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Optimal Control of a Phase Field System Modelling Tumor Growth with Chemotaxis and Singular Potentials

Pierluigi Colli[1] · Andrea Signori[2] · Jürgen Sprekels[3,4]

Abstract
A distributed optimal control problem for an extended model of phase field type for tumor growth is addressed. In this model, the chemotaxis effects are also taken into account. The control is realized by two control variables that design the dispensation of some drugs to the patient. The cost functional is of tracking type, whereas the potential setting has been kept quite general in order to allow regular and singular potentials to be considered. In this direction, some relaxation terms have been introduced in the system. We show the well-posedness of the state system, the Fréchet differentiability of the control-to-state operator in a suitable functional analytic framework, and, lastly, we characterize the first-order necessary conditions of optimality in terms of a variational inequality involving the adjoint variables.

Keywords Distributed optimal control · Tumor growth · Cancer treatment · Phase field system · Evolution equations · Chemotaxis · Adjoint system · Necessary optimality conditions

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✉ Andrea Signori
andrea.signori02@universitadipavia.it

Pierluigi Colli
pierluigi.colli@unipv.it

Jürgen Sprekels
sprekels@wias-berlin.de

1 Dipartimento di Matematica “F. Casorati”, Università di Pavia, via Ferrata 5, 27100 Pavia, Italy

2 Dipartimento di Matematica e Applicazioni, Università di Milano–Bicocca, via Cozzi 55, 20125 Milan, Italy

3 Department of Mathematics, Humboldt-Univesität zu Berlin, Unter den Linden 6, 10099 Berlin, Germany

4 Weierstrass Institute for Applied Analysis and Stochastics, Mohrenstrasse 39, 10117 Berlin, Germany

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1 Introduction

After realizing that tumor cells, like any other material, have to obey physical laws, a significant number of models have been introduced, since from a modelling viewpoint a tumor mass does not behave that different from other special materials investigated by scientists (see [11] and also [12,28,29,33,41,42]). As far as diffuse interface models are concerned, we can identify two main classes. The first one considers the tumor and healthy cells as inertialess fluids and includes effects generated by the fluid flow development by postulating a Darcy law or a Stokes–Brinkman law. In this connection, we refer to [13,14,19–25,41], where also further mechanisms such as chemotaxis and active transport are taken into account. The other class, to which our model belongs, neglects the velocity.

In this framework, let us take $\Omega \subset \mathbb{R}^3$ as an open, bounded, and connected set with smooth boundary Γ; moreover, we set, for $0 < t < T$,

$$Q := \Omega \times (0, T), \quad \Sigma := \Gamma \times (0, T), \quad Q_t := \Omega \times (0, t), \quad Q_t^T := \Omega \times (t, T).$$

The initial-boundary problem under investigation then reads as follows.

$$\alpha \partial_t \mu + \partial_t \varphi - \Delta \mu = (P\sigma - A - u) h(\varphi) \quad \text{in } Q, \tag{1.1}$$

$$\mu = \beta \partial_t \varphi - \Delta \varphi + F'(\varphi) - \chi \sigma \quad \text{in } Q, \tag{1.2}$$

$$\partial_t \sigma - \Delta \sigma = -\chi \Delta \varphi + B(\sigma_s - \sigma) - D\sigma h(\varphi) + w \quad \text{in } Q, \tag{1.3}$$

$$\partial_n \mu = \partial_n \varphi = \partial_n \sigma = 0 \quad \text{on } \Sigma, \tag{1.4}$$

$$\mu(0) = \mu_0, \ \varphi(0) = \varphi_0, \ \sigma(0) = \sigma_0 \quad \text{in } \Omega, \tag{1.5}$$

where the symbol ∂_n indicates the outward normal derivative to Γ. The above state system consists of an extended Cahn–Hilliard type system for the tumor phase coupled with a reaction-diffusion equation for an unknown species acting as a nutrient (e.g., glucose, oxygen, carbohydrates). The system (1.1)–(1.5) is a simplification and relaxed version of the model originally proposed in [24]. Indeed, the velocity contributions are neglected, and two relaxation terms are added. This choice will allow us to consider more general potentials that may exhibit a singular behavior. By assuming different linear phenomenological laws for chemical reactions, a different thermodynamically consistent model was introduced in [27] (see also [12,28,29,33]), and the corresponding mathematical investigations have been addressed in [3–5,17]. In [3–5] the same two relaxation terms $\alpha \partial_t \mu$ and $\beta \partial_t \varphi$ have been introduced. As in the current case, their presence allowed the authors to take into account more general potentials that may be singular and also nonregular. Moreover, in [4,5], the authors pointed out how α and β can be set to zero, by providing the proper framework in which a limit system can be identified and uniquely solved (let us also mention [8–10], where similar problems have been addressed for the case of fractional operators). Next, we mention [18], where a similar nonlocal version was studied for the case of singular potentials and degenerate mobilities. Let us also point out [2,32], where the long-time behavior of these models was analyzed in terms of the convergence to equilibrium and of the existence of a global attractor, respectively. For further models, discussing the case of multispecies, we address the reader to [13,19].

Now, let us briefly describe the role of the occurring symbols from a modeling viewpoint. The variable φ stands for an order parameter and is usually taken between -1 and 1; it represents the healthy cell case and the tumor phase, respectively. Moreover, μ indicates the chemical potential for φ, whereas σ denotes the nutrient extra-cellular water concentration. This latter quantity is usually normalized between 0 and 1, conveying that these values model the nutrient-poor and the nutrient-rich cases. The symbols α and β represent positive constants; let us just note that the term $\beta\partial_t\varphi$ in the second equation corresponds to the classical term of the viscous Cahn–Hilliard equation, while the term $\alpha\partial_t\mu$ gives to Eq. (1.1) a parabolic structure with respect to μ. For more details on these relaxation terms, let us refer to [3–5]. The capital letters A, B, D, P, χ denote positive coefficients that stand for the apoptosis rate, nutrient supply rate, nutrient consumption rate, proliferation rate, and chemotaxis coefficient, in this order. In addition, let us point out that the contributions $\chi\sigma$ and $\chi\Delta\varphi$ model pure chemotaxis, namely, the movement of tumor cells towards regions of high nutrients, and the active transport that describes the movement of the nutrient towards the tumor cells (see [21,22,25] for more details). Furthermore, the function h has been considered in [24] (see also [12,21–23,41]) as an interpolation function between -1 and 1 in order to have $h(-1) = 0$ and $h(1) = 1$, so that the mechanisms modelled by the terms $(P\sigma - A - u)h(\varphi)$ and $D\sigma h(\varphi)$ are switched off in the healthy case, which corresponds to $\varphi = -1$, and are fully active in the tumorous case $\varphi = 1$. Besides, the term σ_s stands for a nonnegative constant modelling the nutrient concentration in a pre-existing vasculature. For further details on the model, we refer the reader to [24] (see also [7,26]). Lastly, the term F' is the derivative of a double-well nonlinearity. Typical examples for this nonlinearity are the regular potential

$$F_{reg}(r) = \frac{1}{4}(r^2 - 1)^2 \quad \text{for } r \in \mathbb{R}, \tag{1.6}$$

and, more relevant for applications, the logarithmic potential

$$F_{log}(r) = (1 + r)\ln(1 + r) + (1 - r)\ln(1 - r) - kr^2 \quad \text{for } r \in (-1, 1), \tag{1.7}$$

where $k > 1$ so that F_{log} is nonconvex. Eventually, the terms u and w are source terms acting as control variables. It is worth noting that we are considering two control variables: u in the phase equation and w in the nutrient equation. In the previous contributions [2,6,34,36,37], the control variable was placed in the nutrient equation, so that it designs an external medication or some nutrient supply. On the other hand, different authors consider the control variable in the phase equation (see, e.g., [15, 16,26]), multiplied by $h(\varphi)$ in order to have the action of the control only in the meaningful region. In that case, it models the introduction of cytotoxic drugs into the system, which has the purpose of eliminating the tumor cells. Thus, with our choice we include both these cases in this paper.

We are now in a position to introduce the distributed optimal control problem we are going to deal with. It consists of finding a solution to the following minimization problem:

(*CP*) Minimize the tracking-type cost functional

$$\mathcal{J}(\varphi, \sigma, u, w) := \frac{\gamma_1}{2} \int_\Omega |\varphi(T) - \varphi_\Omega|^2 + \frac{\gamma_2}{2} \int_Q |\varphi - \varphi_Q|^2 + \frac{\gamma_3}{2} \int_\Omega |\sigma(T) - \sigma_\Omega|^2 + \frac{\gamma_4}{2} \int_Q |\sigma - \sigma_Q|^2 + \frac{\gamma_5}{2} \int_Q |u|^2 + \frac{\gamma_6}{2} \int_Q |w|^2 \qquad (1.8)$$

subject to the condition that (μ, φ, σ) solves the *state system* (1.1)–(1.5) for a control pair (u, w) belonging to the control box

$$\mathcal{U}_{\text{ad}} := \{(u, w) \in (L^\infty(Q))^2 : u_* \le u \le u^* \text{ a.e. in } Q,\ w_* \le w \le w^* \text{ a.e. in } Q\}, \qquad (1.9)$$

where u_*, u^*, w_* and w^* denote some prescribed functions in $L^\infty(Q)$. Moreover, let us point out that the physical meaning of the term $uh(\varphi)$ in the state system requires the control u to be nonnegative. Hence, in the following we will always assume that the lower bound satisfies $u_* \ge 0$ almost everywhere in Q.

As far as control problems for tumor growth models are concerned, the contributions are still scarce. To our knowledge, the first optimal control problem governed by a tumor growth model similar to the one given above is [6]. There, the control problem was investigated for the case of regular potentials enjoying polynomial growth. Then, by adding two relaxation terms, a similar optimal control problem was tackled in [34] by extending the generality of the potentials by allowing singular, but still smooth, potentials like the logarithmic potential to be considered. Next, the same author, using the so-called deep quench asymptotic technique, proved in [35] how nonsmooth potentials like the double obstacle potential can also be admitted. Then, exploiting the results known for the case $\alpha, \beta > 0$, in the following works [36,37] the author showed that it is possible to let α and β approach zero separately in order to recover the existence of optimal controls and to characterize the corresponding first-order necessary conditions for optimality. We also refer to [26], where an optimal treatment time has been performed for a similar system, namely for system (1.1)–(1.5) with the choices $\chi = \alpha = \beta = 0$ and $w \equiv 0$; see also [2], where a similar control problem was investigated for a different model. Moreover, let us mention [39], where an optimal control problem for the two-dimensional Cahn–Hilliard–Darcy system with mass sources is addressed. We also point out [15,16], where the optimal control for a Cahn–Hilliard–Brinkman type system has been tackled. Lastly, we refer to [7], where a different kind of control problem, known as sliding mode control, was performed for a system that is very close to (1.1)–(1.5).

We now comment on (1.1)–(1.5). Let us emphasize that, once the well-posedness of the state system is established, we can properly define the *control-to-state operator* that assigns to a given control (u, w) the unique corresponding solution to (1.1)–(1.5),

$$\mathcal{S} : (u, w) \mapsto \mathcal{S}(u, w) := (\mu, \varphi, \sigma), \qquad (1.10)$$

and attains values in a proper Banach space. Then, we are in a position to eliminate the state variable appearing in the cost functional (1.8) by expressing them as functions of the control. This leads to the *reduced cost functional*

$$\mathcal{J}_{\rm red}(u, w) := \mathcal{J}(\mathcal{S}_2(u, w), \mathcal{S}_3(u, w), u, w), \tag{1.11}$$

where $\mathcal{S}_2(u, w)$ and $\mathcal{S}_3(u, w)$ denote the second and third component of $\mathcal{S}$, respectively. At this formal stage, let us point out that from standard results of convex analysis (see, e.g., [31,40]) it follows the formal first-order necessary condition for optimality characterized by the variational inequality

$$D\mathcal{J}_{\rm red}(\overline{u}, \overline{w})(u - \overline{u}, w - \overline{w}) \geq 0 \quad \text{for every } (u, w) \in \mathcal{U}_{\rm ad}, \tag{1.12}$$

where $D\mathcal{J}_{\rm red}$ stands for the derivative of the reduced cost functional in a proper functional analytic sense.

Therefore, summing up, in this contribution we aim at solving the constrained minimization problem

$$\textbf{(CP)} \quad \text{Minimize } \mathcal{J}(\varphi, \sigma, u, w) \text{ subject to the control constraints (1.9) and under the requirement that the variables } (\varphi, \sigma) \text{ yield a solution to (1.1)–(1.5),} \tag{1.13}$$

and pointing out the corresponding first-order necessary continuations for optimality.

