L^2(Q)} \\ & + \frac{\alpha_{\mathcal{E}}}{2} \int_Q n(x, \varphi) |\mathcal{W}_{,\mathcal{E}}(\varphi, \mathcal{E}(\boldsymbol{u}))|^2 \, dx \, dt \\ & + \frac{\gamma_1}{2} \|w_1\|^2_{L^2(\Sigma)} + \frac{\gamma_2}{2} \|w_2\|^2_{L^2(0,T)} + \frac{\gamma_3}{2} \|w_3\|^2_{L^2(0,T)} \\ & + \gamma_4 \|w_2\|_{L^1(0,T)} + \gamma_5 \|w_3\|_{L^1(0,T)}. \end{aligned} \tag{1.4}$$

It is composed of the standard tracking type with weights α_Q, $\alpha_\Omega \geq 0$ and target functions $\varphi_Q : Q \to \mathbb{R}$ and $\varphi_\Omega : \Omega \to \mathbb{R}$ and L^2-regularizations for the optimal controls $w_1 = \sigma_B$, $w_2 = m(t)$, and $w_3 = s(t)$ with corresponding weights $\gamma_1, \gamma_2, \gamma_3 \geq 0$. Let us stress that the controls w_2 and w_3 are solely functions of time and are spatially constant. Compared to previous works on optimal control with phase field tumor models, we have the presence of a term involving the square of the stress $\mathcal{W}_{,\mathcal{E}}(\varphi, \mathcal{E}(\boldsymbol{u}))$ weighted by a nonnegative coefficient $n(x, \varphi)$ and constant $\alpha_{\mathcal{E}} \geq 0$. Due to the role of mechanical stresses on enhancing tumor growth, we are motivated to minimize stress accumulating in a certain region of the domain, such as important organs (by taking $n(x, \varphi) = \chi_D(x)$ for a subregion $D \subset \Omega$, where χ_D is the characteristic function of the set D) or in certain parts of the tumor microenvironment whose location can be encoded with the help of the phase field variable φ. One example is a function $n(x, \varphi) = \max(0, \min(1, \frac{1}{2}(1 - \varphi)))$, so that n is nonzero in the nontumor region $\{\varphi = -1\}$ and is zero in the tumor region $\{\varphi = 1\}$.

Moreover, we prescribe L^1-regularizations of the drug concentrations w_2 and w_3 with weights $\gamma_4, \gamma_5 \geq 0$ to the cost functional (1.4), with the aim of using the combination of both L^2 and L^1-regularizations to show sparsity; see Theorem 5.1 below for the precise formulation. A first work on sparse controls with phase field tumor models is [41], where directional sparsity [24] of the controls, i.e., sparsity w.r.t. space or w.r.t. time, is shown. Our reasoning for such considerations is in part motivated by the common practice that chemotherapies should be administrated to the patient only in very short periods of time to avoid adverse side effects. In the simulations performed in [12], where an optimal control problem of a similar nature is studied with only L^2-regularization terms in the cost functional, the optimal cytotoxic drug concentration is positive over the treatment period. In practical applications this translates to prolonged exposure and subsequent accumulation of the drugs in the body, potentially invoking damaging side effects, and may even entail a premature abortion of the medical treatment.

The goal of this paper is to study the optimal control problem (1.4) subjected to the state system (1.1). Building on the well-posedness results established in [22], we prove the existence of a minimizer and derive first-order optimality conditions. Our main result is sparsity of the optimal drug concentrations, brought about by the convex nondifferentiable L^1-terms in (1.4). Compared to [41], our analysis includes the elasticity interactions in (1.1b) and in (1.4), covering both cases of $\beta > 0$ and $\beta = 0$ in (1.1d) in a uniform manner, as well as different sparsity conditions for nonnegative drug concentrations $m(t)$ and $s(t)$.

We comment that tracking terms involving the nutrient concentration σ, such as $\|\sigma - \sigma_Q\|^2_{L^2(Q)}$ or $\|\sigma(T) - \sigma_\Omega\|^2_{L^2(\Omega)}$ if $\beta > 0$, can also be inserted into the cost functional. Other terms of interest include the total tumor volume at time T given by the spatial integral of $\frac{1}{2}(1 + \varphi(T))$, and thanks to the well-posedness result for (1.1) (see Theorem 2.1 below), we can consider other parameters as control variables, for instance, the capillary nutrient concentration σ_c, the boundary load $\boldsymbol{g}$, the initial data φ_0, σ_0, the coefficients $\chi, \lambda_p, \lambda_a, \lambda_c$ in (1.1) in the context of parameter estimation [18, 28], and even the magnitude of the treatment time T [8, 21, 40]. One can also consider spatially varying drug concentrations $m(t, x)$ and $s(t, x)$ as in [12, 41] and the corresponding analysis to adapt to these elements would only require minor and straightforward modifications.

The rest of the paper is organized as follows: We recall previous results in section 2, and the existence of a minimizer to the optimal control problem is shown in section 3. Section 4 is devoted to the derivation of first-order optimality conditions, and in section 5, we discuss the sparsity of controls.

2. Mathematical setting and previous results.

2.1. Notation and useful preliminaries. The standard Lebesgue and Sobolev spaces over Ω are denoted by $L^p := L^p(\Omega)$ and $W^{k,p} := W^{k,p}(\Omega)$ for any $p \in [1, \infty]$

and $k > 0$, with corresponding norms $\|\cdot\|_{L^p}$ and $\|\cdot\|_{W^{k,p}}$. In the case $p = 2$, these become Hilbert spaces, and we use the notation $H^k := H^k(\Omega) = W^{k,2}(\Omega)$ and the norm $\|\cdot\|_{H^k}$. For any Banach space Z we denote its dual by Z' and the corresponding duality pairing by $\langle\cdot,\cdot\rangle_Z$. When $Z = H^1(\Omega)$, we use the notation $\langle\cdot,\cdot\rangle = \langle\cdot,\cdot\rangle_{H^1}$. The $L^2(\Omega)$-inner product is denoted by $(\cdot,\cdot)$, while the $L^2(\Gamma)$ and $L^2(\Gamma_N)$-inner products are denoted by $(\cdot,\cdot)_\Gamma$ and $(\cdot,\cdot)_{\Gamma_N}$, respectively. We define the Sobolev space $H^2_{\boldsymbol{n}}(\Omega)$ as the set $\{f \in H^2(\Omega) : \partial_{\boldsymbol{n}} f = 0 \text{ on } \Gamma\}$, and for the displacement $\boldsymbol{u}$, we introduce the following function space:

$$X(\Omega) := \{\mathbf{f} \in H^1(\Omega)^d : \mathbf{f}|_{\Gamma_D} = \mathbf{0}\},$$

where by [10, Thm. 6.15-4, pp. 409–410], a Korn-type inequality is valid in $X(\Omega)$; i.e., there exists a constant $C_K > 0$ such that

$$\|\boldsymbol{u}\|_{H^1} \leq C_K \|\mathcal{E}(\boldsymbol{u})\|_{L^2} \quad \forall\, \boldsymbol{u} \in X(\Omega). \tag{2.1}$$

2.2. Assumptions and previous results. In this work, we make the following assumptions regarding parameters and functions in the model:

(A1) Let $\boldsymbol{g} \in L^2(\Gamma_N)^d$ and $\sigma_B \in L^\infty(\Sigma)$ be given, while $\beta, B, \kappa, \chi, \lambda_a, \lambda_p, \lambda_c, \sigma_c$ are nonnegative constants such that at least one of $\{B, \kappa\}$ is nonzero if $\beta = 0$. Moreover, $\bar{\mathcal{E}}$ and $\mathcal{E}^*$ are constant symmetric second-order tensors, while $\mathcal{C}$ is a constant symmetric, positive definite fourth-order tensor satisfying

$$\mathcal{E} : \mathcal{C}\mathcal{E} \geq c_0 |\mathcal{E}|^2$$

for all symmetric second-order tensors $\mathcal{E} \in \mathbb{R}^{d\times d}_{\mathrm{sym}}$ with a positive constant c_0.

(A2) The potential $\Psi = \Psi_1 + \Psi_2$ is a nonnegative function, $\Psi_i \in C^3(\mathbb{R})$ for $i = 1, 2$, with a convex nonnegative function Ψ_1 such that for all $r, z \in \mathbb{R}$,

$$\begin{gathered}
|\Psi_2''(r)| \leq C, \quad |\Psi_1'''(r)| \leq C(1 + |r|), \\
|\Psi'(r) - \Psi'(z)| \leq C\big(1 + |r|^2 + |z|^2\big)|r - z|, \\
|\Psi''(r) - \Psi''(z)| \leq C\big(1 + |r| + |z|\big)|r - z|
\end{gathered}$$

for some positive constant C.

(A3) The functions f, g, h, and k satisfy $f, h, k \in W^{1,\infty}(\mathbb{R})$, $g \in W^{1,\infty}(\mathbb{R}^{d\times d}, \mathbb{R})$, with Lipschitz constants that shall be denoted by a common symbol $L > 0$. Furthermore, we assume h is nonnegative.

(A4) The cytotoxic and antiangiogenic functions satisfy $m, s \in L^\infty(0, T)$.

(A5) The initial conditions satisfy $\varphi_0 \in H^1(\Omega)$ and $\sigma_0 \in L^2(\Omega)$ with $0 \leq \sigma_0 \leq M := \max(\sigma_c, \|\sigma_B\|_{L^\infty(\Sigma)})$ a.e. in Ω.

To study the optimal control problem, we will need the following:

(A6) We assume f, h, $k \in C^2(\mathbb{R}) \cap W^{2,\infty}(\mathbb{R})$, $g \in C^2(\mathbb{R}^{d\times d}, \mathbb{R}) \cap W^{2,\infty}(\mathbb{R}^{d\times d}, \mathbb{R})$, and
$n : \Omega \times \mathbb{R} \to \mathbb{R}$ is a Carathéodory function such that $n(x, \cdot) \in C^1(\mathbb{R}) \cap W^{1,\infty}(\mathbb{R})$ is nonnegative for a.e. $x \in \Omega$.

(A7) The coefficients $\alpha_Q, \alpha_\Omega, \alpha_{\mathcal{E}}, \gamma_1, \gamma_2, \gamma_3, \gamma_4, \gamma_5$ are nonnegative constants, not all zero. Moreover, γ_2 is positive if γ_4 is positive, and γ_3 is positive when γ_5 is positive.

(A8) The objective data $\varphi_Q : Q \to \mathbb{R}$, $\varphi_\Omega : \Omega \to \mathbb{R}$ are given functions satisfying $\varphi_Q \in L^2(Q), \varphi_\Omega \in L^2(\Omega)$.

Let us mention that from a practical viewpoint, the drug concentrations $m(t)$ and $s(t)$ should be nonnegative functions. However, for the mathematical analysis we perform below, it suffices to work with general $L^\infty(0,T)$-functions as in (A4). We will revisit the nonnegativity of m and s when discussing the sparsity of controls in section 5. It is also worth noting that the conditions expressed in (A2) are fulfilled by the classical quartic potential $\Psi(r) = \frac{1}{4}(r^2-1)^2$. For the motivating example (1.2), for any $\boldsymbol{A} \in \mathbb{R}^{d\times d}$, we use the notation $g'(\boldsymbol{A})$ to denote the tensor derivative of g; i.e., $g'(\boldsymbol{A})$ is a second-order tensor with

$$[g'(\boldsymbol{A})]_{ij} = \frac{\partial}{\partial \boldsymbol{A}_{ij}} g(\boldsymbol{A}) = -\frac{\boldsymbol{A}_{ij}}{(1+|\boldsymbol{A}|^2)^{3/2}} \quad \text{for } 1 \le i,j \le d.$$

On the other hand, we use the notation $g''(\boldsymbol{A})$ to denote the Hessian of g, which is a fourth-order tensor defined as

$$[g''(\boldsymbol{A})]_{ijkl} = \frac{\partial^2}{\partial \boldsymbol{A}_{ij}\partial \boldsymbol{A}_{kl}} g(\boldsymbol{A}) = \frac{3\boldsymbol{A}_{ij}\boldsymbol{A}_{kl}}{(1+|\boldsymbol{A}|^2)^{5/2}} - \frac{\delta_{ik}\delta_{jl}}{(1+|\boldsymbol{A}|^2)^{3/2}} \quad \text{for } 1 \le i,j,k,l \le d.$$

Hence, it is easy to see that for any $\boldsymbol{A} \in \mathbb{R}^{d\times d}$, both $|[g'(\boldsymbol{A})]_{ij}|$ and $|[g''(\boldsymbol{A})]_{ijkl}|$ are bounded for all $1 \le i,j,k,l \le d$. In particular, we can infer that $|g'(\mathcal{W}_{,\mathcal{E}}(\varphi, \mathcal{E}(\boldsymbol{u})))|$ and $|g''(\mathcal{W}_{,\mathcal{E}}(\varphi, \mathcal{E}(\boldsymbol{u}))|$ are bounded a.e. in Q thanks to (A3). For the rest of the paper, the parameters β, $\boldsymbol{g}$, B, κ, χ, λ_a, λ_p, λ_c, σ_c, $\mathcal{C}$, $\bar{\mathcal{E}}$, $\mathcal{E}^*$, as well as initial data φ_0 and σ_0, are kept fixed. We then introduce the notation

$$\boldsymbol{w} = (w_1, w_2, w_3)$$

and the set of admissible controls $\mathcal{U}_{ad} = \mathcal{U}_{ad}^{(1)} \times \mathcal{U}_{ad}^{(2)} \times \mathcal{U}_{ad}^{(3)}$ as

$$\begin{aligned} \mathcal{U}_{ad}^{(1)} &:= \{w_1 \in L^\infty(\Sigma) \,:\, \underline{w}_1 \le w_1 \le \overline{w}_1 \text{ a.e. on } \Sigma\}, \\ \mathcal{U}_{ad}^{(i)} &:= \{w_i \in L^\infty(0,T) \,:\, \underline{w}_i \le w_i \le \overline{w}_i \text{ a.e. in } (0,T)\} \quad \text{for } i = 2,3, \end{aligned} \tag{2.2}$$

with fixed $\underline{w}_1$, $\overline{w}_1 \in L^\infty(\Sigma)$, $\underline{w}_2$, $\overline{w}_2$, $\underline{w}_3$, $\overline{w}_3 \in L^\infty(0,T)$ such that $\underline{w}_1 \le \overline{w}_1$ a.e. on Σ, $\underline{w}_i \le \overline{w}_i$ a.e. in $(0,T)$ for $i = 2,3$, and $\max(\|\underline{w}_1\|_{L^\infty(\Sigma)}, \|\overline{w}_1\|_{L^\infty(\Sigma)}) \le M$. The admissible set of controls $\mathcal{U}_{ad}$ is a nonempty, closed, and convex subset of $\mathcal{U} := L^2(\Sigma) \times L^2(0,T) \times L^2(0,T)$, and we can find a positive constant R such that

$$\mathcal{U}_R := \{(w_1,w_2,w_3) \in \mathcal{U} \,:\, \|w_1\|_{L^2(\Sigma)} + \|w_2\|_{L^2(0,T)} + \|w_3\|_{L^2(0,T)} < R\} \supset \mathcal{U}_{ad}.$$

The following result concerns the well-posedness of the model (1.1).