The paper is organized as follows. The next section brings the mathematical framework and gathers the obtained results. From Sect. 3 onward, we proceed with the proof of the statements. The well-posedness and the continuous dependence results for the state system (1.1)–(1.5) are addressed in Sect. 3, while Sect. 4 is completely devoted to the corresponding control problem. Namely, we prove in this last section the existence of optimal controls and derive the corresponding first-order necessary conditions for optimality.

2 Mathematical Setting and Main Results

To begin with, let us point out some notation. As far as the functional spaces are concerned, it is convenient to set

$$H := L^2(\Omega), \quad V := H^1(\Omega), \quad W := \{v \in H^2(\Omega) : \partial_n v = 0 \text{ on } \Gamma\},$$

and to endow H, V, W with their standard norms. Furthermore, for an arbitrary Banach space X, we denote by $\|\cdot\|_X$ its norm, X^* its topological dual, and by $\langle \cdot, \cdot \rangle_X$ the duality product between X^* and X. Likewise, for every $1 \leq p \leq \infty$, we use the symbol $\|\cdot\|_p$ to indicate the usual norm in $L^p(\Omega)$. Notice that (V, H, V^*) forms a Hilbert triple, that is, the injections $V \subset H \equiv H^* \subset V^*$ are both continuous and dense, where we have the identification

$$\langle u, v \rangle_V = \int_\Omega uv \quad \text{for every } u \in H \text{ and } v \in V.$$

Furthermore, it is convenient to denote the parabolic cylinder and its boundary by

$$Q_t := \Omega \times (0,t) \quad \text{and} \quad \Sigma_t := \Gamma \times (0,t) \quad \text{for every } t \in (0,T],$$
$$Q := Q_T, \quad \text{and} \quad \Sigma := \Sigma_T.$$

For the potential F, we generally assume:

(F1) $F = F_1 + F_2$, where $F_1 : \mathbb{R} \to [0, +\infty]$ is convex and lower semicontinuous with $F_1(0) = 0$.
(F2) There exists an interval (r_-, r_+), with $-\infty \le r_- < 0 < r_+ \le +\infty$, such that the restriction of F_1 to (r_-, r_+) is differentiable with derivative F_1'.
(F3) $F_2 \in C^3(\mathbb{R})$, and F_2' is Lipschitz continuous with Lipschitz constant $L > 0$.
(F4) $F_{|(r_-,r_+)} \in C^3(r_-, r_+)$, and $\lim\limits_{r \to r_\pm} F'(r) = \pm\infty$.

It is worth noting that both (1.6) and (1.7) do fit the above framework with the choices $(r_-, r_+) = (-\infty, +\infty)$ and $(r_-, r_+) = (-1, 1)$, respectively, so that they are allowed to be considered.

For the initial data introduced above, we make the following assumptions:

(A1) $\varphi_0 \in W, \quad \mu_0 \in H^1(\Omega) \cap L^\infty(\Omega), \quad \sigma_0 \in H^1(\Omega) \cap L^\infty(\Omega)$.
(A2) $r_- < \inf \varphi_0 \le \sup \varphi_0 < r_+, \quad$ whence $F(\varphi_0), \; F'(\varphi_0) \in L^\infty(\Omega)$.

Notice that the above requirement can be restrictive for the case of singular potentials. For instance, in the case of the logarithmic potential, we have $r_\pm = \pm 1$ so that by **(A2)** the pure phases (tumor and healthy tissue) can only be approximated by the initial datum.
For the other appearing constants and target functions, we postulate:

(A3) $h \in C^2(\mathbb{R}) \cap W^{2,\infty}(\mathbb{R})$, and h is positive on (r_-, r_+).
(A4) α, β, χ are positive constants, while P, A, B, D, σ_s are nonnegative constants.
(A5) $\gamma_1, \gamma_2, \gamma_3, \gamma_4, \gamma_5, \gamma_6$ are nonnegative constants, but not all zero.
(A6) $\varphi_Q, \sigma_Q \in L^2(Q), \quad \varphi_\Omega, \sigma_\Omega \in L^2(\Omega)$.

Note that **(A3)** entails that h, h' are Lipschitz continuous in $\mathbb{R}$. Let us denote by h_∞, h'_∞ the upper bounds for the $L^\infty(\mathbb{R})$ norms of h and h', and by L_h the Lipschitz constant of h, respectively. Let us also point out that as L_h we can simply take h'_∞.
Moreover, we assume that the control box $\mathcal{U}_{\text{ad}}$ is defined by (1.9), and that

(A7) $u_*, u^* \in L^\infty(Q)$ with $0 \le u_* \le u^*$ a.e. in Q, $w_*, w^* \in L^\infty(Q)$ with $w_* \le w^*$ a.e. in Q.

The latter condition implies that $\mathcal{U}_{\text{ad}}$ is a closed and convex subset of $L^2(Q)$. On the other hand, it will be sometimes convenient to work with an open superset of $\mathcal{U}_{\text{ad}}$. We therefore fix some constant $R > 0$ such that the open ball

$$\mathcal{U}_R := \{(u, w) \in L^2(Q) \times L^2(Q) : \|(u, w)\|_{L^2(Q) \times L^2(Q)} < R\} \text{ contains } \mathcal{U}_{\text{ad}}. \tag{2.1}$$

Remark 2.1 Before diving into the well-posedness result, let us point out a classical issue of control theory. The well-posedness result to be presented below is given in a rather strong setting; this is motivated by the control problem under investigation. However, system (1.1)–(1.5) can be provided with a notion of weak solutions in a rather mild setting. Moreover, it is also possible to extend the analysis for the potentials taking into account singular and nonregular potentials like the well-known double obstacle potential. For this, a Yosida regularization of the maximal monotone operator F_1' has to be introduced. Clearly, the pointwise formulation (1.1)–(1.5) has then to be replaced by a suitable variational formulation. Let us just sketch the expected result here: provided we assume $\mu_0, \varphi_0, \sigma_0 \in L^2(\Omega)$ for the initial data and a potential that fulfills **(F1)–(F3)**, we can prove existence and uniqueness of a weak solution such that $\mu, \varphi, \sigma \in H^1(0, T; V^*) \cap L^\infty(0, T; H) \cap L^2(0, T; V)$. Note that uniqueness will follow from the first continuous dependence estimate that we perform below (cf. (3.19)), which perfectly complies with the above notion of weak solutions.

First, let us present the result regarding the existence and uniqueness of a strong solution to the system (1.1)–(1.5).

Theorem 2.2 *Assume that* **(F1)–(F4)**, **(A1)–(A4)**, *and* **(A7)**, *are fulfilled and that* $(u, w) \in \mathfrak{U}_R$. *Then the state system* (1.1)–(1.5) *admits a unique solution* (μ, φ, σ) *with the regularity*

$$\varphi \in W^{1,\infty}(0, T; H) \cap H^1(0, T; V) \cap L^\infty(0, T; W)\,, \tag{2.2}$$

$$\mu, \sigma \in H^1(0, T; H) \cap L^\infty(0, T; V) \cap L^2(0, T; W) \cap L^\infty(Q)\,. \tag{2.3}$$

Moreover, there exists a positive constant K_1, *which depends only on* Ω, T, R, α, β, *and the data of the system, such that*

$$\|\varphi\|_{W^{1,\infty}(0,T;H)\cap H^1(0,T;V)\cap L^\infty(0,T;W)} + \|\mu\|_{H^1(0,T;H)\cap L^\infty(0,T;V)\cap L^2(0,T;W)\cap L^\infty(Q)} + \|\sigma\|_{H^1(0,T;H)\cap L^\infty(0,T;V)\cap L^2(0,T;W)\cap L^\infty(Q)} \leq K_1\,. \tag{2.4}$$

In addition, there exist some constants r_* *and* r^*, *which satisfy* $r_- < r_* \leq r^* < r_+$ *and depend only on the data of the system, such that*

$$r_* \leq \varphi \leq r^* \quad \textit{a.e. in } Q\,. \tag{2.5}$$

Finally, there exists a positive constant K_2, *which depends only on* Ω, T, R, α, β, *and the data of the system, such that*

$$\|\varphi\|_{L^\infty(Q)} + \max_{i=1,2,3} \|F^{(i)}(\varphi)\|_{L^\infty(Q)} \leq K_2\,. \tag{2.6}$$

Let us point out that (2.5) turns out to be significant for the case of singular potentials such as the logarithmic potential. In that situation, it guarantees that, as soon as **(A2)** is satisfied, the phase variable stays away from the pure phases uniformly during the evolution. This fact, known as the separation principle, in turn, entails that (2.6) holds.

Theorem 2.3 *Suppose that* **(F1)–(F4)** *and* **(A1)–(A7)** *are fulfilled. Then there exists a positive constant* K_3*, which depends only on* Ω*,* T*,* R*,* α*,* β*, and the data of the system, such that the following holds true: whenever two control pairs* $(u_i, w_i) \in \mathcal{U}_R$*,* $i = 1, 2$*, are given and* $(\mu_i, \varphi_i, \sigma_i)$*,* $i = 1, 2$*, are the corresponding states, then*

$$\begin{aligned}
&\|\mu_1 - \mu_2\|_{H^1(0,T;H)\cap L^\infty(0,T;V)\cap L^2(0,T;W)} + \|\varphi_1 - \varphi_2\|_{H^1(0,T;H)\cap L^\infty(0,T;V)\cap L^2(0,T;W)} \\
&\quad + \|\sigma_1 - \sigma_2\|_{H^1(0,T;H)\cap L^\infty(0,T;V)\cap L^2(0,T;W)} \\
&\quad \le K_3 \left(\|u_1 - u_2\|_{L^2(0,T;H)} + \|w_1 - w_2\|_{L^2(0,T;H)} \right). \qquad (2.7)
\end{aligned}$$

For the optimal control problem $(\boldsymbol{CP})$, we will show the following existence result:

Theorem 2.4 *Assume that* **(F1)–(F4)** *and* **(A1)–(A7)** *are satisfied. Then the control problem* $(\boldsymbol{CP})$ *admits at least one solution.*

Finally, we formulate the first-order necessary optimality conditions for $(\boldsymbol{CP})$ that will be shown below. To this end, we assume that $(\overline{u}, \overline{w})$ and $(\overline{\mu}, \overline{\varphi}, \overline{\sigma})$ stand for some fixed control and its associated state, respectively. Sometimes, the same notation is employed to refer to an optimal control with the corresponding optimal state; anyhow, we will specify this whenever it is the case. In the course of our analysis, it will be necessary to establish the Fréchet differentiability of the control-to-state operator $\mathcal{S} : (u, w) \mapsto (\mu, \varphi, \sigma)$ in suitable Banach spaces. To this end, the unique solvability of the corresponding linearized system will have to be shown. This system has for every pair $(k, l) \in (L^2(Q))^2$ the following form:

$$\alpha \partial_t \eta + \partial_t \xi - \Delta \eta = (P\zeta - k) h(\overline{\varphi}) + (P\overline{\sigma} - A - \overline{u}) h'(\overline{\varphi}) \xi \quad \text{in } Q, \qquad (2.8)$$

$$\eta = \beta \partial_t \xi - \Delta \xi + F''(\overline{\varphi}) \xi - \chi \zeta \quad \text{in } Q, \qquad (2.9)$$

$$\partial_t \zeta - \Delta \zeta + B\zeta = -\chi \Delta \xi - D\zeta h(\overline{\varphi}) - D\overline{\sigma} h'(\overline{\varphi}) \xi + l \quad \text{in } Q, \qquad (2.10)$$

$$\partial_n \eta = \partial_n \xi = \partial_n \zeta = 0 \quad \text{on } \Sigma, \qquad (2.11)$$

$$\eta(0) = \xi(0) = \zeta(0) = 0 \quad \text{in } \Omega. \qquad (2.12)$$

Here, the well-posedness result follows.

Theorem 2.5 *Assume that* **(F1)–(F4)***,* **(A1)–(A4)***, and* **(A7)***, are satisfied. Then the linearized system (2.8)–(2.12) admits for every* $(k, l) \in (L^2(Q))^2$ *a unique solution* (η, ξ, ζ) *with the regularity*

$$\eta, \xi, \zeta \in H^1(0, T; H) \cap L^\infty(0, T; V) \cap L^2(0, T; W). \qquad (2.13)$$

Notice that Theorem 2.3 also entails the Lipschitz continuity of the control-to-state operator $\mathcal{S}$ between suitable Banach spaces. We even have Fréchet differentiability, as the following result states.

Theorem 2.6 *Assume that* **(F1)–(F4)**, **(A1)–(A4)**, *and* **(A7)**, *are satisfied, and let* $(\overline{u}, \overline{w}) \in \mathcal{U}_R$ *be a fixed control with the corresponding state* $(\overline{\mu}, \overline{\varphi}, \overline{\sigma})$. *Then the control-to-state operator* $\mathcal{S}$ *is Fréchet differentiable at* $(\overline{u}, \overline{w})$ *as a mapping from* $(L^2(Q))^2$ *into the Banach space* $\mathcal{Y}$, *where*

$$\mathcal{Y} := \big(C^0([0,T]; H) \cap L^2(0,T; V)\big) \times \big(H^1(0,T; H) \cap L^\infty(0,T; V)\big) \\ \times \big(C^0([0,T]; H) \cap L^2(0,T; V)\big). \tag{2.14}$$

Moreover, for every $(k, l) \in (L^2(Q))^2$ *the derivative of* $\mathcal{S}$ *at* $(\overline{u}, \overline{w})$ *is given by the identity* $[D\mathcal{S}(\overline{u}, \overline{w})](k, l) = (\eta, \xi, \zeta)$, *where* (η, ξ, ζ) *is the unique solution to the linearized system* (2.8)–(2.12) *corresponding to* (k, l).

Theorem 2.7 *Assume that* **(F1)–(F4)** *and* **(A1)–(A7)** *are fulfilled, and let* $(\overline{u}, \overline{w})$ *be an optimal control with associated state* $(\overline{\mu}, \overline{\varphi}, \overline{\sigma})$. *Then it holds that*

$$\gamma_1 \int_\Omega (\overline{\varphi}(T) - \varphi_\Omega)\xi(T) + \gamma_2 \int_Q (\overline{\varphi} - \varphi_Q)\xi \\ + \gamma_3 \int_\Omega (\sigma(T) - \sigma_\Omega)\zeta(T) + \gamma_4 \int_Q (\overline{\sigma} - \sigma_Q)\zeta \\ + \gamma_5 \int_Q \overline{u}(u - \overline{u}) + \gamma_6 \int_Q \overline{w}(w - \overline{w}) \geq 0 \quad \text{for every } (u, w) \in \mathcal{U}_{\text{ad}}, \tag{2.15}$$

where the triple (η, ξ, ζ) *is the unique solution to the linearized system* (2.8)–(2.12) *corresponding to* $k = u - \overline{u}$ *and* $l = w - \overline{w}$, *respectively.*

Analyzing the above variational inequality, one realizes that it is not very useful in numerical applications, since for every possible step of the approximation one has to solve the state system and also the linearized system in order to have ξ and ζ at disposal. For this reason, a classical tool is to introduce the so-called adjoint system in order to eliminate these variables. In fact, provided that we choose this auxiliary system properly, the linearized variables can be eliminated from (2.15). The adjoint system to (1.1)–(1.5) can be obtained by the formal Lagrangian method described, e.g., in [40], using integration by parts. Following this route, we arrive at the following (formal) version of the adjoint system:

$$-\alpha\partial_t q - \Delta q - p = 0 \quad \text{in } Q, \tag{2.16}$$

$$-\partial_t q - \beta\partial_t p - \Delta p + \chi\Delta r + F''(\overline{\varphi})p - (P\overline{\sigma} - A - \overline{u})h'(\overline{\varphi})q + D\overline{\sigma}h'(\overline{\varphi})r \\ = \gamma_2(\overline{\varphi} - \varphi_Q) \quad \text{in } Q, \tag{2.17}$$

$$-\partial_t r - \Delta r + Br + Dh(\overline{\varphi})r - \chi p - Ph(\overline{\varphi})q = \gamma_4(\overline{\sigma} - \sigma_Q) \quad \text{in } Q, \tag{2.18}$$

$$\partial_n q = \partial_n p = \partial_n r = 0 \quad \text{on } \Sigma, \tag{2.19}$$

$$q(T) = 0, \ \beta p(T) = \gamma_1(\overline{\varphi}(T) - \varphi_\Omega), \ r(T) = \gamma_3(\overline{\sigma}(T) - \sigma_\Omega) \quad \text{in } \Omega. \tag{2.20}$$

Observe that this is a backward-in-time system with final conditions belonging to $L^2(\Omega)$ (see assumption **(A6)**), so that we cannot expect to recover a strong solution.

Therefore, instead of considering the pointwise Eqs. (2.17)–(2.18), we note that the variables p and r should be understood as weak solutions in the following sense:

$$\begin{aligned}
&-\int_\Omega \partial_t q\, v - \langle \beta \partial_t p, v\rangle_V + \int_\Omega \nabla p\cdot\nabla v - \chi\int_\Omega \nabla r\cdot\nabla v\\
&\quad+\int_\Omega F''(\overline{\varphi})\, p\, v + \int_\Omega D\,\overline{\sigma}\, h'(\overline{\varphi})\, r\, v\\
&\quad-\int_\Omega (P\overline{\sigma} - A - \overline{u})h'(\overline{\varphi})q\, v = \int_\Omega \gamma_2(\overline{\varphi}-\varphi_Q)\, v \quad \text{for all } v\in V \text{ and a.e. in } (0,T),
\end{aligned} \tag{2.21}$$

$$\begin{aligned}
&-\langle \partial_t r, v\rangle_V + \int_\Omega \nabla r\cdot\nabla v + \int_\Omega B r v + \int_\Omega D h(\overline{\varphi}) r\, v - \int_\Omega \chi\, p\, v - \int_\Omega P h(\overline{\varphi}) q\, v\\
&\quad= \int_\Omega \gamma_4(\overline{\sigma}-\sigma_Q) v \quad \text{for all } v\in V \text{ and a.e. in } (0,T),
\end{aligned} \tag{2.22}$$

where, for simplicity, we avoided writing the time variable explicitly. We have the following well-posedness result.

Theorem 2.8 *Assume that* **(F1)**–**(F4)** *and* **(A1)**–**(A7)** *are fulfilled, and let* $(\overline{u},\overline{w})$ *be an optimal control with associated state* $(\overline{\mu},\overline{\varphi},\overline{\sigma})$. *Then the adjoint system* (2.16)–(2.20) *has a unique solution such that*

$$p, r \in H^1(0,T;V^*)\cap C^0([0,T];H)\cap L^2(0,T;V), \tag{2.23}$$

$$q \in H^1(0,T;H)\cap C^0([0,T];V)\cap L^2(0,T;W). \tag{2.24}$$

Theorem 2.9 *Assume that* **(F1)**–**(F4)** *and* **(A1)**–**(A7)** *are fulfilled, and let* $(\overline{u},\overline{w})$ *be an optimal control with associated state* $(\overline{\mu},\overline{\varphi},\overline{\sigma})$ *and adjoint state* (p,q,r). *Then it holds the variational inequality*

$$\int_Q (-h(\overline{\varphi})q + \gamma_5\overline{u})(u-\overline{u}) + \int_Q (r+\gamma_6\overline{w})(w-\overline{w}) \geq 0 \quad \textit{for every } (u,w)\in \mathcal{U}_{\mathrm{ad}}. \tag{2.25}$$

Moreover, whenever $\gamma_5 \neq 0$, *then* $\overline{u}$ *is nothing but the* $L^2(0,T;H)$*-orthogonal projection of* $\gamma_5^{-1}h(\overline{\varphi})q$ *onto the closed and convex set* $\{u \in L^2(Q) : u_* \leq u \leq u^* \text{ a.e. in } Q\}$. *Likewise, if* $\gamma_6 \neq 0$, *then* $\overline{w}$ *reduces to the* $L^2(0,T;H)$*-orthogonal projection of* $-\gamma_6^{-1}r$ *onto* $\{w\in L^2(Q) : w_* \leq w \leq w^* \text{ a.e. in } Q\}$.

Furthermore, since $\mathcal{U}_{\mathrm{ad}}$ is actually a control box, it is possible to explicitly characterize the projection and obtain a pointwise condition.

Corollary 2.10 *Let* **(F1)**–**(F4)** *and* **(A1)**–**(A7)** *be fulfilled, and let* $\gamma_5 > 0$. *Then, the optimal control component* $\overline{u}$ *is implicitly characterized by*

$$\overline{u}(x,t) = \max\big\{u_*(x,t), \min\{u^*(x,t), \gamma_5^{-1}h(\overline{\varphi}(x,t))q(x,t)\}\big\} \quad \textit{for a.a. } (x,t)\in Q.$$

Likewise, if $\gamma_6 > 0$*, then*

$$\overline{w}(x,t) = \max\{w_*(x,t), \min\{w^*(x,t), -\gamma_6^{-1} r(x,t)\}\} \quad \textit{for a.a. } (x,t) \in Q.$$

Let us emphasize a consequence which is of straightforward importance for the numerical approach. Comparing the expected theoretical condition (1.12) with the explicit condition (2.25), via Riesz's representation theorem, the gradient of the reduced cost functional can be recovered as $\nabla \mathcal{J}_{\text{red}}(\overline{u}, \overline{w}) = (-h(\overline{\varphi})q + \gamma_5 \overline{u}\,,\ r + \gamma_6 \overline{w})$. Hence, for the numerical approach, the optimal control problem can be viewed as a constrained minimization of a function, $\mathcal{J}_{red}$, whose gradient is known (think of the well-known projected conjugate gradient method).

In the remainder of this section, we recollect some well-known results that will prove useful later on. To begin with, we recall the standard Sobolev continuous embedding

$$H^1(\Omega) \hookrightarrow L^q(\Omega) \quad \text{for every } q \in [1,6]. \tag{2.26}$$

Furthermore, we often make use of Young's inequality

$$ab \le \delta a^2 + \frac{1}{4\delta} b^2 \quad \text{for every } a, b \ge 0 \text{ and } \delta > 0. \tag{2.27}$$

As far as the constants are concerned, let us set our convention once and for all: the symbol small-case c is used to indicate every constant that depends only on the structural data of the problem, such as T, Ω, R, α or β, the shape of the nonlinearities, and the norms of the involved functions. On the other hand, with capital letters we specify particular constants that will be referred to later on. Therefore, the meaning of the constant c may change from line to line.

3 The State System

3.1 Well-Posedness of the State System

Proof of Theorem 2.2 Here, we do not provide all the details, since the approach is quite standard. Anyhow, let us point out that the argument can be made rigorous by using an approximation technique, e.g., within a Faedo–Galerkin scheme along with the introduction of the Yosida approximation for F_1'. In fact, since the framework for the potential settings is rather general, we cannot assume F_1' to be Lipschitz continuous, in general. In this direction, let $\varepsilon \in (0,1)$ and, for every $r \in \mathbb{R}$, let us set

$$F_{1,\varepsilon}(r) := \min_{s \in \mathbb{R}} \left(\frac{1}{2\varepsilon}(s-r)^2 + F_1(s) \right), \quad F_{1,\varepsilon}'(r) := \frac{d}{dr} F_{1,\varepsilon}(r),$$
$$F_\varepsilon(r) := F_{1,\varepsilon}(r) + F_2(r).$$

It turns out that $F_{1,\varepsilon} \in C^1(\mathbb{R})$ and that the Yosida regularization $F_{1,\varepsilon}'$ is Lipschitz continuous (see, e.g., [1, Prop. 2.11, p. 39]). Furthermore, for every $r \in \mathbb{R}$ the properties

$$0 \le F_{1,\varepsilon}(r) \le F_1(r), \quad F_{1,\varepsilon}(r) \nearrow F_1(r) \quad \text{monotonically as } \varepsilon \searrow 0, \tag{3.1}$$

hold, as well as (cf. [1, Prop. 2.6, p. 28]),

$$\text{for all } r \in (r_-, r_+), \quad |F'_{1,\varepsilon}(r)| \nearrow |F'_1(r)| \quad \text{monotonically as } \varepsilon \searrow 0. \tag{3.2}$$

Hence, the idea is as follows: first we aim at discussing the well-posedness of the approximation of (1.1)–(1.5), namely (1.1)–(1.5) with F' replaced by F'_ε, and then, on account of a priori estimates and monotonicity arguments, using this result to ensure the existence of a solution to the original system. For the sake of simplicity, we denote by $(\mu_\varepsilon, \varphi_\varepsilon, \sigma_\varepsilon)$ the solution to the approximated system, but we avoid writing the subscript ε in the calculations below. Only at the end of each calculation the correct notation is employed. The proof of the uniqueness will follow as a direct consequence of Theorem 2.3.