Theorem 2.1. *Under* (A1)–(A5) *there exists a unique weak solution* $(\varphi, \mu, \sigma, \boldsymbol{u})$ *to* (1.1) *and also an exponent* $p > 2$ *that depends on* d, Ω, Γ_D, *and* $\mathcal{C}$ *such that*

$$\begin{aligned} &\varphi \in H^1(0,T;H^1(\Omega)') \cap L^\infty(0,T;H^1(\Omega)) \cap L^2(0,T;H^2_{\boldsymbol{n}}(\Omega)), \\ &\mu \in L^2(0,T;H^1(\Omega)), \\ &\sigma \in L^2(0,T;H^1(\Omega)) \cap L^\infty(0,T;L^\infty(\Omega)) \text{ with } 0 \le \sigma \le M \text{ a.e. in } Q \\ &\quad \text{and } \sigma \in H^1(0,T;H^1(\Omega)') \cap L^\infty(0,T;L^2(\Omega)) \text{ if } \beta > 0, \\ &\boldsymbol{u} \in L^\infty(0,T;X(\Omega) \cap W^{1,p}(\Omega)), \end{aligned}$$

with $\varphi(0) = \varphi_0$ *in* $L^2(\Omega)$ *as well as* $\sigma(0) = \sigma_0$ *in* $L^2(\Omega)$ *if* $\beta > 0$ *and*

$$0 = \int_0^T \langle \varphi_t, \zeta\rangle + (\nabla\mu, \nabla\zeta) - (U(\varphi, \sigma, \mathcal{E}(\boldsymbol{u})), \zeta)\, dt, \tag{2.3a}$$

$$0 = \int_0^T (\mu, \zeta) - (\nabla\varphi, \nabla\zeta) - (\Psi'(\varphi), \zeta) + \chi(\sigma, \zeta) - (\mathcal{W}_{,\varphi}(\varphi, \mathcal{E}(\boldsymbol{u})), \zeta)\, dt, \tag{2.3b}$$

$$0 = \int_0^T \beta\langle \sigma_t, \zeta\rangle + (\nabla\sigma, \nabla\zeta) + \kappa(\sigma - \sigma_B, \zeta)_\Gamma - (S(\varphi, \sigma), \zeta)\, dt, \tag{2.3c}$$

$$0 = \int_0^T (\mathcal{C}(\mathcal{E}(\boldsymbol{u}) - \bar{\mathcal{E}} - \varphi\mathcal{E}^*), \nabla\boldsymbol{\eta}) - (\boldsymbol{g}, \boldsymbol{\eta})_{\Gamma_N}\, dt \tag{2.3d}$$

for all $\zeta \in L^2(0, T; H^1(\Omega))$ *and* $\boldsymbol{\eta} \in L^2(0, T; X(\Omega))$*. Moreover, there exists a positive constant* K_1 *independent of* β *such that*

$$\begin{aligned} &\|\varphi\|_{H^1(0,T;H^1(\Omega)')\cap L^\infty(0,T;H^1)\cap L^2(0,T;H^2)} + \|\mu\|_{L^2(0,T;H^1)} \\ &\quad + \|\sigma\|_{L^2(0,T;H^1)} + \beta^{\frac{1}{2}}\|\sigma\|_{H^1(0,T;H^1(\Omega)')\cap L^\infty(0,T;L^2)} \\ &\quad + \|\boldsymbol{u}\|_{L^\infty(0,T;X(\Omega)\cap W^{1,p}(\Omega))} \leq K_1\big(1 + \beta^{\frac{1}{2}}\|\sigma_0\|_{L^2}\big). \end{aligned} \tag{2.4}$$

For any pair $\{(\varphi_i, \mu_i, \sigma_i, \boldsymbol{u}_i)\}_{i=1,2}$ *of weak solutions to* (1.1) *corresponding to data*

$$\{(\varphi_{0,i}, \sigma_{0,i}, \boldsymbol{g}_i, \sigma_{B,i}, m_i, s_i)\}_{i=1,2},$$

there exists a constant $K_2 > 0$ *independent of the differences of* $\{(\varphi_i, \mu_i, \sigma_i, \boldsymbol{u}_i)\}_{i=1,2}$ *and* β *such that*

$$\begin{aligned} &\|\varphi_1 - \varphi_2\|_{L^\infty(0,T;H^1)\cap L^2(0,T;H^2)} + \|\mu_1 - \mu_2\|_{L^2(0,T;H^1)} + \|\sigma_1 - \sigma_2\|_{L^2(0,T;H^1)} \\ &\quad + \beta^{\frac{1}{2}}\|\sigma_1 - \sigma_2\|_{L^\infty(0,T;L^2)} + \|\boldsymbol{u}_1 - \boldsymbol{u}_2\|_{L^\infty(0,T;X(\Omega))} \\ &\leq K_2\Big(\|\varphi_{0,1} - \varphi_{0,2}\|_{H^1} + \beta^{\frac{1}{2}}\|\sigma_{0,1} - \sigma_{0,2}\|_{L^2} + \|\boldsymbol{g}_1 - \boldsymbol{g}_2\|_{L^2(\Gamma_N)}\Big) \\ &\quad + K_2\Big(\|\sigma_{B,1} - \sigma_{B,2}\|_{L^2(\Sigma)} + \|m_1 - m_2\|_{L^2(0,T)} + \|s_1 - s_2\|_{L^2(0,T)}\Big). \end{aligned} \tag{2.5}$$

Remark 2.2. The proof of existence can be deduced analogously from [22, sect. 3], and we comment that the subsequent constant K_1 in (2.4) is bounded uniformly in $(\sigma_B, m(t), s(t))$ when we restrict to the open set $\mathcal{U}_R$, whereas a minor modification of [22, sect. 6] using the boundedness of k and h yields the above continuous dependence assertion in the presence of the new coefficients $m(t)$ and $s(t)$. Hence, we omit the details.

Remark 2.3. A closer inspection of the proof in [22, sect. 5.2] allows us to deduce the further regularity statement

$$\varphi \in L^4(0, T; H^2_{\boldsymbol{n}}(\Omega)).$$

We briefly sketch the argument. Testing (1.1b) with $-\Delta\varphi$, integrating by parts for the terms involving μ and $\Psi'(\varphi)$, and then using the convexity of Ψ_1, the bounds for Ψ_2'', the boundedness of σ, and the regularity $\varphi \in L^\infty(0, T; H^1(\Omega))$, and $\boldsymbol{u} \in L^\infty(0, T; X(\Omega))$,

$$\begin{aligned} \tfrac{1}{2}\|\Delta\varphi\|_{L^2}^2 &\leq \|\nabla\mu\|_{L^2}\|\nabla\varphi\|_{L^2} + C\|\nabla\varphi\|_{L^2}^2 + C\|\sigma\|_{L^2}^2 + C\|\mathcal{W}_{,\varphi}(\varphi, \mathcal{E}(\boldsymbol{u}))\|_{L^2}^2 \\ &\leq C\big(1 + \|\nabla\mu\|_{L^2}\big). \end{aligned}$$

Squaring and integrating over $(0, T)$ yields that $\Delta\varphi \in L^4(0, T; L^2(\Omega))$, and elliptic regularity gives the assertion.

3. The optimal control problem. In this section, we show that there exists at least one minimizer to the optimal control problem minimizing the cost functional (1.4) with state system given by (1.1). By Theorem 2.1, we can define the control-to-state operator $\mathcal{S}$, which assigns every admissible control $\boldsymbol{w} = (w_1, w_2, w_3) = (\sigma_B, m, s)$ the corresponding unique solution $(\varphi, \mu, \sigma, \boldsymbol{u})$ to (1.1). Namely, we have

$$\mathcal{S} : \mathcal{U}_{ad} \subset \mathcal{U}_R \to \mathcal{Y}^\beta, \quad (w_1, w_2, w_3) \mapsto (\varphi, \mu, \sigma, \boldsymbol{u}),$$

where the solution space $\mathcal{Y}^\beta$ is defined, according to Theorem 2.1, as

$$\mathcal{Y}^\beta := \begin{cases} H^1(0,T;H^1(\Omega)') \cap L^\infty(0,T;H^1(\Omega)) \cap L^2(0,T;H^2_{\boldsymbol{n}}(\Omega)) \times L^2(0,T;H^1(\Omega)) \\ \times H^1(0,T;H^1(\Omega)') \cap L^\infty(0,T;L^2(\Omega)) \cap L^2(0,T;H^1(\Omega)) \cap L^\infty(Q) \\ \times L^\infty(0,T;X(\Omega) \cap W^{1,p}(\Omega)) \quad \text{if } \beta > 0, \\ \\ H^1(0,T;H^1(\Omega)') \cap L^\infty(0,T;H^1(\Omega)) \cap L^2(0,T;H^2_{\boldsymbol{n}}(\Omega)) \times L^2(0,T;H^1(\Omega)) \\ \times L^2(0,T;H^1(\Omega)) \cap L^\infty(Q) \\ \times L^\infty(0,T;X(\Omega) \cap W^{1,p}(\Omega)) \quad \text{if } \beta = 0. \end{cases}$$

Denoting by $\mathcal{S}_1(\boldsymbol{w}) = \varphi$ the first component and by $\mathcal{S}_4(\boldsymbol{w}) = \boldsymbol{u}$ the fourth component, we can define the reduced cost functional as

$$\mathcal{J}(\boldsymbol{w}) = J(\mathcal{S}_1(\boldsymbol{w}), \mathcal{S}_4(\boldsymbol{w}), \boldsymbol{w}).$$

THEOREM 3.1. *Under* (A1)–(A8)*, there exists at least one minimizer* $\boldsymbol{w} \in \mathcal{U}_{ad}$ *to the optimal control problem*

$$\min_{(z_1,z_2,z_3) \in \mathcal{U}_{ad}} \mathcal{J}(z_1, z_2, z_3).$$

Since the proof is somewhat standard, we omit the details and sketch the main points. The nonnegativity of $\mathcal{J}$ implies the infimum $\inf_{\mathcal{U}_{ad}} \mathcal{J}$ exists and allows us to find a minimizing sequence $\{\boldsymbol{w}_n = (w_{1,n}, w_{2,n}, w_{3,n})\}_{n\in\mathbb{N}} \subset \mathcal{U}_{ad}$ such that $\mathcal{J}(\boldsymbol{w}_n) \to \inf_{\mathcal{U}_{ad}} \mathcal{J}$ as $n \to \infty$. Denoting the corresponding solution as $(\varphi_n, \mu_n, \sigma_n, \boldsymbol{u}_n) = \mathcal{S}(\boldsymbol{w}_n) \in \mathcal{Y}^\beta$, we infer by the bound (2.4) that $\{(\varphi_n, \mu_n, \sigma_n, \boldsymbol{u}_n)\}_{n\in\mathbb{N}}$ is uniformly bounded in $\mathcal{Y}^\beta$. Hence, along a nonrelabeled subsequence there exists a limit triplet $\boldsymbol{w} = (w_1, w_2, w_3) \in \mathcal{U}_{ad}$ such that, as $n \to \infty$,

$$\begin{aligned} (w_{1,n}, w_{2,n}, w_{3,n}) &\to (w_1, w_2, w_3) && \text{weakly* in } L^\infty(\Sigma) \times L^\infty(0,T)^2, \\ (\varphi_n, \mu_n, \sigma_n, \boldsymbol{u}_n) &\to (\varphi, \mu, \sigma, \boldsymbol{u}) = \mathcal{S}(\boldsymbol{w}) && \text{weakly* in } \mathcal{Y}^\beta. \end{aligned}$$

The Aubin–Lions compactness theorem then yields the strong convergence of φ_n to φ in $C^0([0,T];L^2(\Omega)) \cap L^2(0,T;L^2(\Omega))$, allowing us to pass to the limit in the tracking terms of $\mathcal{J}$, and provides strong convergence $\sqrt{n(\varphi_n)}\boldsymbol{\eta} \to \sqrt{n(\varphi)}\boldsymbol{\eta}$ for all $\boldsymbol{\eta} \in L^2(Q)$. Together with the weak convergence of $\mathcal{E}(\boldsymbol{u}_n)$ to $\mathcal{E}(\boldsymbol{u})$ in $L^2(Q)$, we arrive at the weak convergence

$$\sqrt{n(\varphi_n)} \mathcal{W}_{,\mathcal{E}}(\varphi_n, \mathcal{E}(\boldsymbol{u}_n)) \to \sqrt{n(\varphi)} \mathcal{W}_{,\mathcal{E}}(\varphi, \mathcal{E}(\boldsymbol{u})) \quad \text{weakly in } L^2(Q).$$

Then, by the weak lower semicontinuity of L^p-norms for $p \in [1, \infty)$, we deduce that

$$\mathcal{J}(\boldsymbol{w}) \le \liminf_{n\to\infty} \mathcal{J}(\boldsymbol{w}_n) = \inf_{\mathcal{U}_{ad}} \mathcal{J}.$$

4. First-order necessary optimality conditions.

THEOREM 4.1. *Under (A1)–(A8), let* $\boldsymbol{w}^* = (w_1^*, w_2^*, w_3^*) \in \mathcal{U}_{ad}$ *be an optimal control with associated state* $(\varphi, \mu, \sigma, \boldsymbol{u}) = \mathcal{S}(\boldsymbol{w}^*)$. *Then there exist functions* $\lambda_2, \lambda_3 \in L^\infty(0,T)$ *such that, for a.e.* $t \in (0,T)$,

$$\lambda_i(t) \in \begin{cases} \{1\} & \text{if } w_i^*(t) > 0, \\ [-1,1] & \text{if } w_i^*(t) = 0, \\ \{-1\} & \text{if } w_i^*(t) < 0, \end{cases} \quad \text{for } i \in \{2,3\}, \tag{4.1}$$

and for all $\boldsymbol{y} = (y_1, y_2, y_3) \in \mathcal{U}_{ad}$,

$$\begin{aligned} 0 \le & \int_0^T (\kappa r + \gamma_1 w_1^*, y_1 - w_1^*)_\Gamma \, dt \\ & + \int_0^T \Big(\gamma_2 w_2^* + \gamma_4 \lambda_2 - \int_\Omega k(\varphi) p \, dx \Big) (y_2 - w_2^*) \, dt \\ & + \int_0^T \Big(\gamma_3 w_3^* + \gamma_5 \lambda_3 + \int_\Omega h(\varphi) r \, dx \Big) (y_3 - w_3^*) \, dt, \end{aligned} \tag{4.2}$$

where p *and* r *are the first and third components of the associated adjoint variables* $(p, q, r, \boldsymbol{s})$ *satisfying the adjoint system* (4.15).

The proof of Theorem 4.1 proceeds in four steps, which are covered in the following four subsections.

4.1. Linearized state system.

Given $\boldsymbol{w}^* = (w_1^*, w_2^*, w_3^*) \in \mathcal{U}_{ad}$ with associated state $(\varphi, \mu, \sigma, \boldsymbol{u}) = \mathcal{S}(\boldsymbol{w}^*) \in \mathcal{Y}^\beta$, for arbitrary $\boldsymbol{h} = (h_1, h_2, h_3) \in \mathcal{U}$, we study the following linearized state system:

$$\xi_t = \Delta \eta + U_{\mathrm{lin}}(\varphi, \sigma, \mathcal{E}(\boldsymbol{u}), w_2^*, h_2, \xi, \psi, \mathcal{E}(\boldsymbol{v})) \quad \text{in } Q, \tag{4.3a}$$

$$\begin{aligned} U_{\mathrm{lin}} = & \lambda_p g(\mathcal{W}_{,\mathcal{E}}(\varphi, \mathcal{E}(\boldsymbol{u})))(f'(\varphi)\xi\sigma + f(\varphi)\psi) \\ & + \lambda_p \sigma f(\varphi) g'(\mathcal{W}_{,\mathcal{E}}(\varphi, \mathcal{E}(\boldsymbol{u}))) : \mathcal{C}(\mathcal{E}(\boldsymbol{v}) - \xi\mathcal{E}^*) \\ & - (\lambda_a + w_2^*) k'(\varphi)\xi - h_2 k(\varphi) \end{aligned} \tag{4.3b}$$

$$\eta = -\Delta\xi + \Psi''(\varphi)\xi - \chi\psi - \mathcal{C}(\mathcal{E}(\boldsymbol{v}) - \xi\mathcal{E}^*) : \mathcal{E}^* \quad \text{in } Q, \tag{4.3c}$$

$$\beta\psi_t = \Delta\psi + S_{\mathrm{lin}}(\varphi, \sigma, w_3^*, h_3, \xi, \psi) \quad \text{in } Q, \tag{4.3d}$$

$$S_{\mathrm{lin}} = -h'(\varphi)\xi(\lambda_c\sigma - w_3^*) - h(\varphi)(\lambda_c\psi - h_3) - B\psi \tag{4.3e}$$

$$\mathbf{0} = \operatorname{div}(\mathcal{C}(\mathcal{E}(\boldsymbol{v}) - \xi\mathcal{E}^*)) \quad \text{in } Q, \tag{4.3f}$$

$$0 = \xi(0) = \psi(0) \quad \text{in } \Omega, \tag{4.3g}$$

$$0 = \partial_{\boldsymbol{n}}\xi = \partial_{\boldsymbol{n}}\eta, \quad \partial_{\boldsymbol{n}}\psi + \kappa(\psi - h_1) = 0 \quad \text{on } \Sigma, \tag{4.3h}$$

$$\boldsymbol{v} = \mathbf{0} \quad \text{on } \Sigma_D, \tag{4.3i}$$

$$\mathbf{0} = \mathcal{C}(\mathcal{E}(\boldsymbol{v}) - \xi\mathcal{E}^*)\boldsymbol{n} \quad \text{on } \Sigma_N. \tag{4.3j}$$

Introducing the solution space

$$\mathcal{Y}_{\mathrm{lin}}^\beta = \begin{cases} H^1(0,T;H^1(\Omega)') \cap L^\infty(0,T;H^1(\Omega)) \cap L^2(0,T;H^2_{\boldsymbol{n}}(\Omega)) \times L^2(0,T;H^1(\Omega)) \\ \times H^1(0,T;H^1(\Omega)') \cap L^\infty(0,T;L^2(\Omega)) \cap L^2(0,T;H^1(\Omega)) \\ \times L^\infty(0,T;X(\Omega)) \quad \text{if } \beta > 0, \\ \\ H^1(0,T;H^1(\Omega)') \cap L^\infty(0,T;H^1(\Omega)) \cap L^2(0,T;H^2_{\boldsymbol{n}}(\Omega)) \times L^2(0,T;H^1(\Omega)) \\ \times L^2(0,T;H^1(\Omega)) \times L^\infty(0,T;X(\Omega)) \quad \text{if } \beta = 0, \end{cases}$$

we have the following result.

THEOREM 4.2. *For given* $\boldsymbol{w}^* = (w_1^*, w_2^*, w_3^*) \in \mathcal{U}_{ad}$ *with* $(\varphi, \mu, \sigma, \boldsymbol{u}) = \mathcal{S}(\boldsymbol{w}^*) \in \mathcal{Y}^\beta$ *and* $\boldsymbol{h} = (h_1, h_2, h_3) \in \mathcal{U}$*, under* (A1)–(A6)*, there exists a unique solution* $(\xi, \eta, \psi, \boldsymbol{v}) \in \mathcal{Y}^\beta_{\mathrm{lin}}$ *to* (4.3) *with* $\xi(0) = 0$*,* $\psi(0) = 0$ *if* $\beta > 0$*, and*

$$0 = \int_0^T \langle \xi_t, \zeta \rangle + (\nabla \eta, \nabla \zeta) - (U_{\mathrm{lin}}(\varphi, \sigma, \mathcal{E}(\boldsymbol{u}), w_2^*, h_2, \psi, \xi, \mathcal{E}(\boldsymbol{v})), \zeta)\, dt, \tag{4.4a}$$

$$0 = \int_0^T (\eta - \Psi''(\varphi)\xi + \chi\psi + \mathcal{C}(\mathcal{E}(\boldsymbol{v}) - \xi\mathcal{E}^*) : \mathcal{E}^*, \zeta) - (\nabla \xi, \nabla \zeta)\, dt, \tag{4.4b}$$

$$0 = \int_0^T \beta\langle \psi_t, \zeta \rangle + (\nabla \psi, \nabla \zeta) + \kappa(\psi - h_1, \zeta)_\Gamma - (S_{\mathrm{lin}}(\varphi, \sigma, w_3^*, h_3, \xi, \psi), \zeta)\, dt, \tag{4.4c}$$

$$0 = \int_0^T (\mathcal{C}(\mathcal{E}(\boldsymbol{v}) - \xi\mathcal{E}^*), \nabla \boldsymbol{\eta})\, dt \tag{4.4d}$$

for all $\zeta \in L^2(0,T; H^1(\Omega))$ *and* $\boldsymbol{\eta} \in L^2(0,T; X(\Omega))$.

Proof. We proceed with formal estimates that can be justified rigorously with a Galerkin approximation. In the following the positive constants denoted by the symbol C will be independent of the Galerkin parameter, as well as h_1, h_2, and h_3, and might change from line to line. In additon, let us remark that since $\boldsymbol{w}^*$ is fixed, the corresponding state $(\varphi, \mu, \sigma, \boldsymbol{u}) = \mathcal{S}(\boldsymbol{w}^*)$ enjoys the bound (2.4). Let us mention that uniqueness follows from existence thanks to the linearity of the system (4.3).

We test (4.4a) with η and $K\xi$, (4.4b) with $-\xi_t$ and η, (4.4c) with $R\psi$, and (4.4d) with $\boldsymbol{v}_t$ for positive constants K, R to be determined later. After summing and rearranging, we get

$$\begin{aligned}
&\frac{1}{2}\frac{d}{dt}\Big(K\|\xi\|_{L^2}^2 + \|\nabla\xi\|_{L^2}^2 + R\beta\|\psi\|_{L^2}^2\Big) + \frac{d}{dt}\int_\Omega \mathcal{W}^{\mathrm{lin}}(\xi, \mathcal{E}(\boldsymbol{v}))\, dx \\
&\qquad + \|\eta\|_{H^1}^2 + R\|\nabla\psi\|_{L^2}^2 + R\kappa\|\psi\|_{L^2_\Gamma}^2 + RB\|\psi\|_{L^2}^2 \\
&\quad = -K(\nabla\eta, \nabla\xi) + (U_{\mathrm{lin}}, \eta + K\xi) + (\Psi''(\varphi)\xi, \eta - \xi_t) + \chi(\psi, \xi_t - \eta) \\
&\qquad + (\nabla\xi, \nabla\eta) - (\mathcal{C}(\mathcal{E}(\boldsymbol{v}) - \xi\mathcal{E}^*) : \mathcal{E}^*, \eta) + R\kappa(h_1, \psi)_\Gamma + R(S_{\mathrm{lin}}, \psi),
\end{aligned} \tag{4.5}$$

where

$$\mathcal{W}^{\mathrm{lin}}(\xi, \mathcal{E}(\boldsymbol{v})) = \frac{1}{2}(\mathcal{E}(\boldsymbol{v}) - \xi\mathcal{E}^*) : \mathcal{C}(\mathcal{E}(\boldsymbol{v}) - \xi\mathcal{E}^*),$$

and we have used the identity

$$\begin{aligned}
\frac{d}{dt}\int_\Omega \mathcal{W}^{\mathrm{lin}}(\xi, \mathcal{E}(\boldsymbol{v}))\, dx &= (\mathcal{W}^{\mathrm{lin}}_{,\xi}(\xi, \mathcal{E}(\boldsymbol{v})), \xi_t) + (\mathcal{W}^{\mathrm{lin}}_{,\mathcal{E}}(\xi, \mathcal{E}(\boldsymbol{v})), \mathcal{E}(\boldsymbol{v}_t)) \\
&= -(\mathcal{C}(\mathcal{E}(\boldsymbol{v}) - \xi\mathcal{E}^*) : \mathcal{E}^*, \xi_t) + (\mathcal{C}(\mathcal{E}(\boldsymbol{v}) - \xi\mathcal{E}^*), \mathcal{E}(\boldsymbol{v}_t))
\end{aligned}$$

derived with the help of the symmetry of $\mathcal{C}$ and $\mathcal{E}^*$. Furthermore, by the positive definiteness of $\mathcal{C}$ and Young's inequality,

$$\mathcal{W}^{\mathrm{lin}}(\xi, \mathcal{E}(\boldsymbol{v})) \geq \frac{c_0}{4}\|\mathcal{E}(\boldsymbol{v})\|_{L^2}^2 - C\big(1 + \|\xi\|_{L^2}^2\big). \tag{4.6}$$

Next, recalling that w_2^* and w_3^* are constant in space, from the definition of U_{lin} and S_{lin}, using the boundedness of w_2^*, w_3^*, f, g, h, k and their derivatives, as well as the boundedness of σ and of $|g'(\mathcal{W}_{,\mathcal{E}}(\varphi, \mathcal{E}(\boldsymbol{u})))|$, it is easy to see that

$$\|U_{\mathrm{lin}}\|_{L^2} \leq C\big(\|\xi\|_{L^2} + \|\psi\|_{L^2} + \|\mathcal{E}(\boldsymbol{v})\|_{L^2} + |h_2|\big), \tag{4.7}$$

while

$$
\begin{aligned}
R(S_{\mathrm{lin}},\psi) &\le -R\big(B\|\psi\|_{L^2}^2 + \lambda_c(h(\varphi)\psi,\psi)\big) + RC\big(\|\xi\|_{L^2} + |h_3|\big)\|\psi\|_{L^2} \\
&\le -RB\|\psi\|_{L^2}^2 + C\big(\|\xi\|_{L^2}^2 + |h_3|^2\big) + \|\psi\|_{L^2}^2,
\end{aligned}
$$

where we also use the nonnegativity of h and λ_c. Also, using (A2), the inclusion $H^1(\Omega) \subset L^6(\Omega)$, and that $\varphi \in L^\infty(0,T;H^1(\Omega))$,

$$
\|\Psi''(\varphi)\xi\|_{L^2}^2 \le C\|\xi\|_{L^6}^2\big(1 + \|\varphi\|_{L^6}^4\big) \le C\|\xi\|_{H^1}^2.
$$