First estimate To begin with, we add to both sides of (1.2) the term φ. Then, we multiply (1.1) by μ, the new (1.2) by $\partial_t\varphi$, (1.3) by σ, and add the resulting identities. Next, we integrate over Q_t, for an arbitrary $t \in (0, T]$, and by parts. After a cancellation of terms and some rearrangements, we infer that

$$\begin{aligned}
&\frac{\alpha}{2}\|\mu(t)\|_H^2 + \int_{Q_t} |\nabla\mu|^2 + \beta\int_{Q_t} |\partial_t\varphi|^2 + \frac{1}{2}\|\varphi(t)\|_H^2 + \frac{1}{2}\|\nabla\varphi(t)\|_H^2 \\
&\quad + \int_\Omega F_{1,\varepsilon}(\varphi(t)) + \frac{1}{2}\|\sigma(t)\|_H^2 + B\int_{Q_t} |\sigma|^2 + \int_{Q_t} |\nabla\sigma|^2 \\
&\quad = \frac{\alpha}{2}\|\mu_0\|_H^2 + \frac{1}{2}\|\varphi_0\|_H^2 + \frac{1}{2}\|\nabla\varphi_0\|_H^2 + \frac{1}{2}\|\sigma_0\|_H^2 + \int_\Omega F_{1,\varepsilon}(\varphi_0) \\
&\quad + \int_{Q_t} (P\sigma - A - u)h(\varphi)\mu + \chi\int_{Q_t} \sigma\,\partial_t\varphi + \int_{Q_t} (\varphi - F'_2(\varphi))\partial_t\varphi \\
&\quad + \chi\int_{Q_t} \nabla\varphi\cdot\nabla\sigma + \int_{Q_t} B\sigma_s\sigma - \int_{Q_t} Dh(\varphi)|\sigma|^2 + \int_{Q_t} w\sigma.
\end{aligned}$$

Obviously, all of the summands on the left-hand side are nonnegative, and the first four summands on the right-hand side are bounded, by virtue of **(A1)**, **(A2)**, and the general assumptions on F_1 and F_2. Besides, (3.1) implies that the fifth term verifies

$$\int_\Omega F_{1,\varepsilon}(\varphi_0) \le \int_\Omega F_1(\varphi_0) \le c.$$

It remains to estimate the remaining terms on the right-hand side, which we denote by I_1, ..., I_7, in this order. This can easily be done by means of Young's inequality. In fact, we have that

$$|I_1| \le \int_{Q_t} |\sigma|^2 + T|\Omega| + \int_{Q_t} |u|^2 + \frac{h_\infty^2\big(P^2 + A^2 + 1\big)}{4}\int_{Q_t} |\mu|^2.$$

Furthermore, we also infer that

$$\sum_{i=2}^{7} |I_i| \le \frac{\beta}{2}\int_{Q_t} |\partial_t\varphi|^2 + \frac{\chi^2}{\beta}\int_{Q_t} |\sigma|^2 + \frac{2(1+L^2)}{\beta}\int_{Q_t} |\varphi|^2 + \frac{\chi^2}{2}\int_{Q_t} |\nabla\varphi|^2$$
$$+ \frac{1}{2}\int_{Q_t} |\nabla\sigma|^2 + \frac{1}{2}\int_{Q_t} |\sigma|^2 + \frac{B^2\sigma_s^2}{2} T\,|\Omega|$$
$$+ Dh_\infty \int_{Q_t} |\sigma|^2 + \frac{1}{2}\int_{Q_t} (|\sigma|^2 + |w|^2)$$
$$\le \frac{\beta}{2}\int_{Q_t} |\partial_t\varphi|^2 + \frac{1}{2}\int_{Q_t} |\nabla\sigma|^2$$
$$+ \Big(\frac{\chi^2}{\beta} + Dh_\infty + 1\Big)\int_{Q_t} |\sigma|^2 + \frac{2(1+L^2)}{\beta}\int_{Q_t} |\varphi|^2$$
$$+ \frac{\chi^2}{2}\int_{Q_t} |\nabla\varphi|^2 + \frac{1}{2}\int_{Q_t} |w|^2 + \frac{B^2\sigma_s^2}{2} T\,|\Omega|.$$

Therefore, a Gronwall argument yields that

$$\|\mu_\varepsilon\|_{L^\infty(0,T;H)\cap L^2(0,T;V)} + \|\varphi_\varepsilon\|_{H^1(0,T;H)\cap L^\infty(0,T;V)} + \|\sigma_\varepsilon\|_{L^\infty(0,T;H)\cap L^2(0,T;V)}$$
$$+ \|F_{1,\varepsilon}(\varphi)\|^{1/2}_{L^\infty(0,T;L^1(\Omega))} \le c\,(1 + \|u\|_{L^2(0,T;H)} + \|w\|_{L^2(0,T;H)}). \tag{3.3}$$

Second estimate We multiply (1.2) by $-\Delta\varphi$, write $F'_\varepsilon = F'_{1,\varepsilon} + F'_2$, integrate over Q_t, where $t \in (0,T]$, and by parts, to obtain that

$$\frac{\beta}{2}\|\nabla\varphi(t)\|_H^2 + \int_{Q_t} |\Delta\varphi|^2 + \int_{Q_t} F''_{1,\varepsilon}(\varphi)|\nabla\varphi|^2$$
$$= \frac{\beta}{2}\|\nabla\varphi_0\|_H^2 - \int_{Q_t} F''_2(\varphi)|\nabla\varphi|^2 - \int_{Q_t} \chi\sigma\,\Delta\varphi - \int_{Q_t} \mu\,\Delta\varphi,$$

where the terms on the right-hand side are denoted by $I_1, \ldots, I_4$, in this order. At first, the convexity (recall assumption **(F1)**) of F_1 and the well-known properties of the Yosida regularization entail that $F''_{1,\varepsilon}(\varphi) \ge 0$, so that the third term on the left-hand side is nonnegative. Furthermore, the first term I_1 on the right-hand side is bounded due to **(A1)**, whereas the other terms can be dealt with by accounting for Young's inequality and the above estimate. In fact, we have that

$$\sum_{i=2}^{4} |I_i| \le L\int_{Q_t} |\nabla\varphi|^2 + \chi^2\int_{Q_t} |\sigma|^2 + \int_{Q_t} |\mu|^2 + \frac{1}{2}\int_{Q_t} |\Delta\varphi|^2.$$

Therefore, we realize that $\|\Delta\varphi\|^2_{L^2(0,T;H)} \le c$. The elliptic regularity theory, along with the smooth boundary condition in (1.4), and then a comparison in (1.2), give us that

$$\|\varphi_\varepsilon\|_{L^2(0,T;W)} + \|F'_{1,\varepsilon}(\varphi_\varepsilon)\|_{L^2(0,T;H)} \le c\,(1 + \|u\|_{L^2(0,T;H)} + \|w\|_{L^2(0,T;H)}). \tag{3.4}$$

Third estimate We now multiply (1.3) by $\partial_t\sigma$, and integrate over Q_t and by parts, to infer that

$$\begin{aligned}&\int_{Q_t} |\partial_t\sigma|^2 + \frac{B}{2}\|\sigma(t)\|_H^2 + \frac{1}{2}\|\nabla\sigma(t)\|_H^2\\ &\quad= \frac{B}{2}\|\sigma_0\|_H^2 + \frac{1}{2}\|\nabla\sigma_0\|_H^2 - \chi\int_{Q_t} \Delta\varphi\,\partial_t\sigma + \int_{Q_t} B\sigma_s\,\partial_t\sigma\\ &\qquad- \int_{Q_t} D\sigma h(\varphi)\partial_t\sigma + \int_{Q_t} w\,\partial_t\sigma.\end{aligned}$$

Here, it suffices to recall **(A1)**, (3.3), (3.4), and to employ Young's inequality several times, to deduce that

$$\|\sigma_\varepsilon\|_{H^1(0,T;H)\cap L^\infty(0,T;V)} \le c\,(1 + \|u\|_{L^2(0,T;H)} + \|w\|_{L^2(0,T;H)}). \tag{3.5}$$

Fourth estimate Next, we differentiate (1.2) with respect to time and multiply the resulting equality by $\partial_t\varphi$ to infer that

$$\begin{aligned}&\frac{\beta}{2}\|\partial_t\varphi(t)\|_H^2 + \int_{Q_t} |\nabla\partial_t\varphi|^2 + \int_{Q_t} F''_{1,\varepsilon}(\varphi)|\partial_t\varphi|^2\\ &\quad= \frac{\beta}{2}\|\partial_t\varphi(0)\|_H^2 - \int_{Q_t} F''_2(\varphi)|\partial_t\varphi|^2 + \int_{Q_t} \partial_t\mu\,\partial_t\varphi + \int_{Q_t} \chi\,\partial_t\sigma\,\partial_t\varphi.\end{aligned}$$

Again, the third term on the left-hand side is nonnegative. On the other hand, the first term on the right-hand side is under control by virtue of assumptions **(A1)**, **(A2)**, **(F2)** and (3.2) which imply that $F'_\varepsilon(\varphi_0)$ is uniformly bounded in $L^\infty(\Omega)$. In fact, evaluating (1.2) at $t = 0$, we see that

$$\partial_t\varphi(0) = \frac{1}{\beta}[\mu_0 + \Delta\varphi_0 - F'_\varepsilon(\varphi_0) + \chi\sigma_0],$$

and all of the terms on the right-hand side are bounded in $L^2(\Omega)$. Lastly, thanks to the Young inequality, we have that

$$\sum_{i=2}^{4}|I_i| \le \frac{1}{2}\int_{Q_t} |\partial_t\mu|^2 + \left(\frac{1+\chi^2}{2} + L\right)\int_{Q_t} |\partial_t\varphi|^2 + \frac{1}{2}\int_{Q_t} |\partial_t\sigma|^2.$$

Thus, owing to the previous estimates, we infer that

$$\|\varphi_\varepsilon\|_{W^{1,\infty}(0,T;H)\cap H^1(0,T;V)} \le c\,(1 + \|u\|_{L^2(0,T;H)} + \|w\|_{L^2(0,T;H)}). \tag{3.6}$$

Next, by multiplying (1.2) by $-\Delta\varphi$ and integrating over Ω, we obtain

$$\int_\Omega |\Delta\varphi|^2 + \int_\Omega F''_{1,\varepsilon}(\varphi)|\nabla\varphi|^2 = \int_\Omega (\beta\partial_t\varphi + F'_2(\varphi) - \chi\sigma - \mu)\Delta\varphi.$$

Then, making use of previous estimates and elliptic regularity results, we easily deduce that

$$\|\varphi_\varepsilon\|_{L^\infty(0,T;W)} \le c\,(1 + \|u\|_{L^2(0,T;H)} + \|w\|_{L^2(0,T;H)}), \tag{3.7}$$

which, accounting for the Sobolev embedding $H^2(\Omega) \subset L^\infty(\Omega)$, also yields that

$$\|\varphi_\varepsilon\|_{L^\infty(Q)} \le c\,(1 + \|u\|_{L^2(0,T;H)} + \|w\|_{L^2(0,T;H)}). \tag{3.8}$$

Fifth estimate Next, we observe that the equation (1.3) has parabolic structure with respect to the variable σ, since we can rewrite it as

$$\begin{cases} \partial_t\sigma - \Delta\sigma + B\sigma = f & \text{in } Q, \quad \text{with} \quad f := -\chi\Delta\varphi + B\sigma_s - D\sigma h(\varphi) + w, \\ \sigma(0) = \sigma_0 & \text{in } \Omega. \end{cases}$$

By virtue of the above estimates and **(A7)**, the reader can easily check that f is bounded in $L^\infty(0,T;H)$, which allows us to recover the full parabolic regularity

$$\|\sigma_\varepsilon\|_{H^1(0,T;H)\cap L^\infty(0,T;V)\cap L^2(0,T;W)} \le c\,(1 + \|u\|_{L^2(0,T;H)} + \|w\|_{L^2(0,T;H)}). \tag{3.9}$$

Moreover, provided we assume $\sigma_0 \in L^\infty(\Omega)$, as in **(A1)**, we can invoke [30, Thm. 7.1, p. 181] to conclude that

$$\|\sigma_\varepsilon\|_{L^\infty(Q)} \le c\,(1 + \|u\|_{L^2(0,T;H)} + \|w\|_{L^\infty(0,T;H)}). \tag{3.10}$$

Sixth estimate Now, we note that the Eq. (1.1) shows a parabolic structure with respect to μ; indeed, it can be rewritten as

$$\begin{cases} \alpha\partial_t\mu - \Delta\mu = f & \text{in } Q, \quad \text{with} \quad f := (P\sigma - A - u)h(\varphi) - \partial_t\varphi, \\ \mu(0) = \mu_0 & \text{in } \Omega. \end{cases} \tag{3.11}$$

On the other hand, owing to the above estimates, the source term f is bounded in $L^2(0,T;H)$ and the initial datum is regular, so that the parabolic regularity theory yields that

$$\|\mu_\varepsilon\|_{H^1(0,T;H)\cap L^\infty(0,T;V)\cap L^2(0,T;W)} \le c\,(1 + \|u\|_{L^2(0,T;H)} + \|w\|_{L^2(0,T;H)}). \tag{3.12}$$