Hence, the right-hand side of (4.5) can be estimated as

$$
\begin{aligned}
\mathrm{RHS} \le{}& \frac{1}{4}\|\eta\|_{H^1}^2 + c\|\psi\|_{L^2}^2 + C\big(\|\xi\|_{H^1}^2 + \|\mathcal{E}(\boldsymbol{v})\|_{L^2}^2 + \|h_1\|_{L^2_\Gamma}^2 + |h_2|^2 + |h_3|^2\big) \\
&+ (\chi\psi - \Psi''(\varphi)\xi, \xi_t) + \frac{R\kappa}{2}\|\psi\|_{L^2_\Gamma}^2 - RB\|\psi\|_{L^2}^2
\end{aligned}
$$

with a positive constant c that is independent of R. To handle the term involving ξ_t, we use (4.4a) and (4.7) to deduce that

$$
\begin{aligned}
\|\xi_t\|_{H^1(\Omega)'} &\le \|\nabla\eta\|_{L^2} + \|U_{\mathrm{lin}}\|_{L^2} \\
&\le \|\nabla\eta\|_{L^2} + C\big(\|\xi\|_{L^2} + \|\psi\|_{L^2} + \|\mathcal{E}(\boldsymbol{v})\|_{L^2} + |h_2|\big),
\end{aligned} \tag{4.8}
$$

while invoking the assumption (A2) for Ψ'' and Ψ''' leads to

$$
\begin{aligned}
\|\Psi''(\varphi)\xi\|_{H^1} &\le \|\Psi''(\varphi)\xi\|_{L^2} + \|\xi\Psi'''(\varphi)\nabla\varphi\|_{L^2} + \|\Psi''(\varphi)\nabla\xi\|_{L^2} \\
&\le C\|\xi\|_{H^1} + \|\Psi'''(\varphi)\|_{L^6}\|\xi\|_{L^6}\|\nabla\varphi\|_{L^6} + \|\Psi''(\varphi)\|_{L^\infty}\|\nabla\xi\|_{L^2} \\
&\le C\big(1 + \|\varphi\|_{H^2}^2\big)\|\xi\|_{H^1}.
\end{aligned}
$$

Then, via Young's inequality,

$$
|(\Psi''(\varphi)\xi,\xi_t)| \le \frac{1}{8}\|\nabla\eta\|_{L^2}^2 + C\big(1 + \|\varphi\|_{H^2}^4\big)\|\xi\|_{H^1}^2 + C\big(\|\psi\|_{L^2}^2 + \|\mathcal{E}(\boldsymbol{v})\|_{L^2}^2 + |h_2|^2\big).
$$

Meanwhile, by a similar argument,

$$
|(\chi\psi,\xi_t)| \le \frac{1}{8}\|\nabla\eta\|_{L^2}^2 + C\big(\|\psi\|_{H^1}^2 + \|\mathcal{E}(\boldsymbol{v})\|_{L^2}^2 + |h_2|^2 + \|\xi\|_{L^2}^2\big),
$$

and so, collecting the above estimates for the right-hand side of (4.5), we deduce the existence of two positive constants c_1 and c_2 independent of R such that

$$
\begin{aligned}
&\frac{1}{2}\frac{d}{dt}\Big(K\|\xi\|_{L^2}^2 + \|\nabla\xi\|_{L^2}^2 + R\beta\|\psi\|_{L^2}^2\Big) + \frac{d}{dt}\int_\Omega \mathcal{W}^{\mathrm{lin}}(\xi,\mathcal{E}(\boldsymbol{v}))\,dx \\
&\quad + \frac{1}{2}\|\eta\|_{H^1}^2 + (R - c_1)\|\nabla\psi\|_{L^2}^2 + \frac{R\kappa}{2}\|\psi\|_{L^2_\Gamma}^2 + (RB - c_2)\|\psi\|_{L^2}^2 \\
&\le C\big(1 + \|\varphi\|_{H^2}^4\big)\big(\|\mathcal{E}(\boldsymbol{v})\|_{L^2} + \|\xi\|_{H^1}^2\big) + C\big(\|h_1\|_{L^2_\Gamma}^2 + |h_2|^2 + |h_3|^2\big) \\
&\le C\big(1 + \|\varphi\|_{H^2}^4\big)\big(\|\mathcal{W}^{\mathrm{lin}}(\xi,\mathcal{E}(\boldsymbol{v}))\|_{L^1} + \|\xi\|_{H^1}^2\big) + C\big(\|h_1\|_{L^2_\Gamma}^2 + |h_2|^2 + |h_3|^2\big),
\end{aligned}
$$

where we have also used the lower bound (4.6). In the case $\beta > 0$, we can directly employ Gronwall's inequality to handle the terms on the right-hand side, whereas in the case $\beta = 0$, we proceed as follows: If $B > 0$, we can choose $R > \max(2c_1, \frac{2c_2}{B})$, and if $B = 0$, then $\kappa > 0$ by (A1), and we employ the generalized Poincaré inequality

$$\|f\|_{L^2} \le C\big(\|\nabla f\|_{L^2} + \|f\|_{L^2_\Gamma}\big) \quad \forall f \in H^1(\Omega)$$

to handle the term $c_2\|\psi\|_{L^2}^2$ on the left-hand side after choosing R sufficiently large. Invoking Gronwall's inequality, keeping in mind that $\varphi \in L^4(0,T;H^2(\Omega))$, there exists a constant C independent of β such that

$$\begin{aligned} &\|\xi\|^2_{L^\infty(0,T;H^1)} + \beta\|\psi\|^2_{L^\infty(0,T;L^2)} + \|\mathcal{W}^{\mathrm{lin}}(\xi,\mathcal{E}(\boldsymbol{v}))\|^2_{L^\infty(0,T;L^1)} \\ &\quad + \|\eta\|^2_{L^2(0,T;H^1)} + \|\nabla\psi\|^2_{L^2(Q)} + \kappa\|\psi\|^2_{L^2(\Sigma)} + B\|\psi\|^2_{L^2(Q)} \\ &\le C\big(\|h_1\|^2_{L^2(\Sigma)} + \|h_2\|^2_{L^2(0,T)} + \|h_3\|^2_{L^2(0,T)}\big). \end{aligned} \tag{4.9}$$

In view of $\xi(0) = 0$, we note that from (4.3) the initial data $\boldsymbol{v}_0$ assigned to $\boldsymbol{v}$ satisfies the elliptic equation

$$\begin{cases} \mathrm{div}(\mathcal{C}(\mathcal{E}(\boldsymbol{v}_0))) = \mathbf{0} & \text{in } \Omega, \\ \boldsymbol{v}_0 = \mathbf{0} & \text{on } \Gamma_D, \\ \mathcal{C}(\mathcal{E}(\boldsymbol{v}_0))\boldsymbol{n} = \mathbf{0} & \text{on } \Gamma_N. \end{cases}$$

Testing with $\boldsymbol{v}_0$ and using Korn's inequality shows that

$$\|\boldsymbol{v}_0\|_{H^1} \le C_K\|\mathcal{E}(\boldsymbol{v}_0)\|_{L^2} \le \frac{C_K}{c_0}(\mathcal{C}\mathcal{E}(\boldsymbol{v}_0), \mathcal{E}(\boldsymbol{v}_0)) = 0,$$

which explains the absence of initial data on the right-hand side of (4.9). Then, recalling the lower bound (4.6) and employing Korn's inequality, we have

$$\begin{aligned} &\|\xi\|^2_{L^\infty(0,T;H^1)} + \beta\|\psi\|^2_{L^\infty(0,T;L^2)} + \|\boldsymbol{v}\|^2_{L^\infty(0,T;H^1)} + \|\eta\|^2_{L^2(0,T;H^1)} + \|\psi\|^2_{L^2(0,T;H^1)} \\ &\quad \le C\big(\|h_1\|^2_{L^2(\Sigma)} + \|h_2\|^2_{L^2(0,T)} + \|h_3\|^2_{L^2(0,T)}\big), \end{aligned}$$

which also implies the uniqueness of solution since the difference of two solutions to the linear system (4.3) satisfies (4.3) with $h_1 = h_2 = h_3 = 0$. To complete the proof, we return to (4.8) to deduce that

$$\|\xi_t\|_{L^2(0,T;H^1(\Omega)')} \le C\big(\|h_1\|_{L^2(\Sigma)} + \|h_2\|_{L^2(0,T)} + \|h_3\|_{L^2(0,T)}\big),$$

while if $\beta > 0$, from (4.4c), we also have

$$\|\psi_t\|_{L^2(0,T;H^1(\Omega)')} \le C\big(\|h_1\|_{L^2(\Sigma)} + \|h_2\|_{L^2(0,T)} + \|h_3\|_{L^2(0,T)}\big).$$

Finally, after passing to the limit in the Galerkin approximation, we obtain limit functions $(\xi,\eta,\psi,\boldsymbol{v}) \in \mathcal{Y}^\beta_{\mathrm{lin}}$ satisfying (4.3) except for the $L^2(0,T;H^2_{\boldsymbol{n}}(\Omega))$ regularity of ξ. This can be obtained from viewing (4.4b) as the variational formulation of the elliptic problem

$$\begin{cases} -\Delta\xi = \tilde{f} := \eta - \Psi''(\varphi)\xi + \chi\psi + \mathcal{C}(\mathcal{E}(\boldsymbol{v}) - \xi\mathcal{E}^*) : \mathcal{E}^* & \text{in } Q, \\ \partial_{\boldsymbol{n}}\xi = 0 & \text{on } \Sigma, \end{cases}$$

with a right-hand side $\tilde{f} \in L^2(Q)$, and with the help of elliptic regularity, we then infer that $\xi \in L^2(0,T;H^2_{\boldsymbol{n}}(\Omega))$. Hence, we have shown that $(\xi,\eta,\psi,\boldsymbol{v}) \in \mathcal{Y}^\beta_{\mathrm{lin}}$, and this concludes the proof. ∎

4.2. Differentiability of the solution operator. In this section, we establish the Fréchet differentiability of the solution operator $\mathcal{S}$ between suitable Banach spaces, and that the derivative at $\boldsymbol{w}^* = (w_1^*, w_2^*, w_3^*) \in \mathcal{U}_{ad}$ in direction $\boldsymbol{h} = (h_1, h_2, h_3) \in \mathcal{U}$ is the unique solution $(\xi, \eta, \psi, \boldsymbol{v})$ obtained from Theorem 4.2. This is formulated as follows.

THEOREM 4.3. *Under* (A1)–(A6)*, for given* $\boldsymbol{w}^* \in \mathcal{U}_{ad}$ *with* $(\varphi, \mu, \sigma, \boldsymbol{u}) = \mathcal{S}(\boldsymbol{w}^*) \in \mathcal{Y}^\beta$*, the control-to-state operator* $\mathcal{S}$ *is Fréchet differentiable at* $\boldsymbol{w}^*$ *when viewed as a mapping from* $\mathcal{U}$ *to* $\mathcal{X}^\beta$*, where*

$$\mathcal{X}^\beta = \begin{cases} L^\infty(0,T;L^2(\Omega)) \cap L^2(0,T;H^2_{\boldsymbol{n}}(\Omega)) \times L^2(Q) \\ \times L^\infty(0,T;L^2(\Omega)) \cap L^2(0,T;H^1(\Omega)) \times L^2(0,T;X(\Omega)) & \text{if } \beta > 0, \\ \\ L^\infty(0,T;L^2(\Omega)) \cap L^2(0,T;H^2_{\boldsymbol{n}}(\Omega)) \times L^2(Q) \\ \times L^2(0,T;H^1(\Omega)) \times L^2(0,T;X(\Omega)) & \text{if } \beta = 0. \end{cases}$$

Moreover, for all $\boldsymbol{h} = (h_1, h_2, h_3) \in \mathcal{U}$*, the directional derivative*

$$D\mathcal{S}(\boldsymbol{w}^*)[\boldsymbol{h}] = (\xi, \eta, \psi, \boldsymbol{v})$$

is the unique solution to (4.3) *associated to* $\boldsymbol{h}$*.*

Proof. We denote

$$(\varphi_h, \mu_h, \sigma_h, \boldsymbol{u}_h) = \mathcal{S}(\boldsymbol{w}^* + \boldsymbol{h})$$

and aim to show

$$\frac{\|\mathcal{S}(\boldsymbol{w}^* + \boldsymbol{h}) - \mathcal{S}(\boldsymbol{w}^*) - D\mathcal{S}(\boldsymbol{w}^*)[\boldsymbol{h}]\|_{\mathcal{X}^\beta}}{\|\boldsymbol{h}\|_{\mathcal{U}}} \to 0 \qquad \text{as } \|\boldsymbol{h}\|_{\mathcal{U}} \to 0.$$

This is done via establishing for functions

$$\Phi := \varphi_h - \varphi - \xi, \quad \lambda := \mu_h - \mu - \eta, \quad \theta := \sigma_h - \sigma - \psi, \quad \boldsymbol{z} := \boldsymbol{u}_h - \boldsymbol{u} - \boldsymbol{v}$$

the inequality

$$\|(\Phi, \lambda, \theta, \boldsymbol{z})\|_{\mathcal{X}^\beta} \le C \|\boldsymbol{h}\|_{\mathcal{U}}^2 \tag{4.10}$$

with a positive constant C independent of $(\Phi, \lambda, \theta, \boldsymbol{z})$ and $\boldsymbol{h}$. To this end, we recall from Theorems 2.1 and 4.2 that the new variables $(\Phi, \lambda, \theta, \boldsymbol{z}) \in \mathcal{Y}^\beta_{\mathrm{lin}}$ satisfy

$$\begin{aligned} \text{(4.11a)} \quad & 0 = \langle \Phi_t, \zeta \rangle + (\nabla \lambda, \nabla \zeta) + (\lambda_p X_h, \zeta) \\ & \qquad - ((\lambda_a + w_2^*)[k(\varphi_h) - k(\varphi) - k'(\varphi)\xi], \zeta) - ((k(\varphi_h) - k(\varphi))h_2, \zeta), \\ \text{(4.11b)} \quad & 0 = (\lambda, \zeta) - (\nabla \Phi, \nabla \zeta) - (\Psi'(\varphi_h) - \Psi'(\varphi) - \Psi''(\varphi)\xi, \zeta) \\ & \qquad + (\chi\theta, \zeta) - (\mathcal{C}(\mathcal{E}(\boldsymbol{z}) - \Phi\mathcal{E}^*) : \mathcal{E}^*, \zeta), \\ \text{(4.11c)} \quad & 0 = \beta\langle \theta_t, \zeta \rangle + (\nabla \theta, \nabla \zeta) + (B\theta + \lambda_c h(\varphi)\theta, \zeta) + (\kappa\theta, \zeta)_\Gamma \\ & \qquad + \lambda_c((\sigma - w_3^*)[h(\varphi_h) - h(\varphi) - h'(\varphi)\xi], \zeta) - \lambda_c((h(\varphi_h) - h(\varphi))h_3, \zeta) \\ & \qquad + \lambda_c((h(\varphi_h) - h(\varphi))(\sigma_h - \sigma), \zeta), \\ \text{(4.11d)} \quad & 0 = (\mathcal{C}(\mathcal{E}(\boldsymbol{z}) - \Phi\mathcal{E}^*), \nabla \boldsymbol{\eta}) \end{aligned}$$

for all $\zeta \in H^1(\Omega)$ and $\boldsymbol{\eta} \in X(\Omega)$ and for a.e. $t \in (0,T)$, where

$$\begin{aligned} X_h &= \big(g(\mathcal{W}_{,\mathcal{E}}(\varphi_h, \mathcal{E}(\boldsymbol{u}_h))) - g(\mathcal{W}_{,\mathcal{E}}(\varphi, \mathcal{E}(\boldsymbol{u})))\big) \\ &\qquad \times \Big[(f(\varphi_h) - f(\varphi))(\sigma_h - \sigma) + f(\varphi)(\sigma_h - \sigma) + (f(\varphi_h) - f(\varphi))\sigma\Big] \\ &\quad + g(\mathcal{W}_{,\mathcal{E}}(\varphi, \mathcal{E}(\boldsymbol{u}))) \\ &\qquad \times \Big[(f(\varphi_h) - f(\varphi))(\sigma_h - \sigma) + \sigma[f(\varphi_h) - f(\varphi) - f'(\varphi)\xi] + f(\varphi)\theta\Big] \\ &\quad + \Big[g(\mathcal{W}_{,\mathcal{E}}(\varphi_h, \mathcal{E}(\boldsymbol{u}_h))) - g(\mathcal{W}_{,\mathcal{E}}(\varphi, \mathcal{E}(\boldsymbol{u}))) - g'(\mathcal{W}_{,\mathcal{E}}(\varphi, \mathcal{E}(\boldsymbol{u}))) : \mathcal{C}(\mathcal{E}(\boldsymbol{v}) - \xi\mathcal{E}^*)\Big] \\ &\qquad \times f(\varphi)\sigma. \end{aligned}$$

Take note that h_1 does not appear in (4.11) since the state system (1.1) is linear in $w_1^* = \sigma_B$. We invoke Taylor's theorem with integral remainder for $f \in W^{2,\infty}(\mathbb{R})$,

$$f(x) - f(a) - f'(a)(x-a) = (x-a)^2 \int_0^1 f''(a + z(x-a))(1-z)\,dz \quad \text{ for } a, x \in \mathbb{R},$$

to deduce that

$$\begin{aligned} f(\varphi_h) - f(\varphi) - f'(\varphi)\xi &= f'(\varphi)\Phi + (\varphi_h - \varphi)^2 R_f, \\ h(\varphi_h) - h(\varphi) - h'(\varphi)\xi &= h'(\varphi)\Phi + (\varphi_h - \varphi)^2 R_h, \\ k(\varphi_h) - k(\varphi) - k'(\varphi)\xi &= k'(\varphi)\Phi + (\varphi_h - \varphi)^2 R_k, \\ \Psi'(\varphi_h) - \Psi'(\varphi) - \Psi''(\varphi)\xi &= \Psi''(\varphi)\Phi + (\varphi_h - \varphi)^2 R_\Psi, \end{aligned}$$

where

$$\begin{aligned} R_f &= \int_0^1 f''(\varphi + z(\varphi_h - \varphi))(1-z)\,dz, \quad R_h = \int_0^1 h''(\varphi + z(\varphi_h - \varphi))(1-z)\,dz, \\ R_k &= \int_0^1 k''(\varphi + z(\varphi_h - \varphi))(1-z)\,dz, \quad R_\Psi = \int_0^1 \Psi'''(\varphi + z(\varphi_h - \varphi))(1-z)\,dz, \end{aligned}$$

and in light of the regularity assumption (A6), as well as (A2) and (2.4), there exists a positive constant C such that

$$\begin{aligned} &\|R_f\|_{L^\infty} + \|R_h\|_{L^\infty} + \|R_k\|_{L^\infty} \leq C, \\ &\|R_\Psi\|_{L^6} \leq C\big(1 + \|\varphi\|_{L^6} + \|\varphi_h\|_{L^6}\big) \leq C. \end{aligned} \tag{4.12}$$

Next, we test (4.11a) with Φ, (4.11b) with λ, (4.11c) with $M\theta$, and (4.11d) with $K\boldsymbol{z}$ for positive constants M, K yet to be determined, and on adding the resulting equations, we arrive at

$$\begin{aligned} &\frac{1}{2}\frac{d}{dt}\Big(\|\Phi\|_{L^2}^2 + \beta M\|\theta\|_{L^2}^2\Big) + \|\lambda\|_{L^2}^2 + M\|\nabla\theta\|^2 \\ &\quad + M(B\theta + \lambda_c h(\varphi)\theta, \theta) + M\kappa\|\theta\|_{L^2_\Gamma}^2 + Kc_0\|\mathcal{E}(\boldsymbol{z})\|^2 \\ &\leq -(\lambda_p X_h, \Phi) + \big((\lambda_a + w_2^*)[k(\varphi_h) - k(\varphi) - k'(\varphi)\xi] + h_2(k(\varphi_h) - k(\varphi)), \Phi\big) \\ &\quad + (\Psi'(\varphi_h) - \Psi'(\varphi) - \Psi''(\varphi)\xi, \lambda) - (\chi\theta, \lambda) + (\mathcal{C}(\mathcal{E}(\boldsymbol{z}) - \Phi\mathcal{E}^*) : \mathcal{E}^*, \lambda) \\ &\quad - M\lambda_c((\sigma - w_3^*)[h(\varphi_h) - h(\varphi) - h'(\varphi)\xi], \theta) + M\lambda_c((h(\varphi_h) - h(\varphi))h_3, \theta) \\ &\quad - M\lambda_c((h(\varphi_h) - h(\varphi))(\sigma_h - \sigma), \theta) + K(\mathcal{C}(\Phi\mathcal{E}^*), \mathcal{E}(\boldsymbol{z})). \end{aligned} \tag{4.13}$$

Looking at the terms involving $\boldsymbol{z}$, we see

$$\begin{aligned}&(\mathcal{C}(\mathcal{E}(\boldsymbol{z}) - \Phi\mathcal{E}^*) : \mathcal{E}^*, \lambda) + K(\mathcal{C}(\Phi\mathcal{E}^*), \mathcal{E}(\boldsymbol{z}))\\ &\quad \leq \frac{1}{8}\|\lambda\|_{L^2}^2 + C\|\mathcal{E}(\boldsymbol{z})\|_{L^2}^2 + C(1+K^2)\|\Phi\|_{L^2}^2\end{aligned}$$

for a positive constant C independent of K. Next, for terms involving θ, we employ the boundedness of σ and w_3^* and the Lipschitz continuity of h to obtain

$$\begin{aligned}&-(\chi\theta, \lambda) - M\lambda_c((h(\varphi_h) - h(\varphi))(\sigma_h - \sigma), \theta)\\ &\qquad - M\lambda_c((\sigma - w_3^*)[h(\varphi_h) - h(\varphi) - h'(\varphi)\xi], \theta) + M\lambda_c((h(\varphi_h) - h(\varphi))h_3, \theta)\\ &\quad \leq \frac{1}{8}\|\lambda\|_{L^2}^2 + C\|\theta\|_{L^2}^2 + M^2C\|\varphi_h - \varphi\|_{L^4}^2\|\sigma_h - \sigma\|_{L^4}^2\\ &\qquad + M^2C\|h''(\varphi)\Phi + (\varphi_h - \varphi)^2R_h\|_{L^2}^2 + M^2C\|\varphi_h - \varphi\|_{L^2}^2|h_3|^2\\ &\quad \leq CM^2\big(\|\Phi\|_{L^2}^2 + \|\varphi_h - \varphi\|_{H^1}^2\big(\|\sigma_h - \sigma\|_{H^1}^2 + \|\varphi_h - \varphi\|_{H^1}^2 + |h_3|^2\big)\big)\\ &\qquad + \frac{1}{8}\|\lambda\|_{L^2}^2 + C\|\theta\|_{L^2}^2\end{aligned}$$

for a positive constant C independent of M. Next, for the terms involving k in (4.13), we similarly have

$$\begin{aligned}&((\lambda_a + w_2^*)[k(\varphi_h) - k(\varphi) - k'(\varphi)\xi] + h_2(k(\varphi_h) - k(\varphi)), \Phi)\\ &\quad \leq C\|\Phi\|_{L^2}^2 + C\|\varphi_h - \varphi\|_{L^4}^4 + C\|\varphi_h - \varphi\|_{L^2}^2|h_2|^2\\ &\quad \leq C\|\Phi\|_{L^2}^2 + C\big(|h_2|^2 + \|\varphi_h - \varphi\|_{H^1}^2\big)\|\varphi_h - \varphi\|_{H^1}^2\end{aligned}$$

and, for the terms involving Ψ',

$$\begin{aligned}&(\Psi'(\varphi_h) - \Psi'(\varphi) - \Psi''(\varphi)\xi, \lambda) = (\Psi''(\varphi)\Phi + R_\Psi(\varphi_h - \varphi)^2, \lambda)\\ &\quad \leq \|\Psi''(\varphi)\|_{L^\infty}\|\Phi\|_{L^2}\|\lambda\|_{L^2} + \|R_\Psi\|_{L^6}\|\varphi_h - \varphi\|_{L^6}^2\|\lambda\|_{L^2}\\ &\quad \leq \frac{1}{8}\|\lambda\|_{L^2}^2 + C\big(1 + \|\varphi\|_{H^2}^4\big)\|\Phi\|_{L^2}^2 + C\|\varphi_h - \varphi\|_{H^1}^4,\end{aligned}$$

where we used (A2), (2.5), and (4.12). Finally, we tackle the term involving X_h. First, we observe with the assumption $g \in W^{2,\infty}(\mathbb{R}^{d\times d}, \mathbb{R})$ from (A6) that

$$\begin{aligned}|g(\mathcal{W}_{,\mathcal{E}}(\varphi_h, \mathcal{E}(\boldsymbol{u}_h))) - g(\mathcal{W}_{,\mathcal{E}}(\varphi, \mathcal{E}(\boldsymbol{u})))| &= \left|\int_0^1 g'(\cdot)\, dz : \mathcal{C}(\mathcal{E}(\boldsymbol{u}_h - \boldsymbol{u}) - (\varphi_h - \varphi)\mathcal{E}^*)\right|\\ &\leq C|\mathcal{E}(\boldsymbol{u}_h) - \mathcal{E}(\boldsymbol{u})| + C|\varphi_h - \varphi|,\end{aligned}$$

where $g'(\cdot)$ is evaluated at $z\mathcal{W}_{,\mathcal{E}}(\varphi_h, \mathcal{E}(\boldsymbol{u}_h)) + (1-z)\mathcal{W}_{,\mathcal{E}}(\varphi, \mathcal{E}(\boldsymbol{u}))$, and

$$\begin{aligned}&g(\mathcal{W}_{,\mathcal{E}}(\varphi_h, \mathcal{E}(\boldsymbol{u}_h))) - g(\mathcal{W}_{,\mathcal{E}}(\varphi, \mathcal{E}(\boldsymbol{u}))) - g'(\mathcal{W}_{,\mathcal{E}}(\varphi, \mathcal{E}(\boldsymbol{u}))) : \mathcal{C}(\mathcal{E}(\boldsymbol{v}) - \xi\mathcal{E}^*)\\ &\quad = g'(\mathcal{W}_{,\mathcal{E}}(\varphi, \mathcal{E}(\boldsymbol{u}))) : \mathcal{C}(\mathcal{E}(\boldsymbol{z}) - \Phi\mathcal{E}^*)\\ &\qquad + \Big(\int_0^1 (1-z)g''(\cdot)\, dz\Big)[\mathcal{C}(\mathcal{E}(\boldsymbol{u}_h - \boldsymbol{u}) - (\varphi_h - \varphi)\mathcal{E}^*)] : [\mathcal{C}(\mathcal{E}(\boldsymbol{u}_h - \boldsymbol{u}) - (\varphi_h - \varphi)\mathcal{E}^*)]\\ &\quad \leq g'(\mathcal{W}_{,\mathcal{E}}(\varphi, \mathcal{E}(\boldsymbol{u}))) : \mathcal{C}(\mathcal{E}(\boldsymbol{z}) - \Phi\mathcal{E}^*) + C|\mathcal{C}(\mathcal{E}(\boldsymbol{u}_h - \boldsymbol{u}) - (\varphi_h - \varphi)\mathcal{E}^*)|^2,\end{aligned}$$

where $g''(\cdot)$ is evaluated at $(1-z)\mathcal{W}_{,\mathcal{E}}(\varphi, \mathcal{E}(\boldsymbol{u})) + z\mathcal{W}_{,\mathcal{E}}(\varphi_h, \mathcal{E}(\boldsymbol{u}_h))$. Hence, using the boundedness of $f(\varphi)$, $g(\cdot)$, $g'(\cdot)$, $g''(\cdot)$, σ, and σ_h that are independent of $\|\boldsymbol{h}\|_{\mathcal{U}}$, we obtain for a positive constant $\varepsilon > 0$ to be determined later

$$\begin{aligned}(\lambda_p X_h, \Phi) &\le \varepsilon\|\Phi\|_{H^2}^2 + C\|X_h\|_{L^1}^2 \\ &\le \varepsilon\|\Phi\|_{H^2}^2 + C\|\mathcal{E}(\boldsymbol{u}_h) - \mathcal{E}(\boldsymbol{u})\|_{L^2}^2\|\varphi_h - \varphi\|_{L^4}^2\|\sigma_h - \sigma\|_{L^4}^2 \\ &\quad + C\|\mathcal{E}(\boldsymbol{u}_h) - \mathcal{E}(\boldsymbol{u})\|_{L^2}^2\big(\|\sigma_h - \sigma\|_{L^2}^2 + \|\varphi_h - \varphi\|_{L^2}^2\big) \\ &\quad + C\|\varphi_h - \varphi\|_{L^4}^4\|\sigma_h - \sigma\|_{L^2}^2 + C\|\varphi_h - \varphi\|_{L^2}^4 + C\|\varphi_h - \varphi\|_{L^2}^2\|\sigma_h - \sigma\|_{L^2}^2 \\ &\quad + C\|\Phi\|_{L^2}^2 + C\|\theta\|_{L^2}^2 + C\|\mathcal{E}(\boldsymbol{z})\|_{L^2}^2 + C\|\mathcal{E}(\boldsymbol{u}_h) - \mathcal{E}(\boldsymbol{u})\|_{L^2}^4 \\ &\le \varepsilon\|\Phi\|_{H^2}^2 + C(\|\boldsymbol{h}\|_{\mathcal{U}}^4 + \|\boldsymbol{h}\|_{\mathcal{U}}^6).\end{aligned}$$