Seventh estimate Moreover, the above estimates also entail that the right-hand side f in (3.11) is bounded in $L^\infty(0,T;H)$. By virtue of the assumption $\mu_0 \in L^\infty(\Omega)$, we can again invoke [30, Thm. 7.1, p. 181] in order to realize that

$$\|\mu_\varepsilon\|_{L^\infty(Q)} \le c\,(1 + \|u\|_{L^\infty(0,T;H)} + \|w\|_{L^\infty(0,T;H)}). \tag{3.13}$$

Passage to the limit Upon collecting the above estimates, all of them independent of ε, it is a standard matter to realize that there is a subsequence of $(\mu_\varepsilon, \varphi_\varepsilon, \sigma_\varepsilon)$ suitably converging, as $\varepsilon \to 0$, to a solution (μ, φ, σ) of (1.1)–(1.5) that verifies (2.4). We can argue, for instance, as in [3] and just point out that in the limit procedure we have to use the maximal monotonicity of F_1' (intended as a subdifferential operator) and a weak-strong convergence argument to identify the limit of $F_{1,\varepsilon}'(\varphi_\varepsilon)$ as $F_1'(\varphi)$.
Separation property At this point, we can rewrite the second equation (1.2) in the form

$$\beta\partial_t\varphi - \Delta\varphi + F'(\varphi) = g, \quad \text{with} \quad g := \mu + \chi\sigma, \tag{3.14}$$

and, on account of the previous estimates, we know that g is bounded in $L^\infty(Q)$, so that there exists a positive constant g_* for which $\|g\|_{L^\infty(Q)} \le g_*$. Besides, the growth assumption **(F4)** implies the existence of some constants r_* and r^* such that $r_- < r_* \le r^* < r_+$ and

$$r_* \le \inf_{x\in\Omega} \operatorname{ess} \varphi_0(x), \quad r^* \ge \sup_{x\in\Omega} \operatorname{ess} \varphi_0(x), \tag{3.15}$$

$$F'(r) + g_* \le 0 \quad \forall r \in (r_-, r_*), \quad F'(r) - g_* \ge 0 \quad \forall r \in (r^*, r_+). \tag{3.16}$$

Then, let us set, for convenience, $\vartheta := (\varphi - r^*)^+$, multiply equation (3.14) by ϑ, and integrate over Q_t, where $t \in (0, T]$, and by parts, to obtain that

$$\frac{\beta}{2}\|\vartheta(t)\|_H^2 + \int_{Q_t} |\nabla\vartheta|^2 + \int_{Q_t} (F'(\varphi) - g)\vartheta = 0,$$

where we also applied (3.15) to conclude that $\vartheta(0) = 0$. Moreover, the last term is nonnegative due to (3.16), so that $\vartheta = (\varphi - r^*)^+ = 0$, which in turn implies that $\varphi \le r^*$ almost everywhere in Q. In a similar manner, we easily conclude that $\varphi \ge r_*$ almost everywhere in Q by testing (3.14) by $-(\varphi - r_*)^-$. Thus, we have just shown that

$$r_* \le \varphi \le r^* \quad \text{a.e. in } Q. \tag{3.17}$$

Now, we note that (2.5) and **(F1)**–**(F4)** directly imply (2.6). In fact, (3.17) ensures that the phase variable φ stays away from the boundary of (r_-, r_+), so that F and its derivatives turn out to be uniformly bounded in $[r_*, r^*]$. □

3.2 Continuous Dependence Results

The continuous dependence result to be shown below will in turn prove the uniqueness of the solution to the state system (1.1)–(1.5).

Proof of Theorem 2.3 First of all, let us set

$$u := u_1 - u_2,\ w := w_1 - w_2,\ \mu := \mu_1 - \mu_2,\ \varphi := \varphi_1 - \varphi_2,\ \sigma := \sigma_1 - \sigma_2. \tag{3.18}$$

In view of **(A7)**, the controls (u_i, w_i), $i = 1, 2$, belong to the admissible set $\mathcal{U}_{\mathrm{ad}}$ defined in (1.9), and the respective states $(\mu_i, \varphi_i, \sigma_i)$, $i = 1, 2$, satisfy (2.4)–(2.6), as solutions to the state system (1.1)–(1.5).

First estimate To begin with, we add to both sides of (1.2) the term φ. Next, we multiply the difference of (1.1) by μ, the difference of the new (1.2) by $\partial_t\varphi$, and the difference of (1.3) by σ. By integrating over Q_t, with $t \in (0, T]$, and adding everything, we obtain a cancellation of terms and arrive at

$$\begin{aligned}
&\frac{\alpha}{2}\|\mu(t)\|_H^2 + \int_{Q_t} |\nabla\mu|^2 + \beta\int_{Q_t} |\partial_t\varphi|^2 + \frac{1}{2}\|\varphi(t)\|_V^2 \\
&\quad + \frac{1}{2}\|\sigma(t)\|_H^2 + \int_{Q_t} B|\sigma|^2 + \int_{Q_t} |\nabla\sigma|^2 = -\int_{Q_t} (F'(\varphi_1) - F'(\varphi_2))\partial_t\varphi \\
&\quad + \int_{Q_t} \big((P\sigma - u)h(\varphi_1) + (P\sigma_2 - A - u_2)(h(\varphi_1) - h(\varphi_2))\big)\mu \\
&\quad + \chi\int_{Q_t} \sigma\,\partial_t\varphi + \int_{Q_t} \varphi\,\partial_t\varphi + \chi\int_{Q_t} \nabla\varphi\cdot\nabla\sigma - \int_{Q_t} Dh(\varphi_1)|\sigma|^2 \\
&\quad - \int_{Q_t} D\sigma_2(h(\varphi_1) - h(\varphi_2))\sigma + \int_{Q_t} w\sigma\,.
\end{aligned}$$

We now estimate the terms on the right-hand side, which we denote by I_1, ..., I_8, in this order. We first infer from (2.5) that the nonlinear term F' turns out to be Lipschitz continuous in the range of interesting arguments, so that we obtain from Young's inequality that

$$-\int_{Q_t} (F'(\varphi_1) - F'(\varphi_2))\partial_t\varphi \le L\int_{Q_t} |\varphi||\partial_t\varphi| \le \frac{\beta}{4}\int_{Q_t} |\partial_t\varphi|^2 + \frac{L^2}{\beta}\int_{Q_t} |\varphi|^2,$$

where L here stands for a Lipschitz constant of F'. Moreover, accounting for the Young inequality, it is easy to see that

$$\begin{aligned}
|I_2| &\le Ph_\infty \int_{Q_t} |\sigma||\mu| \\
&\qquad + h_\infty\int_{Q_t} |u||\mu| + \big(P\|\sigma_2\|_{L^\infty(Q)} + A + \|u_2\|_{L^\infty(Q)}\big)L_h\int_{Q_t} |\varphi||\mu| \\
&\le c\int_{Q_t} (|\mu|^2 + |\varphi|^2 + |\sigma|^2 + |u|^2),
\end{aligned}$$

where we have have used the fact that σ_2 is a solution to (1.1)–(1.5), and thus has to satisfy (2.4) and also that u_2 is an admissible control. Furthermore, using Young's inequality once more, we have that

$$|I_3| + |I_4| + |I_5| \leq \frac{\beta}{4} \int_{Q_t} |\partial_t \varphi|^2 + \frac{2}{\beta} \int_{Q_t} (|\sigma|^2 + |\varphi|^2) \\ + \frac{\chi^2}{2} \int_{Q_t} |\nabla \varphi|^2 + \frac{1}{2} \int_{Q_t} |\nabla \sigma|^2.$$

Finally, Young's inequality, along with the Lipschitz continuity of h, leads us to

$$|I_6| + |I_7| + |I_8| \leq D h_\infty \int_{Q_t} |\sigma|^2 + D L_h \|\sigma_2\|_{L^\infty(Q)} \int_{Q_t} |\varphi||\sigma| + \int_{Q_t} |w||\sigma| \\ \leq c \int_{Q_t} (|\varphi|^2 + |\sigma|^2 + |w|^2).$$

At this point, we collect the above estimates, and apply Gronwall's lemma, to conclude that

$$\|\mu_1 - \mu_2\|_{L^\infty(0,T;H)\cap L^2(0,T;V)} + \|\varphi_1 - \varphi_2\|_{H^1(0,T;H)\cap L^\infty(0,T;V)} \\ + \|\sigma_1 - \sigma_2\|_{L^\infty(0,T;H)\cap L^2(0,T;V)} \leq c \left(\|u_1 - u_2\|_{L^2(0,T;H)} + \|w_1 - w_2\|_{L^2(0,T;H)}\right). \tag{3.19}$$

Second estimate We multiply the difference of (1.2) by $-\Delta\varphi$, and use the Young inequality several times, the previous estimates, and the elliptic regularity theory, to obtain that

$$\|\varphi_1 - \varphi_2\|_{L^2(0,T;W)} \leq c \left(\|u_1 - u_2\|_{L^2(0,T;H)} + \|w_1 - w_2\|_{L^2(0,T;H)}\right). \tag{3.20}$$

Third estimate Next, we test the difference of (1.1) by $\partial_t \mu$ and integrate over time and by parts to realize that

$$\alpha \int_{Q_t} |\partial_t \mu|^2 + \frac{1}{2} \|\nabla \mu(t)\|_H^2 = - \int_{Q_t} \partial_t \varphi \partial_t \mu + \int_{Q_t} (P\sigma - u) h(\varphi_1) \partial_t \mu \\ + \int_{Q_t} (P\sigma_2 - A - u_2)(h(\varphi_1) - h(\varphi_2)) \partial_t \mu.$$

Let us indicate by I_1, I_2, and I_3 the integrals on the right-hand side. They can be handled, with the help of the Young inequality and the previous estimates, as follows:

$$\sum_{i=1}^{3} |I_i| \leq \frac{\alpha}{2} \int_{Q_t} |\partial_t \mu|^2 + \frac{1}{\alpha} \int_{Q_t} |\partial_t \varphi|^2 + \frac{2h_\infty^2}{\alpha} \int_{Q_t} (P^2 |\sigma|^2 + |u|^2) \\ + L_h \Big(P \|\sigma_2\|_{L^\infty(Q)} \int_{Q_t} |\varphi| \, |\partial_t \mu| \\ + A \int_{Q_t} |\varphi||\partial_t \mu| + \|u_2\|_{L^\infty(Q)} \int_{Q_t} |\varphi| \, |\partial_t \mu| \Big)$$

$$
\begin{aligned}
&\leq \frac{3\alpha}{4}\int_{Q_t}|\partial_t\mu|^2+\frac{1}{\alpha}\int_{Q_t}|\partial_t\varphi|^2+\frac{2h_\infty^2}{\alpha}\int_{Q_t}(P^2|\sigma|^2+|u|^2)\\
&\quad+\frac{3L_h^2}{\alpha}\Big(P^2K_1^2+A^2+\|u^*\|^2_{L^\infty(Q)}\Big)\int_{Q_t}|\varphi|^2,
\end{aligned}
$$

where we use the boundedness of σ_2 once more, whereas u_2 belongs to the class $\mathcal{U}_{\text{ad}}$ of admissible controls (cf. (1.9) and **(A7)**). Thus, the above estimates yield that

$$
\|\mu_1-\mu_2\|_{H^1(0,T;H)\cap L^\infty(0,T;V)}\leq c\left(\|u_1-u_2\|_{L^2(0,T;H)}+\|w_1-w_2\|_{L^2(0,T;H)}\right). \tag{3.21}
$$

Fourth estimate Arguing as in the second estimate, that is, using comparison in the difference of (1.1) and elliptic regularity theory, we find that

$$
\|\mu_1-\mu_2\|_{L^2(0,T;W)}\leq c\left(\|u_1-u_2\|_{L^2(0,T;H)}+\|w_1-w_2\|_{L^2(0,T;H)}\right). \tag{3.22}
$$

Fifth estimate We multiply the difference of (1.3) by $\partial_t\sigma$, and integrate over Q_t and by parts, to obtain that

$$
\begin{aligned}
&\int_{Q_t}|\partial_t\sigma|^2+\frac{1}{2}\|\nabla\sigma(t)\|_H^2+\frac{B}{2}\|\sigma(t)\|_H^2\\
&\quad=-\chi\int_{Q_t}\Delta\varphi\,\partial_t\sigma-\int_{Q_t}D\sigma h(\varphi_1)\,\partial_t\sigma\\
&\qquad-\int_{Q_t}D\sigma_2(h(\varphi_1)-h(\varphi_2))\,\partial_t\sigma+\int_{Q_t}w\,\partial_t\sigma.
\end{aligned}
$$

Here, we denote by I_1, ..., I_4 the terms on the right-hand side. Using Young's inequality four times, along with the Lipschitz continuity of h, we realize that the integrals on the right-hand side can be estimated as follows:

$$
\begin{aligned}
\sum_{i=1}^4|I_i|&\leq\chi\int_{Q_t}|\Delta\varphi|\,|\partial_t\sigma|+Dh_\infty\int_{Q_t}|\sigma|\,|\partial_t\sigma|\\
&\quad+DL_h\|\sigma_2\|_{L^\infty(Q)}\int_{Q_t}|\varphi|\,|\partial_t\sigma|+\int_{Q_t}|w|\,|\partial_t\sigma|\\
&\leq\frac{1}{2}\int_{Q_t}|\partial_t\sigma|^2+2\chi^2\int_{Q_t}|\Delta\varphi|^2+2D^2h_\infty^2\int_{Q_t}|\sigma|^2\\
&\quad+2D^2L_h^2K_1^2\int_{Q_t}|\varphi|^2+2\int_{Q_t}|w|^2,
\end{aligned}
$$

where we again exploit the uniform bound for $\|\sigma_2\|_{L^\infty(Q)}$. Therefore, we deduce that

$$
\|\sigma_1-\sigma_2\|_{H^1(0,T;H)\cap L^\infty(0,T;V)}\leq c\left(\|u_1-u_2\|_{L^2(0,T;H)}+\|w_1-w_2\|_{L^2(0,T;H)}\right). \tag{3.23}
$$

Sixth estimate Finally, by comparison in the difference of (1.2), and applying elliptic regularity theory, we have that

$$\|\sigma_1 - \sigma_2\|_{L^2(0,T;W)} \le c\left(\|u_1 - u_2\|_{L^2(0,T;H)} + \|w_1 - w_2\|_{L^2(0,T;H)}\right). \tag{3.24}$$

Upon collecting all of the estimates (3.19)–(3.24), we find that (2.7) is shown, so that Theorem 2.3 is completely proved. □

4 The Control Problem

From now on, we are going to focus our attention on the control problem. The main results are the existence of optimal controls and the first-order necessary conditions for optimality.

4.1 Existence of Optimal Controls

Proof of Theorem 2.4 The proof makes use of the direct method from the calculus of variations. In fact, the cost functional is nonnegative, convex, and weakly lower semicontinuous. To this end, let us pick a minimizing sequence $\{(u_n, w_n)\}_{n\in\mathbb{N}} \subset \mathcal{U}_{\rm ad}$ such that, setting $(\mu_n, \varphi_n, \sigma_n) = \mathcal{S}(u_n, w_n)$, and recalling the notations (1.8)–(1.11), there holds

$$\lim_{n\to\infty} \mathcal{J}(\varphi_n, \sigma_n, u_n, w_n) = \lim_{n\to\infty} \mathcal{J}_{\rm red}(u_n, w_n) = \inf_{(u,w)\in\mathcal{U}_{\rm ad}} \mathcal{J}_{\rm red}(u, w).$$

On the other hand, $\{(u_n, w_n)\}_{n\in\mathbb{N}}$ is bounded in $L^\infty(Q)\times L^\infty(Q)$, and also the bounds (2.4) and (2.6) are at our disposal, for every $n \in \mathbb{N}$ and for the corresponding triplet $(\mu_n, \varphi_n, \sigma_n)$. Hence, accounting for standard weak compactness arguments (see, e.g., [38, Sec. 8, Cor. 4]), it is a standard matter to infer the existence of a pair $(\overline{u}, \overline{w})$ and a triplet $(\overline{\mu}, \overline{\varphi}, \overline{\sigma})$ such that the following convergence properties are (possibly only on a subsequence) fulfilled as $n \to \infty$:

$$(u_n, w_n) \to (\overline{u}, \overline{w}) \quad \text{weakly star in } (L^\infty(Q))^2, \tag{4.1}$$

$$\begin{aligned}\mu_n \to \overline{\mu} \quad &\text{weakly star in } H^1(0,T;H) \cap L^\infty(0,T;V) \cap L^2(0,T;W) \cap L^\infty(Q)\\ &\text{and strongly in } C^0([0,T];H) \cap L^2(0,T;V),\end{aligned} \tag{4.2}$$

$$\begin{aligned}\varphi_n \to \overline{\varphi} \quad &\text{weakly star in } W^{1,\infty}(0,T;H) \cap H^1(0,T;V) \cap L^\infty(0,T;W)\\ &\text{and strongly in } C^0(\overline{Q}),\end{aligned} \tag{4.3}$$

$$\begin{aligned}\sigma_n \to \overline{\sigma} \quad &\text{weakly star in } H^1(0,T;H) \cap L^\infty(0,T;V) \cap L^2(0,T;W) \cap L^\infty(Q)\\ &\text{and strongly in } C^0([0,T];H) \cap L^2(0,T;V).\end{aligned} \tag{4.4}$$

Clearly, as the convex set $\mathcal{U}_{\rm ad}$ is weakly sequentially closed, we have that $(\overline{u}, \overline{w}) \in \mathcal{U}_{\rm ad}$; besides, the strong convergence properties show that the Cauchy conditions (1.5) are fulfilled by $(\overline{\mu}, \overline{\varphi}, \overline{\sigma})$. Moreover, the strong convergence in (4.3) and the assumptions **(F1)**–**(F4)** and **(A3)** imply that

$$h(\varphi_n) \to h(\overline{\varphi}) \text{ and } F'(\varphi_n) \to F'(\overline{\varphi}) \quad \text{strongly in } C^0(\overline{Q}), \quad \text{as } n \to \infty.$$

Therefore, passing to the limit as $n \to \infty$ in the corresponding time-integrated version of (1.1)–(1.5), written for (u_n, w_n) and $(\mu_n, \varphi_n, \sigma_n)$, we easily see that $(\overline{\mu}, \overline{\varphi}, \overline{\sigma})$ solves (1.1)–(1.5) with $(u, w) = (\overline{u}, \overline{w})$, which yields that $(\overline{\mu}, \overline{\varphi}, \overline{\sigma}) = \mathcal{S}(\overline{u}, \overline{w})$. Finally, we combine the weak sequential lower semicontinuity of the cost functional with the assumption that (u_n, w_n) is a minimizing sequence to deduce that $(\overline{u}, \overline{w})$ is indeed an optimal control. □

4.2 The Linearized System

At this point, our aim is to find the necessary conditions for optimality. Actually, we would like to express the formal variational inequality (1.12) in an explicit form. For this purpose, we have to prove the Fréchet differentiability of the reduced cost functional $\mathcal{J}_{\text{red}}$, which is the composition of $\mathcal{J}$ with the control-to-state operator $\mathcal{S}$. However, $\mathcal{J}$ is straightforwardly Fréchet differentiable. Therefore, it suffices to prove that $\mathcal{S}$ is Fréchet differentiable as well, and then invoke the chain rule to write (1.12) in an explicit way.

The expectation is that, provided we find the proper Banach spaces, the Fréchet derivative of $\mathcal{S}$ applied to the pair (k, l) is given by the unique solution to the linearized system (2.8)–(2.12). With this in mind, we begin by establishing the well-posedness of the linearized system (2.8)–(2.12).

Proof of Theorem 2.5 For the sake of simplicity, we proceed formally by providing some estimates. Here, let us just mention that a rigorous proof can be carried out, e.g., using a Galerkin scheme: first showing the rigorous counterpart of the following estimates so to ensure that they are independent of the discretization parameter, and then passing to the limit with respect to the discretization parameter. Moreover, the system (2.8)–(2.12) is linear, so that the uniqueness directly follows from the uniform estimates. In addition, some of the forthcoming estimates follow the same lines as the ones of the state system, which allows us to be less detailed below.

First estimate First of all, we add to both sides of (2.9) the term ξ. Then, we multiply (2.8) by η, the new (2.9) by $\partial_t \xi$, (2.10) by ζ, add the resulting equations, and integrate over Q_t and by parts for an arbitrary $t \in (0, T]$. After a cancellation of terms and some rearrangements, and making use of the initial conditions (2.12), we obtain that

$$\begin{aligned}
&\frac{\alpha}{2}\|\eta(t)\|_H^2 + \int_{Q_t} |\nabla \eta|^2 + \beta \int_{Q_t} |\partial_t \xi|^2 + \frac{1}{2}\|\xi(t)\|_V^2 + \frac{1}{2}\|\zeta(t)\|_H^2 \\
&\quad + B \int_{Q_t} |\zeta|^2 + \int_{Q_t} |\nabla \zeta|^2 = \int_{Q_t} (P\zeta - k) h(\overline{\varphi}) \eta + \int_{Q_t} (P\overline{\sigma} - A - \overline{u}) h'(\overline{\varphi}) \xi \eta \\
&\quad + \int_{Q_t} \xi\, \partial_t \xi - \int_{Q_t} F''(\overline{\varphi}) \xi\, \partial_t \xi + \chi \int_{Q_t} \zeta\, \partial_t \xi + \chi \int_{Q_t} \nabla \xi \cdot \nabla \zeta - \int_{Q_t} D h(\overline{\varphi}) |\zeta|^2 \\
&\quad - \int_{Q_t} D\overline{\sigma} h'(\overline{\varphi}) \xi \zeta + \int_{Q_t} l \zeta\, .
\end{aligned}$$

We denote by I_1, ..., I_9 the integrals on the right-hand side. Using the Young inequality, we infer that

$$
\begin{aligned}
|I_1| + |I_2| \leq P h_\infty \int_{Q_t} |\zeta||\eta| + h_\infty \int_{Q_t} |k||\eta| + h'_\infty \big(P \|\overline{\sigma}\|_{L^\infty(Q)} + A + \|\overline{u}\|_{L^\infty(Q)}\big) \\
+ \int_{Q_t} |\xi||\eta| \\
\leq \frac{P h_\infty}{2} \int_{Q_t} (|\zeta|^2 + |\eta|^2) + \frac{h_\infty}{2} \int_{Q_t} (|k|^2 + |\eta|^2) \\
+ \frac{h'_\infty \big(P K_1 + A + \|u^*\|_{L^\infty(Q)}\big)}{2} \int_{Q_t} (|\xi|^2 + |\eta|^2),
\end{aligned}
$$

where we use the fact that $\overline{\sigma}$ satisfies (2.4) and $\overline{u}$ belongs to the class of admissible controls. Moreover, from Young's inequality, combined with (2.6), it follows that

$$
\begin{aligned}
\sum_{i=3}^{5} |I_i| &\leq \int_{Q_t} |\xi||\partial_t \xi| + \|F''(\overline{\varphi})\|_{L^\infty(Q)} \int_{Q_t} |\xi||\partial_t \xi| + \chi \int_{Q_t} |\zeta||\partial_t \xi| \\
&\leq \frac{\beta}{2} \int_{Q_t} |\partial_t \xi|^2 + \frac{3}{2\beta}\big(K_2^2 + 1\big) \int_{Q_t} |\xi|^2 + \frac{3\chi^2}{2\beta} \int_{Q_t} |\zeta|^2
\end{aligned}
$$

and also that

$$
\begin{aligned}
\sum_{i=7}^{9} |I_i| &\leq D h_\infty \int_{Q_t} |\zeta|^2 + D h'_\infty \|\overline{\sigma}\|_{L^\infty(Q)} \int_{Q_t} |\xi||\zeta| + \int_{Q_t} |l||\zeta| \\
&\leq \left(D h_\infty + \frac{(D h'_\infty K_1)^2 + 1}{4}\right) \int_{Q_t} |\zeta|^2 + \int_{Q_t} (|\xi|^2 + |l|^2).
\end{aligned}
$$

Furthermore, using Young's inequality once more, we infer that

$$
|I_6| \leq \frac{1}{2} \int_{Q_t} |\nabla \zeta|^2 + \frac{\chi^2}{2} \int_{Q_t} |\nabla \xi|^2.
$$

At this point, we collect all of the above estimates and apply Gronwall's lemma to deduce that

$$
\begin{aligned}
&\|\eta\|_{L^\infty(0,T;H) \cap L^2(0,T;V)} + \|\xi\|_{H^1(0,T;H) \cap L^\infty(0,T;V)} + \|\zeta\|_{L^\infty(0,T;H) \cap L^2(0,T;V)} \\
&\quad \leq c \left(\|k\|_{L^2(Q)} + \|l\|_{L^2(Q)}\right). \qquad (4.5)
\end{aligned}
$$