To close the estimate, we require an estimate, for $\|\Phi\|_{H^2}^2$, which can be obtained from (4.11b). Using that $(\Phi, \lambda, \theta, \boldsymbol{z}) \in \mathcal{Y}_{\mathrm{lin}}^{\beta}$, we see that

$$\begin{aligned}\|\Delta\Phi\|_{L^2}^2 &\le C\|\lambda\|_{L^2}^2 + C\|\Psi'(\varphi_h) - \Psi'(\varphi) - \Psi''(\varphi)\xi\|_{L^2}^2 \\ &\quad + C\|\theta\|_{L^2}^2 + C\|\mathcal{E}(\boldsymbol{z})\|_{L^2}^2 + C\|\Phi\|_{L^2}^2 \\ &\le C\big(1 + \|\varphi\|_{H^2}^4\big)\|\Phi\|_{L^2}^2 + C\|\boldsymbol{h}\|_{\mathcal{U}}^4 + C\big(\|\theta\|_{L^2}^2 + \|\mathcal{E}(\boldsymbol{z})\|_{L^2}^2 + \|\lambda\|_{L^2}^2\big).\end{aligned}$$

By elliptic regularity, there exists a positive constant C_0 independent of $(\Phi, \lambda, \theta, \boldsymbol{z})$ and $\boldsymbol{h}$, as well as M and K, such that

$$\|\Phi\|_{H^2}^2 \le C\big(1 + \|\varphi\|_{H^2}^4\big)\|\Phi\|_{L^2}^2 + C\|\boldsymbol{h}\|_{\mathcal{U}}^4 + C_0\big(\|\theta\|_{L^2}^2 + \|\mathcal{E}(\boldsymbol{z})\|_{L^2}^2 + \|\lambda\|_{L^2}^2\big). \tag{4.14}$$

Let α be a positive constant such that

$$\alpha C_0 \le \tfrac{1}{8}.$$

Multiplying (4.14) with α and adding to (4.13), then employing the estimates for the right-hand side and choosing $\varepsilon = \frac{\alpha}{2}$, we obtain

$$\begin{aligned}&\frac{1}{2}\frac{d}{dt}\Big(\|\Phi\|_{L^2}^2 + \beta M\|\theta\|_{L^2}^2\Big) + \frac{1}{2}\|\lambda\|_{L^2}^2 + \frac{\alpha}{2}\|\Phi\|_{H^2}^2 \\ &\qquad + M\|\nabla\theta\|_{L^2}^2 + MB\|\theta\|_{L^2}^2 + M\kappa\|\theta\|_{L^2_\Gamma}^2 - \hat{C}\|\theta\|_{L^2}^2 + (Kc_0 - \hat{C})\|\mathcal{E}(\boldsymbol{z})\|_{L^2}^2 \\ &\quad \le C\big(1 + \|\varphi\|_{H^2}^4\big)\|\Phi\|_{L^2}^2 + C\|\varphi_h - \varphi\|_{H^1}^2\big(|h_2|^2 + |h_3|^2\big) \\ &\qquad + C\|\varphi_h - \varphi\|_{H^1}^2\big(\|\sigma_h - \sigma\|_{H^1}^2 + \|\varphi_h - \varphi\|_{H^1}^2 + \|\mathcal{E}(\boldsymbol{u}_h) - \mathcal{E}(\boldsymbol{u})\|_{L^2}^2\big) \\ &\qquad + C\|\mathcal{E}(\boldsymbol{u}_h) - \mathcal{E}(\boldsymbol{u})\|_{L^2}^2\big(\|\mathcal{E}(\boldsymbol{u}_h) - \mathcal{E}(\boldsymbol{u})\|_{L^2}^2 + \|\sigma_h - \sigma\|_{L^2}^2\big) + C(\|\boldsymbol{h}\|_{\mathcal{U}}^4 + \|\boldsymbol{h}\|_{\mathcal{U}}^6) \\ &\quad =: C\big(1 + \|\varphi\|_{H^2}^4\big)\|\Phi\|_{L^2}^2 + C\|\varphi_h - \varphi\|_{H^1}^2\big(|h_2|^2 + |h_3|^2\big) + \mathcal{R}_h,\end{aligned}$$

where the positive constants $\hat{C}$ appearing on the left-hand side are independent of M and K. Hence, choosing M and K sufficiently large, with Gronwall's inequality and Korn's inequality, as well as $\Phi(0) = \theta(0) = 0$, we have

$$\begin{aligned}&\|\Phi\|_{L^\infty(0,T;L^2)}^2 + \beta\|\theta\|_{L^\infty(0,T;L^2)}^2 + \|\lambda\|_{L^2(Q)}^2 + \|\Phi\|_{L^2(0,T;H^2)}^2 \\ &\qquad + \|\theta\|_{L^2(0,T;H^1)}^2 + \|\boldsymbol{z}\|_{L^2(0,T;X(\Omega))}^2 \\ &\quad \le C\exp\Big(C + C\|\varphi\|_{L^4(0,T;H^2)}^4\Big)\int_0^T \|\varphi_h - \varphi\|_{H^1}^2\big(|h_2|^2 + |h_3|^2\big) + \mathcal{R}_h\, dt \\ &\quad \le C(\|\boldsymbol{h}\|_{\mathcal{U}}^4 + \|\boldsymbol{h}\|_{\mathcal{U}}^6),\end{aligned}$$

where the last inequality comes from the application of (2.5). This completes the proof as (4.10) has been shown. ∎

4.3. Adjoint system. Associated to an optimal control $\boldsymbol{w}^* \in \mathcal{U}_{ad}$ and its corresponding solution $(\varphi, \mu, \sigma, \boldsymbol{u})$ are the adjoint variables $(p, q, r, \boldsymbol{s})$ that satisfy the following adjoint system written in strong form:

$$f_1 = -p_t - \Delta q + \mathcal{G}, \quad q = -\Delta p \qquad \text{in } Q, \tag{4.15a}$$
$$0 = -\beta r_t - \Delta r + Br + \mathcal{K} \qquad \text{in } Q, \tag{4.15b}$$
$$\operatorname{div}(\boldsymbol{f}_2) = \operatorname{div}(\mathcal{C}(\mathcal{E}(\boldsymbol{s}) + \mathcal{H})) \qquad \text{in } Q, \tag{4.15c}$$
$$p(T) = \alpha_\Omega(\varphi(T) - \varphi_\Omega), \quad r(T) = 0 \qquad \text{in } \Omega, \tag{4.15d}$$
$$0 = \partial_{\boldsymbol{n}} p = \partial_{\boldsymbol{n}} q, \quad \partial_{\boldsymbol{n}} r + \kappa r = 0 \qquad \text{on } \Sigma, \tag{4.15e}$$
$$\boldsymbol{0} = (\mathcal{C}(\mathcal{E}(\boldsymbol{s}) + \mathcal{H}) - \boldsymbol{f}_2)\boldsymbol{n} \qquad \text{on } \Sigma_D, \tag{4.15f}$$
$$\boldsymbol{s} = \boldsymbol{0} \qquad \text{on } \Sigma_N, \tag{4.15g}$$

where using the notation $n'(\cdot, \varphi) = \frac{\partial n}{\partial \varphi}(\cdot, \varphi)$

$$\begin{aligned}
f_1 &= f_1(\varphi, \mathcal{E}(\boldsymbol{u})) = \alpha_Q(\varphi - \varphi_Q) + \tfrac{\alpha_{\mathcal{E}}}{2} n'(\cdot, \varphi)|\mathcal{W}_{,\mathcal{E}}(\varphi, \mathcal{E}(\boldsymbol{u}))|^2 \\
&\quad - \alpha_{\mathcal{E}} n(\cdot, \varphi) \mathcal{W}_{,\mathcal{E}}(\varphi, \mathcal{E}(\boldsymbol{u})) : \mathcal{C}\mathcal{E}^*, \\
\boldsymbol{f}_2 &= \boldsymbol{f}_2(\varphi, \mathcal{E}(\boldsymbol{u})) = -\alpha_{\mathcal{E}} n(\cdot, \varphi) \mathcal{C} \mathcal{W}_{,\mathcal{E}}(\varphi, \mathcal{E}(\boldsymbol{u})), \\
\mathcal{G} &= \mathcal{G}(\varphi, \sigma, \mathcal{E}(\boldsymbol{u}), p, q, r, \mathcal{E}(\boldsymbol{s}), w_2^*, w_3^*) = \Psi''(\varphi) q + (\lambda_a + w_2^*) k'(\varphi) p + q \mathcal{C}\mathcal{E}^* : \mathcal{E}^* \\
&\quad - \lambda_p \sigma p \big(f'(\varphi) g(\mathcal{W}_{,\mathcal{E}}(\varphi, \mathcal{E}(\boldsymbol{u}))) + f(\varphi) g'(\mathcal{W}_{,\mathcal{E}}(\varphi, \mathcal{E}(\boldsymbol{u}))) : \mathcal{C}\mathcal{E}^*\big) \\
&\quad + h'(\varphi)(\lambda_c \sigma - w_3^*) r + \mathcal{C}\mathcal{E}^* : \mathcal{E}(\boldsymbol{s}), \\
\mathcal{K} &= \mathcal{K}(\varphi, \mathcal{E}(\boldsymbol{u}), p, q, r) = h(\varphi) \lambda_c r - \lambda_p f(\varphi) g(\mathcal{W}_{,\mathcal{E}}(\varphi, \mathcal{E}(\boldsymbol{u}))) p - \chi q, \\
\mathcal{H} &= \mathcal{H}(\varphi, \sigma, \mathcal{E}(\boldsymbol{u}), p, q) = q \mathcal{E}^* + \lambda_p p \sigma f(\varphi) g'(\mathcal{W}_{,\mathcal{E}}(\varphi, \mathcal{E}(\boldsymbol{u}))).
\end{aligned}$$

We introduce the solution space

$$\mathcal{Z}^\beta = \begin{cases} H^1(0,T; H^2_{\boldsymbol{n}}(\Omega)') \cap L^2(0,T; H^2_{\boldsymbol{n}}(\Omega)) \times L^2(Q) \\ \times H^1(0,T; H^1(\Omega)') \cap L^2(0,T; H^1(\Omega)) \times L^2(0,T; X(\Omega)) & \text{if } \beta > 0, \\ \\ H^1(0,T; H^2_{\boldsymbol{n}}(\Omega)') \cap L^2(0,T; H^2_{\boldsymbol{n}}(\Omega)) \times L^2(Q) \\ \times L^2(0,T; H^1(\Omega)) \times L^2(0,T; X(\Omega)) & \text{if } \beta = 0. \end{cases}$$

THEOREM 4.4. *For given $\boldsymbol{w}^* \in \mathcal{U}_{ad}$ with $(\varphi, \mu, \sigma, \boldsymbol{u}) = \mathcal{S}(\boldsymbol{w}^*) \in \mathcal{Y}^\beta$, under* (A1)–(A8)*, there exists a unique solution $(p, q, r, \boldsymbol{s}) \in \mathcal{Z}^\beta$ to the adjoint system* (4.15) *with $p(T) = \alpha_\Omega(\varphi(T) - \varphi_\Omega)$, $r(T) = 0$ if $\beta > 0$, and*

$$0 = \int_0^T -\langle p_t, \zeta \rangle_{H^2} - (q, \Delta \zeta) + (\mathcal{G} - f_1, \zeta)\, dt, \tag{4.16a}$$
$$0 = \int_0^T -(q, \phi) + (\nabla p, \nabla \phi)\, dt, \tag{4.16b}$$
$$0 = \int_0^T \beta \langle -r_t, \phi \rangle + (\nabla r, \nabla \phi) + (Br, \phi) + \kappa (r, \phi)_\Gamma + (\mathcal{K}, \phi)\, dt, \tag{4.16c}$$
$$0 = \int_0^T (\mathcal{C}(\mathcal{E}(\boldsymbol{s}) + \mathcal{H}) - \boldsymbol{f}_2, \nabla \boldsymbol{\eta})\, dt \tag{4.16d}$$

for all $\zeta \in L^2(0,T; H^2_{\boldsymbol{n}}(\Omega))$, $\phi \in L^2(0,T; H^1(\Omega))$, and $\boldsymbol{\eta} \in L^2(0,T; X(\Omega))$.