Second estimate We now observe that the Eq. (2.8) shows a parabolic structure with respect to the variable η. In fact, we can write (2.8) in the form

$$
\alpha \partial_t \eta - \Delta \eta = f_1 \quad \text{with} \quad f_1 := (P\zeta - k) h(\overline{\varphi}) + (P\overline{\sigma} - A - \overline{u}) h'(\overline{\varphi}) \xi - \partial_t \xi,
$$

where, owing to the above estimate, we easily verify that $f_1 \in L^2(0,T;H)$ and

$$\|f_1\|_{L^2(0,T;H)} \leq c\,(\|k\|_{L^2(Q)} + \|l\|_{L^2(Q)}). \tag{4.6}$$

So, recalling the boundary and initial conditions (2.11)–(2.12), it is a standard matter to recover the full parabolic regularity and infer that

$$\|\eta\|_{H^1(0,T;H)\cap L^\infty(0,T;V)\cap L^2(0,T;W)} \leq c\,(\|k\|_{L^2(Q)} + \|l\|_{L^2(Q)}). \tag{4.7}$$

Third estimate In the same way, we also have

$$\begin{aligned}\beta\partial_t\xi - \Delta\xi &= f_2 \quad \text{with} \quad f_2 := -F''(\overline{\varphi})\xi + \chi\zeta + \eta,\\ \partial_t\zeta - \Delta\zeta &= f_3 \quad \text{with} \quad f_3 := -\chi\Delta\xi - B\zeta - D\zeta h(\overline{\varphi}) - D\overline{\sigma}h'(\overline{\varphi})\xi + l.\end{aligned}$$

Then, we first note that f_2 belongs to $L^2(0,T;H)$ and satisfies the same estimate as in (4.6), so that the regularity theory for parabolic equation with regular initial datum and homogeneous Neumann boundary conditions allows us to to infer that

$$\|\xi\|_{H^1(0,T;H)\cap L^\infty(0,T;V)\cap L^2(0,T;W)} \leq c\,(\|k\|_{L^2(Q)} + \|l\|_{L^2(Q)}). \tag{4.8}$$

Besides, also f_3 belongs to $L^2(0,T;H)$, and similar reasoning leads to the conclusion that

$$\|\zeta\|_{H^1(0,T;H)\cap L^\infty(0,T;V)\cap L^2(0,T;W)} \leq c\,(\|k\|_{L^2(Q)} + \|l\|_{L^2(Q)}), \tag{4.9}$$

which concludes the proof of Theorem 2.5. □

4.3 Differentiability of the Control-to-State Operator

Now we are going to show the Fréchet differentiability of the operator $\mathcal{S}$ and to characterize its Fréchet derivative.

Proof of Theorem 2.6 At first, let us fix a control pair $(\overline{u},\overline{w}) \in \mathcal{U}_{\text{ad}} \subset \mathcal{U}_R$ with the corresponding state $(\overline{\mu},\overline{\varphi},\overline{\sigma})$. Then, whenever (k,l) belongs to $(L^2(Q))^2$, we denote with (η,ξ,ζ) the corresponding solution to system (2.8)–(2.12). Moreover, let us recall that $\mathcal{U}_R$ is an open set, so that, provided that we consider small perturbations, we also have $(\overline{u}+k,\overline{w}+l) \in \mathcal{U}_R$. Namely, there exist some positive constant δ_* such that $(\overline{u}+k,\overline{w}+l) \in \mathcal{U}_R$ for every (k,l) such that $\|k\|_{L^2(Q)} + \|l\|_{L^2(Q)} \leq \delta_*$. In the following, we always assume that this is the case. Lastly, we denote with $(\widehat{\mu},\widehat{\varphi},\widehat{\sigma})$ the unique solution to (1.1)–(1.5) corresponding to the incremented control $(\overline{u}+k,\overline{w}+l)$. Let us point out that Theorem 2.5 entails that the map $(k,l) \mapsto (\eta,\xi,\zeta)$ is linear and continuous between $(L^2(Q))^2$ and $(H^1(0,T;H) \cap L^\infty(0,T;V) \cap L^2(0,T;W))^3$.

Here, we aim at directly checking the definition of Fréchet differentiability for $\mathcal{S}$. Namely, we are going to show that

$$\mathcal{S}(\overline{u}+k,\overline{w}+l)=\mathcal{S}(\overline{u},\overline{w})+[D\mathcal{S}(\overline{u},\overline{w})](k,l)+o(\|(k,l)\|_{L^2(Q)\times L^2(Q)})\quad\text{in } \mathcal{Y}$$
$$\text{as }\ \|(k,l)\|_{L^2(Q)\times L^2(Q)}\to 0, \tag{4.10}$$

for the Banach space $\mathcal{Y}$ introduced in (2.14). To this end, it is convenient to set

$$\psi:=\widehat{\mu}-\overline{\mu}-\eta,\quad y:=\widehat{\varphi}-\overline{\varphi}-\xi,\quad z:=\widehat{\sigma}-\overline{\sigma}-\zeta.$$

With this notation, (4.10) takes the form

$$\|(\psi,y,z)\|_{\mathcal{Y}}=o(\|(k,l)\|_{L^2(Q)\times L^2(Q)})\quad\text{as}\ \ \|(k,l)\|_{L^2(Q)\times L^2(Q)}\to 0.$$

Obviously, the validity of this condition implies that $\mathcal{S}$ is Fréchet differentiable at $(\overline{u},\overline{w})$ and that $[D\mathcal{S}(\overline{u},\overline{w})](k,l)=(\eta,\xi,\zeta)$ for every $(k,l)\in(L^2(Q))^2$. To verify this condition, it suffices to construct an increasing function $G:(0,\delta_*)\to(0,+\infty)$ such that $\|(\psi,y,z)\|_{\mathcal{Y}}^2\le G\big(\|(k,l)\|_{L^2(Q)\times L^2(Q)}\big)$ and

$$\lim_{\lambda\to 0}\frac{G(\lambda)}{\lambda^2}=0. \tag{4.11}$$

This is actually the estimate we are going to check with the choice $G(\lambda)=c\lambda^4$ for some positive constant c.

At this stage, let us recall that since $(\widehat{\mu},\widehat{\varphi},\widehat{\sigma})$ and $(\overline{\mu},\overline{\varphi},\overline{\sigma})$ are fixed, they both verify (2.4) and (2.6), as well as the following continuous dependence estimate

$$\begin{aligned}&\|\widehat{\mu}-\overline{\mu}\|_{H^1(0,T;H)\cap L^\infty(0,T;V)\cap L^2(0,T;W)}+\|\widehat{\varphi}-\overline{\varphi}\|_{H^1(0,T;H)\cap L^\infty(0,T;V)\cap L^2(0,T;W)}\\&\quad+\|\widehat{\sigma}-\overline{\sigma}\|_{H^1(0,T;H)\cap L^\infty(0,T;V)\cap L^2(0,T;W)}\\&\le K_3\left(\|k\|_{L^2(0,T;H)}+\|l\|_{L^2(0,T;H)}\right),\end{aligned} \tag{4.12}$$

which directly follows from (2.7).

Besides, a system for (ψ,y,z) can be constructed in light of the systems (1.1)–(1.5) corresponding to $(u,w)=(\overline{u}+k,\overline{w}+l)$, (1.1)–(1.5) for $(u,w)=(\overline{u},\overline{w})$, and (2.8)–(2.12). By combining them, we obtain the following system:

$$\begin{aligned}&\alpha\partial_t\psi+\partial_t y-\Delta\psi=Pzh(\overline{\varphi})+(P\overline{\sigma}-A-\overline{u})(h(\widehat{\varphi})-h(\overline{\varphi})-h'(\overline{\varphi})\xi)\\&\quad-k(h(\widehat{\varphi})-h(\overline{\varphi}))+P(\widehat{\sigma}-\overline{\sigma})(h(\widehat{\varphi})-h(\overline{\varphi}))\quad\text{in } Q,\end{aligned} \tag{4.13}$$
$$\psi=\beta\partial_t y-\Delta y+(F'(\widehat{\varphi})-F'(\overline{\varphi})-F''(\overline{\varphi})\xi)-\chi z\quad\text{in } Q, \tag{4.14}$$
$$\begin{aligned}&\partial_t z-\Delta z+Bz=-\chi\Delta y-D[\overline{\sigma}(h(\widehat{\varphi})-h(\overline{\varphi})-h'(\overline{\varphi})\xi)\\&\quad+(\widehat{\sigma}-\overline{\sigma})(h(\widehat{\varphi})-h(\overline{\varphi}))+h(\overline{\varphi})z]\quad\text{in } Q,\end{aligned} \tag{4.15}$$
$$\partial_n\psi=\partial_n y=\partial_n z=0\quad\text{on } \Sigma, \tag{4.16}$$
$$\psi(0)=y(0)=z(0)=0\quad\text{in } \Omega. \tag{4.17}$$

Note that (2.2)–(2.3) and (2.13) entail that

$$\psi,y,z\in H^1(0,T;H)\cap L^\infty(0,T;V)\cap L^2(0,T;W).$$

First estimate First of all, we add to both sides of (4.14) the term y. Next, we multiply (4.13) by ψ, the new (4.14) by $\partial_t y$, and (4.15) by z. Then, we add the resulting identities, integrate over Q_t, where $t \in (0, T]$, and by parts, to find that

$$
\begin{aligned}
&\frac{\alpha}{2}\|\psi(t)\|_H^2 + \int_{Q_t} |\nabla\psi|^2 + \beta\int_{Q_t} |\partial_t y|^2 + \frac{1}{2}\|y(t)\|_V^2 + \frac{1}{2}\|z(t)\|_H^2 \\
&\quad + B\int_{Q_t} |z|^2 + \int_{Q_t} |\nabla z|^2 \\
&\quad = \int_{Q_t} Pzh(\overline{\varphi})\psi + \int_{Q_t} (P\overline{\sigma} - A - \overline{u})(h(\widehat{\varphi}) - h(\overline{\varphi}) - h'(\overline{\varphi})\xi)\psi \\
&\qquad - \int_{Q_t} k(h(\widehat{\varphi}) - h(\overline{\varphi}))\psi + \int_{Q_t} P(\widehat{\sigma} - \overline{\sigma})(h(\widehat{\varphi}) - h(\overline{\varphi}))\psi \\
&\qquad - \int_{Q_t} (F'(\widehat{\varphi}) - F'(\overline{\varphi}) - F''(\overline{\varphi})\xi)\partial_t y + \int_{Q_t} \chi z\partial_t y \\
&\qquad + \int_{Q_t} y\partial_t y + \chi\int_{Q_t} \nabla y\cdot\nabla z - \int_{Q_t} D\overline{\sigma}(h(\widehat{\varphi}) - h(\overline{\varphi}) - h'(\overline{\varphi})\xi)z \\
&\qquad - \int_{Q_t} D(\widehat{\sigma} - \overline{\sigma})(h(\widehat{\varphi}) - h(\overline{\varphi}))z - \int_{Q_t} Dh(\overline{\varphi})|z|^2,
\end{aligned}
$$

where we denote by $I_1, ..., I_{11}$ the integrals on the right-hand side. Moreover, in the above calculations we also owe to the fact that the initial data are zero by (4.17). Using the Hölder and Young inequalities, the Lipschitz continuity of h and the Sobolev embedding (2.26) with $q = 4$, we have that

$$
\begin{aligned}
|I_1| + |I_3| + |I_4| &\le Ph_\infty \int_{Q_t} |z||\psi| + L_h\int_0^t \|k(s)\|_2\|\widehat{\varphi}(s) - \overline{\varphi}(s)\|_4\|\psi(s)\|_4\,ds \\
&\quad + PL_h\int_0^t \|\widehat{\sigma}(s) - \overline{\sigma}(s)\|_4\|\widehat{\varphi}(s) - \overline{\varphi}(s)\|_4\|\psi\|_2\,ds \\
&\le \frac{Ph_\infty}{2}\int_{Q_t} (|z|^2 + |\psi|^2) \\
&\quad + \frac{1}{2}\int_0^t \|\psi(s)\|_V^2\,ds + c\,\|\widehat{\varphi} - \overline{\varphi}\|^2_{L^\infty(0,T;V)}\int_{Q_t} |k|^2 \\
&\quad + c\,\|\widehat{\sigma} - \overline{\sigma}\|^2_{L^\infty(0,T;V)}\|\widehat{\varphi} - \overline{\varphi}\|^2_{L^\infty(0,T;V)} + \int_{Q_t} |\psi|^2 \\
&\le \frac{1}{2}\int_0^t \|\psi(s)\|_V^2\,ds + c\left(\|k\|^4_{L^2(0,T;H)} + \|l\|^4_{L^2(0,T;H)}\right) \\
&\quad + c\int_{Q_t} (|z|^2 + |\psi|^2)\,,
\end{aligned}
$$

where we also invoked the continuous dependence estimate (4.12). Before moving on, let us recall the Taylor formula with integral remainder which will be useful to estimate some terms. For an arbitrary function $g \in C^1(\mathbb{R})$ with g' Lipschitz continuous, we have that

$$g(x) = g(\overline{x}) + g'(\overline{x})(x-\overline{x}) \\ + (x-\overline{x})^2 \int_0^1 g''(\overline{x}+s(x-\overline{x}))(1-s)\,ds \quad \text{for every } x \in \mathbb{R}. \tag{4.18}$$