Remark 4.5. Let us notice that the test function space $H^2_{\boldsymbol{n}}(\Omega)$ in (4.16a) can be weakened by assuming a more regular target function φ_Ω. In fact, formally testing (4.16a) by q and (4.16b) by p_t will lead to the regularity $q \in L^2(0,T;H^1(\Omega))$ and $p \in L^\infty(0,T;H^1(\Omega))$ provided that $p(T) = \alpha_\Omega(\varphi(T) - \varphi_\Omega) \in H^1(\Omega)$, which is fulfilled if $\varphi_\Omega \in H^1(\Omega)$.

Proof. We proceed with formal estimates that can be rigorously derived with a standard Galerkin approximation, and let us note that in the following, positive constants denoted by the symbol C will be independent of the Galerkin parameter. Then, testing $\zeta = Kp$ in (4.16a), $\phi = -Kq$ and $\phi = p$ in (4.16b), $\phi = Hr$ in (4.16c), and $\boldsymbol{\eta} = Z\boldsymbol{s}$ in (4.16d) for some positive constants K, H, and Z yet to be determined, we obtain after summing the resulting equalities

$$
\begin{aligned}
&-\frac{1}{2}\frac{d}{dt}\Big(K\|p\|^2_{L^2} + H\beta\|r\|^2_{L^2}\Big) + K\|q\|^2_{L^2} + \|\nabla p\|^2_{L^2} \\
&\quad + H\|\nabla r\|^2_{L^2} + H\kappa\|r\|^2_{L^2_\Gamma} + HB\|r\|^2_{L^2} + Zc_0\|\mathcal{E}(\boldsymbol{s})\|^2_{L^2} \\
&\le -(K(\mathcal{G} - f_1), p) + (q,p) - (H\mathcal{K}, r) - (Z(\mathcal{C}\mathcal{H} - \boldsymbol{f}_2), \mathcal{E}(\boldsymbol{s})).
\end{aligned} \tag{4.17}
$$

First, we obtain from (4.16b) and elliptic regularity that

$$
\|p\|^2_{H^2} \le C\|\Delta p\|^2_{L^2} + C\|p\|^2_{L^2} \le C\|q\|^2_{L^2} + C\|p\|^2_{L^2}. \tag{4.18}
$$

Then a short calculation involving the embedding $H^2(\Omega) \subset L^\infty(\Omega)$ shows that

$$
\begin{aligned}
(K(\mathcal{G} - f_1), p) &\le \frac{1}{2}\|q\|^2_{L^2} + C\big(1 + \|\Psi''(\varphi)\|^2_{L^\infty}\big)\|p\|^2_{L^2} + C\|r\|^2_{L^2} + C\|\varphi\|^2_{L^2} \\
&\quad + C\|\mathcal{E}(\boldsymbol{u})\|^2_{L^2} + C\|\mathcal{E}(\boldsymbol{s})\|^2_{L^2} + \tfrac{1}{2}\|p\|^2_{H^2} + C\|\varphi - \varphi_Q\|^2_{L^2}, \\
(q,p) &\le \frac{1}{2}\|q\|^2_{L^2} + C\|p\|^2_{L^2}, \\
(H\mathcal{K}, r) &\le H^2\|q\|^2_{L^2} + C\big(\|r\|^2_{L^2} + \|p\|^2_{L^2}\big), \\
(Z(\mathcal{C}\mathcal{H} - \boldsymbol{f}_2), \mathcal{E}(\boldsymbol{s})) &\le Z^2\|q\|^2_{L^2} + CZ^2\big(\|p\|^2_{L^2} + \|\varphi\|^2_{L^2} + \|\mathcal{E}(\boldsymbol{u})\|^2_{L^2}\big) + C\|\mathcal{E}(\boldsymbol{s})\|^2_{L^2},
\end{aligned}
$$

with positive constants C independent of H and Z. Adding (4.18) to (4.17) and substituting the above yields

$$
\begin{aligned}
&-\frac{1}{2}\frac{d}{dt}\Big(K\|p\|^2_{L^2} + H\beta\|r\|^2_{L^2}\Big) + (K - (1 + C + H^2 + Z^2))\|q\|^2_{L^2} + \tfrac{1}{2}\|p\|^2_{H^2} \\
&\quad + H\|\nabla r\|^2_{L^2} + H\kappa\|r\|^2_{L^2_\Gamma} + (HB - C)\|r\|^2_{L^2} + (Zc_0 - C)\|\mathcal{E}(\boldsymbol{s})\|^2_{L^2} \\
&\le C\big(1 + \|\varphi\|^4_{H^2}\big)\|p\|^2_{L^2} + C\|\varphi - \varphi_Q\|^2_{L^2} + C\big(\|\varphi\|^2_{L^2} + \|\mathcal{E}(\boldsymbol{u})\|^2_{L^2}\big).
\end{aligned}
$$

If $B > 0$, we choose $HB > C$; otherwise, we use the generalized Poincaré inequality with H sufficiently large so that

$$
H\|\nabla r\|^2_{L^2} + H\kappa\|r\|^2_{L^2_\Gamma} \ge (C+1)\|r\|^2_{L^2}.
$$

Then, choosing Z sufficiently large so that $Zc_0 > C$ and then finally K sufficiently large, we obtain via Gronwall's inequality (applied backward in time) and Korn's inequality that

$$
\begin{aligned}
&\|p\|^2_{L^\infty(0,T;L^2)} + \beta\|r\|^2_{L^\infty(0,T;L^2)} + \|q\|^2_{L^2(Q)} \\
&\quad + \|p\|^2_{L^2(0,T;H^2)} + \|r\|^2_{L^2(0,T;H^1)} + \|\boldsymbol{s}\|^2_{L^2(0,T;X(\Omega))} \\
&\le C\|\varphi - \varphi_Q\|^2_{L^2(Q)} + C\|\varphi\|^2_{L^2(Q)} + C\|\mathcal{E}(\boldsymbol{u})\|^2_{L^2(Q)}.
\end{aligned} \tag{4.19}
$$

Then, from (4.16a), we infer

$$\|p_t\|_{L^2(0,T;H^2_{\boldsymbol{n}}(\Omega)')} \leq C\big(1 + \|\Psi''(\varphi)\|_{L^\infty(0,T;L^2)}\big)\|q\|_{L^2(Q)} + C\|p\|_{L^2(Q)} + C\|r\|_{L^2(Q)} \\ + C\|\mathcal{E}(\boldsymbol{s})\|_{L^2(Q)} + C\big(1 + \|\varphi - \varphi_Q\|_{L^2(Q)}\big),$$

and if $\beta > 0$, a comparison of terms in (4.16c) gives

$$\|r_t\|_{L^2(0,T;H^1(\Omega)')} \leq C\|r\|_{L^2(0,T;H^1)} + C\|p\|_{L^2(Q)} + C\|q\|_{L^2(Q)}.$$

These estimates are sufficient to pass to the limit and deduce the existence of a solution $(p, q, r, \boldsymbol{s}) \in \mathcal{Z}^\beta$ to (4.15) in the sense that (4.16) is fulfilled. Moreover, as the adjoint system is linear in $(p, q, r, \boldsymbol{s})$, the difference of any two solutions satisfies (4.16), where the terms involving $n(\cdot, \varphi)$ and $\varphi - \varphi_Q$ are absent in f_1 and $\boldsymbol{f}_2$. Consequently, we arrive at an analogue of (4.19) for the difference of two solutions where the right-hand side is zero, which in turn leads to uniqueness of solutions. ∎

4.4. Optimality conditions. Finally, we exploit the differentiability property of $\mathcal{S}$ established so far to obtain the first-order necessary conditions for optimality. In this direction, we first express the reduced cost functional $\mathcal{J}$ as the sum

$$\mathcal{J}(\boldsymbol{w}) := \mathcal{J}_1(\boldsymbol{w}) + \mathcal{J}_2(\boldsymbol{w}),$$

where

$$\begin{aligned} \mathcal{J}_1(\boldsymbol{w}) &= \frac{\alpha_\Omega}{2}\|\mathcal{S}_1(\boldsymbol{w}) - \varphi_\Omega\|^2_{L^2(\Omega)} + \frac{\alpha_Q}{2}\|\mathcal{S}_1(\boldsymbol{w}) - \varphi_Q\|^2_{L^2(Q)} \\ &\quad + \frac{\alpha_{\mathcal{E}}}{2}\int_Q n(x, \mathcal{S}_1(\boldsymbol{w}))|\mathcal{W}_{,\mathcal{E}}(\mathcal{S}_1(\boldsymbol{w}), \mathcal{E}(\mathcal{S}_4(\boldsymbol{w})))|^2\, dx\, dt \\ &\quad + \frac{\gamma_1}{2}\|w_1\|^2_{L^2(\Sigma)} + \frac{\gamma_2}{2}\|w_2\|^2_{L^2(0,T)} + \frac{\gamma_3}{2}\|w_3\|^2_{L^2(0,T)}, \\ \mathcal{J}_2(\boldsymbol{w}) &= \gamma_4\|w_2\|_{L^1(0,T)} + \gamma_5\|w_3\|_{L^1(0,T)}. \end{aligned}$$

Then, for arbitrary $\boldsymbol{y} \in \mathcal{U}_{ad}$ and an optimal control $\boldsymbol{w}^* \in \mathcal{U}_{ad}$ with corresponding state $(\varphi, \mu, \sigma, \boldsymbol{u}) = \mathcal{S}(\boldsymbol{w}^*) \in \mathcal{Y}^\beta$ and linearized state variables $(\xi, \eta, \psi, \boldsymbol{v}) \in \mathcal{Y}^\beta_{\text{lin}}$ to (4.4) corresponding to $\boldsymbol{h} = \boldsymbol{y} - \boldsymbol{w}^*$, the differentiability of the solution operator $\mathcal{S} : \mathcal{U} \to \mathcal{Y}^\beta$ and the chain rule shows that

$$\begin{aligned} &D\mathcal{J}_1(\boldsymbol{w}^*)[\boldsymbol{h}] = D\mathcal{J}_1(\boldsymbol{w}^*)[\boldsymbol{y} - \boldsymbol{w}^*] \\ &\quad = \int_\Omega \alpha_\Omega(\varphi(T) - \varphi_\Omega)\xi(T)\, dx + \int_Q \alpha_Q(\varphi - \varphi_Q)\xi\, dx\, dt \\ &\qquad + \alpha_{\mathcal{E}}\int_Q \tfrac{1}{2}n'(x,\varphi)\xi|\mathcal{W}_{,\mathcal{E}}|^2 + n(x,\varphi)\mathcal{W}_{,\mathcal{E}} : \mathcal{C}(\mathcal{E}(\boldsymbol{v}) - \xi\mathcal{E}^*)\, dx\, dt \\ &\qquad + \int_0^T \gamma_1(w_1^*, h_1)_\Gamma\, dt + \int_0^T \gamma_2 w_2^* h_2 + \gamma_3 w_3^* h_3\, dt, \end{aligned} \tag{4.20}$$

where $\mathcal{W}_{,\mathcal{E}}$ is evaluated at $(\varphi, \mathcal{E}(\boldsymbol{u}))$. On the other hand, optimality of $\boldsymbol{w}^*$ and the convexity of $\mathcal{J}_2$ leads to

$$\begin{aligned} 0 &\leq \mathcal{J}(\boldsymbol{w}^* + t(\boldsymbol{y} - \boldsymbol{w}^*)) - \mathcal{J}(\boldsymbol{w}^*) \\ &= \mathcal{J}_1(\boldsymbol{w}^* + t(\boldsymbol{y} - \boldsymbol{w}^*)) - \mathcal{J}_1(\boldsymbol{w}^*) + \mathcal{J}_2((1-t)\boldsymbol{w}^* + t\boldsymbol{y}) - \mathcal{J}_2(\boldsymbol{w}^*) \\ &\leq \mathcal{J}_1(\boldsymbol{w}^* + t(\boldsymbol{y} - \boldsymbol{w}^*)) - \mathcal{J}_1(\boldsymbol{w}^*) + t[\mathcal{J}_2(\boldsymbol{y}) - \mathcal{J}_2(\boldsymbol{w}^*)] \end{aligned}$$

for all $t \in (0,1)$ and arbitrary $\boldsymbol{y} \in \mathcal{U}_{ad}$. Dividing by t and passing to the limit $t \to 0$ yields the inequality

$$0 \le D\mathcal{J}_1(\boldsymbol{w}^*)[\boldsymbol{y} - \boldsymbol{w}^*] + \mathcal{J}_2(\boldsymbol{y}) - \mathcal{J}_2(\boldsymbol{w}^*) \quad \forall \boldsymbol{y} \in \mathcal{U}_{ad}. \tag{4.21}$$

Arguing as in [41, sects. 3 and 4], the inequality (4.21) allows us to interpret $\boldsymbol{w}^*$ as a solution to the convex minimization problem

$$\min_{\boldsymbol{y} \in \mathcal{U}} \Big(D\mathcal{J}_1(\boldsymbol{w}^*)[\boldsymbol{y}] + \mathcal{J}_2(\boldsymbol{y}) + \mathbb{I}_{\mathcal{U}_{ad}}(\boldsymbol{y}) \Big), \quad \text{where} \quad \mathbb{I}_{\mathcal{U}_{ad}}(\boldsymbol{y}) = \begin{cases} 0 & \text{if } \boldsymbol{y} \in \mathcal{U}_{ad}, \\ +\infty & \text{otherwise} \end{cases}$$

denotes the indicator function of the set $\mathcal{U}_{ad}$. Using the definition of subdifferentials, the inequality (4.21) can also be interpreted as

$$\mathbf{0} \in \partial \Big(D\mathcal{J}_1(\boldsymbol{w}^*) + \mathcal{J}_2 + \mathbb{I}_{\mathcal{U}_{ad}} \Big)(\boldsymbol{w}^*) = \{ D\mathcal{J}_1(\boldsymbol{w}^*) \} + \partial \mathcal{J}_2(\boldsymbol{w}^*) + \partial \mathbb{I}_{\mathcal{U}_{ad}}(\boldsymbol{w}^*),$$

where the equality is due to the well-known sum rule for subdifferentials of convex functionals. This implies that there exist elements $\boldsymbol{\zeta} \in \partial \mathbb{I}_{\mathcal{U}_{ad}}(\boldsymbol{w}^*)$, and $\lambda_2(t) \in \partial \|w_2^*(t)\|_{L^1(0,T)}$, $\lambda_3(t) \in \partial \|w_3^*(t)\|_{L^1(0,T)}$ with $\lambda_2, \lambda_3 \in L^\infty(0,T)$ satisfy (4.1) for a.e. $t \in (0,T)$ (see, e.g., [41, sect. 4.2] for similar ideas regarding the derivation) such that

$$\mathbf{0} = D\mathcal{J}_1(\boldsymbol{w}^*) + \boldsymbol{\lambda} + \boldsymbol{\zeta}$$

for $\boldsymbol{\lambda} = (0, \gamma_4 \lambda_2, \gamma_5 \lambda_3)^\top$. From the definition of $\partial \mathbb{I}_{\mathcal{U}_{ad}}$, we have

$$(\boldsymbol{\zeta}, \boldsymbol{y} - \boldsymbol{w}^*) \le \mathbb{I}_{\mathcal{U}_{ad}}(\boldsymbol{y}) - \mathbb{I}_{\mathcal{U}_{ad}}(\boldsymbol{w}^*) = 0 \quad \text{as} \quad \boldsymbol{y}, \boldsymbol{w}^* \in \mathcal{U}_{ad},$$

where we use $(\cdot,\cdot)$ to denote the inner product on $\mathcal{U}$. Hence, from (4.21), we deduce that $\boldsymbol{w}^* \in \mathcal{U}_{ad}$ satisfies

$$0 \le D\mathcal{J}_1(\boldsymbol{w}^*)[\boldsymbol{y} - \boldsymbol{w}^*] + (\boldsymbol{\lambda}, \boldsymbol{y} - \boldsymbol{w}^*) \quad \forall \boldsymbol{y} \in \mathcal{U}_{ad}. \tag{4.22}$$

Next, we aim to simplify (4.20) with the help of the adjoint variables. The standard procedure is to test (4.4a) with $\zeta = p$, (4.4b) with $\zeta = -q$, (4.4c) with $\zeta = r$, and (4.4d) with $\boldsymbol{\eta} = \boldsymbol{s}$, then take the sum and compare with the resulting equality obtained from the sum of (4.16a) with $\zeta = \xi$, (4.16b) with $\phi = \eta$, (4.16c) with $\phi = \psi$, and (4.16d) with $\boldsymbol{\eta} = -\boldsymbol{v}$, which yields the relations

$$\begin{aligned} &\int_0^T \kappa(h_1, r)_\Gamma + (h_3 h(\varphi), r) - (h'(\varphi)\xi(\lambda_c \sigma - w_3^*), r)\, dt \\ &\quad = \int_0^T (\lambda_p f(\varphi) g(\mathcal{W}_{,\mathcal{E}}(\varphi, \mathcal{E}(\boldsymbol{u}))) p, \psi) - (\chi q, \psi)\, dt \end{aligned}$$

and

$$\begin{aligned} &\alpha_Q \int_Q (\varphi - \varphi_Q)\xi \, dx\, dt + \alpha_\Omega \int_\Omega (\varphi(T) - \varphi_\Omega)\xi(T)\, dx \\ &\quad + \int_Q \frac{\alpha_{\mathcal{E}}}{2} n'(x,\varphi)\xi |\mathcal{W}_{,\mathcal{E}}(\varphi, \mathcal{E}(\boldsymbol{u}))|^2 + \alpha_{\mathcal{E}} n(x,\varphi) \mathcal{W}_{,\mathcal{E}}(\varphi, \mathcal{E}(\boldsymbol{u})) : \mathcal{C}(\mathcal{E}(\boldsymbol{v}) - \xi \mathcal{E}^*)\, dx\, dt \\ &= \int_0^T (h'(\varphi)(\lambda_c \sigma - w_3^*) r, \xi) - (h_2 k(\varphi), p) - (\chi \psi, q)\, dt \\ &\quad + \int_0^T (\lambda_p f(\varphi) \psi g(\mathcal{W}_{,\mathcal{E}}(\varphi, \mathcal{E}(\boldsymbol{u}))), p)\, dt. \end{aligned}$$

Combining these two leads to the simplification

$$\begin{aligned} D\mathcal{J}_1(\boldsymbol{w}^*)[\boldsymbol{h}] &= \int_0^T \kappa(h_1, r)_\Gamma - h_2(k(\varphi), p) + h_3(h(\varphi), r)\, dt \\ &\quad + \int_0^T \gamma_1(w_1^*, h_1)_\Gamma \, dt + \int_0^T \gamma_2 w_2^* h_2 + \gamma_3 w_3^* h_3 \, dt, \end{aligned}$$

and (4.2) is then a consequence of (4.22).

5. Sparsity of nonnegative optimal controls. In the medical context, the control variables $w_2 = m(t)$ and $w_3 = s(t)$ should be nonnegative, and so we modify the admissible control subsets $\mathcal{U}_{ad}^{(2)}$ and $\mathcal{U}_{ad}^{(3)}$ to the following:

$$\mathcal{U}_{ad}^{(i)} = \{w_i \in L^\infty(0,T) : 0 \leq w_i(t) \leq \overline{w} \text{ for a.e. } t \in (0,T)\} \quad \text{for } i = 2, 3, \tag{5.1}$$

where $\overline{w}$ is a fixed positive constant. If $\gamma_1 > 0$, from the optimality condition (4.2), substituting $y_2 = w_2^*$ and $y_3 = w_3^*$ and then using the Hilbert projection theorem allows us to infer that w_1^* is the $L^2(\Sigma)$-orthogonal projection of $-\kappa r/\gamma_1$ onto the closed and convex subset $\mathcal{U}_{ad}^{(1)}$ of $L^2(\Sigma)$, leading to the representation formula

$$w_1^*(x,t) = \min\left(\overline{w}_1(x,t),\, \max\left(\underline{w}_1(x,t),\, -\tfrac{\kappa}{\gamma_1} r(x,t)\right)\right) \quad \text{for a.e. } (x,t) \in \Sigma.$$

In a similar fashion, if $\gamma_2, \gamma_4 > 0$, substituting $y_1 = w_1^*$ and $y_3 = w_3^*$ in (4.2) leads to the representation formula

$$w_2^*(t) = \mathbb{P}_{[0,\overline{w}]}\left(\frac{1}{\gamma_2}\left(\int_\Omega k(\varphi(x,t))p(x,t)\, dx - \gamma_4 \lambda_2(t)\right)\right) \quad \text{for a.e. } t \in (0,T), \tag{5.2}$$

where $\mathbb{P}_{[a,b]} : \mathbb{R} \to [a,b]$ denotes the pointwise projection function

$$\mathbb{P}_{[a,b]}(s) = \min(b, \max(a, s)).$$

Similarly, if $\gamma_3, \gamma_5 > 0$, then substituting $y_1 = w_1^*$ and $y_2 = w_2^*$ in (4.2) leads to the representation formula

$$w_3^*(t) = \mathbb{P}_{[0,\overline{w}]}\left(-\frac{1}{\gamma_3}\left(\gamma_5 \lambda_3(t) + \int_\Omega h(\varphi(x,t))r(x,t)\, dx\right)\right) \quad \text{for a.e. } t \in (0,T).$$

Due to the L^1-regularization for w_2 and w_3 in the optimal control problem, we can expect the optimal controls w_2^* and w_3^* to vanish on certain parts of the time interval $[0,T]$. This is formulated as follows.

THEOREM 5.1. *Under* (A1)–(A8)*, let* $\boldsymbol{w}^* = (w_1^*, w_2^*, w_3^*) \in \mathcal{U}_{ad}$ *be an optimal control where* $\mathcal{U}_{ad}^{(2)}$ *and* $\mathcal{U}_{ad}^{(3)}$ *are now given as* (5.1) *with the associated state* $(\varphi, \mu, \sigma, \boldsymbol{u}) = \mathcal{S}(\boldsymbol{w}^*)$ *and adjoint variables* $(p, q, r, \boldsymbol{s})$*. Then we have the following characterizations:*

- *If* $\gamma_2, \gamma_4 > 0$*, for a.e.* $t \in (0,T)$*,*

$$w_2^*(t) = 0 \iff \int_\Omega k(\varphi(x,t))p(x,t)\, dx \leq \gamma_4. \tag{5.3}$$

- *If* $\gamma_3, \gamma_5 > 0$*, for a.e.* $t \in (0,T)$*,*

$$w_3^*(t) = 0 \iff \int_\Omega h(\varphi(x,t))r(x,t)\, dx \geq -\gamma_5. \tag{5.4}$$

Remark 5.2. Similar one-sided inequalities characterizing sparsity of optimal controls are common when the lower bound in the admissible control sets $\mathcal{U}_{ad}^{(i)}$ is zero; see, e.g., [6, Thm. 3.1] or [7, Thm. 3.3]. If we allow $\underline{w}_2(t), \underline{w}_3(t)$ in the definition (2.2) of $\mathcal{U}_{ad}^{(2)}$ and $\mathcal{U}_{ad}^{(3)}$ to be a negative constant $\underline{w}$, then it is possible to provide a representation formula also for λ_2 and λ_3; see [41] in the context of Cahn–Hilliard tumor models and also [6, 7, 42] for classical parabolic and elliptic control problems. However, a negative lower bound for the controls may not be applicable in a medical context.

Remark 5.3. We point out that if $w_2^*(t_0) = 0$ for some $t_0 \in (0,T)$, then there exists an open subinterval $I \subset (0,T)$ with $t_0 \in I$ such that $w_2^*(t) = 0$ for all $t \in I$. The same assertion also holds for w_3^* provided that $\beta > 0$. This is due to the fact that the mappings

$$\begin{aligned} &t \mapsto \int_\Omega k(\varphi(x,t))p(x,t)\,dx, \\ &t \mapsto \int_\Omega h(\varphi(x,t))r(x,t)\,dx \text{ if } \beta > 0 \end{aligned}$$

are continuous in light of the regularities $\varphi \in C^0([0,T];L^2(\Omega))$ from Theorem 2.1 and $p \in C^0([0,T];L^2(\Omega))$ and $r \in C^0([0,T];L^2(\Omega))$ if $\beta > 0$ from Theorem 4.4. In particular, this behavior where the optimal controls are zero over an interval is consistent with the prevailing medical practice in which there are periods in the overall treatment where radiation/cytotoxic therapies are not applied to patients.

Proof. Let us just present the details for (5.3), as (5.4) can be derived in an analogous manner. Due to the modification to $\mathcal{U}_{ad}^{(2)}$, we observe from (4.1) that $\lambda_2(t) \in L^\infty(0,T)$ satisfies

$$\lambda_2(t) \in \begin{cases} \{1\} & \text{if } w_2^*(t) > 0, \\ [-1,1] & \text{if } w_2^*(t) = 0 \end{cases} \tag{5.5}$$

for a.e. $t \in (0,T)$. The left implication proceeds as follows: Consider the set $E = \{t \in (0,T) : w_2^*(t) = 0\}$, where by the representation formula (5.2), we see that

$$\int_\Omega k(\varphi(x,t))p(x,t)\,dx - \gamma_4\lambda_2(t) \le 0 \quad \text{for all } t \in E.$$

Using (5.5) and rearranging, we obtain the left implication of (5.3). For the right implication we argue by contrapositive: Suppose $w_2^*(t) > 0$. Then, from (5.5), we have $\lambda_2(t) = 1$, and thus by the representation formula it holds that

$$\int_\Omega k(\varphi(x,t))p(x,t)\,dx - \gamma_4\lambda_2(t) = \int_\Omega k(\varphi(x,t))p(x,t)\,dx - \gamma_4 > 0.$$

On rearranging, we obtain the assertion

$$w_2^*(t) > 0 \quad \Longrightarrow \quad \int_\Omega k(\varphi(x,t))p(x,t)\,dx > \gamma_4,$$

which gives the right implication of (5.3). ∎

An interesting consequence is that we can identify $w_2^*(t) \equiv 0$ as a local optimal control provided that γ_4 is sufficiently large and similarly that $w_3^*(t) \equiv 0$ is a local optimal control provided that γ_5 is sufficiently large.

Corollary 5.4. *Suppose* (A1)–(A8) *and* $\gamma_2 > 0$. *Then there exists* $\gamma_* > 0$ *such that for* $\gamma_4 > \gamma_*$, $w_2^*(t) \equiv 0$ *for all* $t \in (0,T)$ *is an optimal control for* (1.4). *Similarly, suppose* $\gamma_3 > 0$ *and* $\beta > 0$. *Then there exists* $\gamma^* > 0$ *such that for* $\gamma_5 > \gamma^*$, $w_3^*(t) \equiv 0$ *for all* $t \in (0,T)$ *is an optimal control for* (1.4).

Proof. It suffices to use conditions (5.3) and (5.4). In light of the admissible control subsets defined in (5.1), where $\overline{w}$ is a fixed constant, the constant K_1 in (2.4) is independent of the weights $\{\alpha_Q, \alpha_\Omega, \alpha_\mathcal{E}, \gamma_1, \gamma_2, \gamma_3, \gamma_4, \gamma_5\}$ in the optimal control problem (1.4). Then, revisiting the proof of Theorem 4.4, we note that $\{\gamma_i\}_{i=1}^5$ do not appear in the adjoint system (4.15). Consequently, the positive constants on the right-hand side of (4.19) are independent of $\{\gamma_i\}_{i=1}^5$. Employing (A3) on the boundedness of h and k, we deduce that

$$\int_\Omega k(\varphi(x,t))p(x,t)\,dx \leq C_1 \qquad \text{for a.e. } t \in (0,T),$$
$$\int_\Omega h(\varphi(x,t))r(x,t)\,dx \geq -C_2 \qquad \text{for a.e. } t \in (0,T) \text{ if } \beta > 0$$

for positive constants C_1 and C_2 independent of $\{\gamma_i\}_{i=1}^5$. The assertion now follows from (5.3) and (5.4) by choosing $\gamma_* = C_1$ and $\gamma^* = C_2$. ∎

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