Applying the above formula to F' and h, respectively, we infer that

$$F'(\widehat{\varphi}) - F'(\overline{\varphi}) - F''(\overline{\varphi})\xi \;=\; F''(\overline{\varphi})y + R_1(\widehat{\varphi}-\overline{\varphi})^2, \tag{4.19}$$

$$h(\widehat{\varphi}) - h(\overline{\varphi}) - h'(\overline{\varphi})\xi \;=\; h'(\overline{\varphi})y + R_2(\widehat{\varphi}-\overline{\varphi})^2, \tag{4.20}$$

with the remainders

$$R_1 := \int_0^1 F'''(\overline{\varphi}+s(\widehat{\varphi}-\overline{\varphi}))(1-s)ds\,, \quad R_2 := \int_0^1 h''(\overline{\varphi}+s(\widehat{\varphi}-\overline{\varphi}))(1-s)ds\,.$$

Taking advantage of (2.6) and **(A3)**, we see that

$$\|R_1\|_{L^\infty(Q)} \le R_1^*, \quad \|R_2\|_{L^\infty(Q)} \le R_2^*,$$

for some positive constants R_1^*, R_2^*. Thus, making use of (4.20), we are now in a position to estimate I_2 as follows:

$$\begin{aligned}
|I_2| &\le (P\|\overline{\sigma}\|_{L^\infty(Q)} + A + \|\overline{u}\|_{L^\infty(Q)}) \int_{Q_t} (h'_\infty|y| + R_2^*(\widehat{\varphi}-\overline{\varphi})^2)|\psi| \\
&\le \frac{(PK_1 + A + \|u^*\|_{L^\infty(Q)})h'_\infty}{2} \int_{Q_t} (|y|^2 + |\psi|^2) \\
&\quad + (PK_1 + A + \|u^*\|_{L^\infty(Q)})R_2^* \int_0^t \|\widehat{\varphi}(s) - \overline{\varphi}(s)\|_4^2\, \|\psi(s)\|_2\, ds \\
&\le \frac{(PK_1 + A + \|u^*\|_{L^\infty(Q)})h'_\infty}{2} \int_{Q_t} (|y|^2 + |\psi|^2) \\
&\quad + c\|\widehat{\varphi}-\overline{\varphi}\|^4_{L^\infty(0,T;V)} + \int_{Q_t} |\psi|^2 \\
&\le c\int_{Q_t} (|y|^2 + |\psi|^2) + c(\|k\|^4_{L^2(Q)} + \|l\|^4_{L^2(Q)})\,,
\end{aligned}$$

where we also use (4.12), the fact that $\overline{\sigma}$ is bounded for (2.4), whereas $\overline{u}$ is bounded since it is an admissible control. As for I_5, thanks to the Young inequality and (4.19), we have that

$$\begin{aligned}
|I_5| &\le \frac{\beta}{4}\int_{Q_t} |\partial_t y|^2 + \frac{2\|F''(\overline{\varphi})\|^2_{L^\infty(Q)}}{\beta} \int_{Q_t} |y|^2 + 2R_1^{*2}\|\widehat{\varphi}-\overline{\varphi}\|^4_{L^\infty(0,T;L^4(\Omega))} \\
&\le \frac{\beta}{4}\int_{Q_t} |\partial_t y|^2 + \frac{2K_2^2}{\beta}\int_{Q_t} |y|^2 + c\,(\|k\|^4_{L^2(Q)} + \|l\|^4_{L^2(Q)}).
\end{aligned}$$

Moreover, using the Young inequality once more, we have that

$$\sum_{i=6}^{8} |I_i| \le \frac{1}{2}\int_{Q_t} |\nabla z|^2 + \frac{\chi^2}{2}\int_{Q_t} |\nabla y|^2 + \frac{\beta}{4}\int_{Q_t} |\partial_t y|^2 + \frac{2\chi^2}{\beta}\int_{Q_t} |z|^2 + \frac{2}{\beta}\int_{Q_t} |y|^2.$$

Lastly, by similar reasoning, we obtain that

$$\begin{aligned}
\sum_{i=9}^{11} |I_i| &\le D\|\overline{\sigma}\|_{L^\infty(Q)} \int_{Q_t} (h'_\infty |y| + R_2^*(\widehat{\varphi}-\overline{\varphi})^2)|z| \\
&\quad + DL_h \int_0^t \|\widehat{\sigma}(s)-\overline{\sigma}(s)\|_4 \, \|\widehat{\varphi}(s)-\overline{\varphi}(s)\|_4 \, \|z(s)\|_2 \, ds + Dh_\infty \int_{Q_t} |z|^2 \\
&\le \frac{DK_1 h'_\infty}{2} \int_{Q_t} (|y|^2+|z|^2) + DK_1 R_2^* \int_0^t \|\widehat{\varphi}(s)-\overline{\varphi}(s)\|_4^2 \, \|z(s)\|_2 \, ds \\
&\quad + \frac{D^2 L_h^2}{4} \|\widehat{\sigma}-\overline{\sigma}\|^2_{L^\infty(0,T;L^4(\Omega))} \|\widehat{\varphi}-\overline{\varphi}\|^2_{L^\infty(0,T;L^4(\Omega))} + \int_{Q_t} |z|^2 \\
&\quad + Dh_\infty \int_{Q_t} |z|^2 \\
&\le \frac{DK_1 h'_\infty}{2} \int_{Q_t} (|y|^2+|z|^2) + c\|\widehat{\varphi}-\overline{\varphi}\|^4_{L^\infty(0,T;V)} \\
&\quad + c\|\widehat{\sigma}-\overline{\sigma}\|^2_{L^\infty(0,T;V)} \|\widehat{\varphi}-\overline{\varphi}\|^2_{L^\infty(0,T;V)} + (Dh_\infty+1)\int_{Q_t} |z|^2 \\
&\le c\int_{Q_t} (|y|^2+|z|^2) + c(\|k\|^4_{L^2(Q)} + \|l\|^4_{L^2(Q)}).
\end{aligned}$$

Hence, applying Gronwall's lemma, we deduce that

$$\begin{aligned}
&\|\psi\|^2_{C^0([0,T];H)\cap L^2(0,T;V)} + \|y\|^2_{H^1(0,T;H)\cap L^\infty(0,T;V)} + \|z\|^2_{C^0([0,T];H)\cap L^2(0,T;V)} \\
&\quad \le C\|(k,l)\|^4_{L^2(Q)\times L^2(Q)},
\end{aligned}$$

which in turn implies the validity of (4.11) with the choice $G(\lambda) = C\lambda^4$. This concludes the proof of the assertion. □

4.4 First-Order Necessary Optimality Conditions

As already pointed out in Sect. 2, we would like to employ the adjoint variables in order to eliminate the linearized variables from the variational inequality (2.15). Here, we begin with the task of establishing the well-posedness of the adjoint system. In this direction, let us set

$$Q_t^T = (t,T)\times\Omega \quad \text{for every } t \in (0,T).$$

Proof of Theorem 2.8 The rigorous proof should employ an approximation technique. Anyhow, since the system is linear and the arguments are standard, we simply point out the estimates which allow us to conclude, leaving the details to the reader. It is worth recalling that the adjoint system is linear, so that the uniqueness directly follows from our estimates.

First estimate First, we add to both sides of (2.16) the term $-q$. Then, we multiply the new (2.16) by $-\partial_t q$, (2.17) by p, (2.18) by $\chi^2 r$, add the resulting equations, and integrate over Q_t^T and by parts. We obtain a cancellation and deduce that

$$\alpha \int_{Q_t^T} |\partial_t q|^2 + \frac{1}{2}\|q(t)\|_V^2 + \frac{\beta}{2}\|p(t)\|_H^2 + \int_{Q_t^T} |\nabla p|^2 + \frac{\chi^2}{2}\|r(t)\|_H^2$$
$$+ \chi^2 \int_{Q_t^T} |\nabla r|^2 + \chi^2 B \int_{Q_t^T} |r|^2$$
$$= \frac{\gamma_1^2}{2\beta}\|\overline{\varphi}(T) - \varphi_\Omega\|_H^2 + \frac{\chi^2\gamma_3^2}{2}\|\overline{\sigma}(T) - \sigma_\Omega\|_H^2 + \int_{Q_t^T} q\partial_t q$$
$$+ \chi \int_{Q_t^T} \nabla r \cdot \nabla p - \int_{Q_t^T} F''(\overline{\varphi})|p|^2 + \int_{Q_t^T} (P\overline{\sigma} - A - \overline{u})h'(\overline{\varphi})qp$$
$$- \int_{Q_t^T} D\overline{\sigma}h'(\overline{\varphi})rp + \int_{Q_t^T} \gamma_2(\overline{\varphi} - \varphi_Q)p - \chi^2 \int_{Q_t^T} Dh(\overline{\varphi})|r|^2$$
$$+ \chi^3 \int_{Q_t^T} pr + \chi^2 \int_{Q_t^T} Ph(\overline{\varphi})qr + \chi^2 \int_{Q_t^T} \gamma_4(\overline{\sigma} - \sigma_Q)r,$$

where we used the information (2.20) on the final data. In the above equality, the terms on the left-hand side are nonnegative, whereas we denote the integrals on the right-hand side by I_1, ..., I_{12}, in this order. As far as the right-hand side is concerned, the first four terms can be easily handled with the aid of (2.4), assumption **(A6)**, and the Young inequality. Indeed, we have

$$\sum_{i=1}^{4} |I_i| \le c + \frac{\alpha}{2}\int_{Q_t^T} |\partial_t q|^2 + \frac{1}{2\alpha}\int_{Q_t^T} |q|^2 + \frac{1}{2}\int_{Q_t^T} |\nabla p|^2 + \frac{\chi^2}{2}\int_{Q_t^T} |\nabla r|^2.$$

Using Young's inequality, we can deal with I_6 as follows:

$$|I_6| \le \frac{(P\|\overline{\sigma}\|_{L^\infty(Q)} + A + \|\overline{u}\|_{L^\infty(Q)})h'_\infty}{2}\int_{Q_t^T} (|q|^2 + |p|^2),$$

where we employ that $\overline{\sigma}$ satisfies (2.4) and that $\overline{u}$ is an admissible control. The rest of the terms can be handled using several times the Young inequality to get that

$$|I_5| + \sum_{i=7}^{12} |I_i| \le \frac{Ph_\infty\chi^2}{2}\int_{Q_t^T} |q|^2$$
$$+ \left(\|F''(\overline{\varphi})\|_{L^\infty(Q)} + \frac{2 + D\|\overline{\sigma}\|_{L^\infty(Q)}h'_\infty + \chi^3}{2}\right)\int_{Q_t^T} |p|^2$$

$$+\left(\frac{2+D\|\overline{\sigma}\|_{L^\infty(Q)}h'_\infty+\chi^3}{2}+\chi^2 Dh_\infty+\frac{Ph_\infty\chi^2}{2}\right)\int_{Q_t^T}|r|^2$$
$$+\frac{(\gamma_2^2+\chi^4\gamma_4^2)}{4}\int_{Q_t^T}(|\overline{\varphi}-\varphi_Q|^2+|\overline{\sigma}-\sigma_Q|^2).$$

Thus, the backward-in-time Gronwall lemma yields that

$$\|q\|_{H^1(0,T;H)\cap L^\infty(0,T;V)}+\|p\|_{L^\infty(0,T;H)\cap L^2(0,T;V)}+\|r\|_{L^\infty(0,T;H)\cap L^2(0,T;V)}\le c. \tag{4.21}$$

Second estimate By (4.21) and a comparison argument in (2.17) and (2.18), we obtain that

$$\|\partial_t p\|_{L^2(0,T;V^*)}+\|\partial_t r\|_{L^2(0,T;V^*)}\le c, \tag{4.22}$$

which, in turn, gives sense to the final conditions (2.20). In fact, from the standard embedding of $H^1(0,T;V^*)\cap L^2(0,T;V)$ in $C^0([0,T];H)$, we deduce that $p, r\in C^0([0,T];H)$.

Third estimate Next, a comparison in (2.16) produces $\Delta q\in L^2(0,T;H)$, and the elliptic regularity theory yields that

$$\|q\|_{L^2(0,T;W)}\le c, \tag{4.23}$$

which also allows us to recover $q\in C^0([0,T];V)$ from well-known embedding results.

Summing up, we realize that the estimate

$$\|q\|_{H^1(0,T;H)\cap C^0([0,T];V)\cap L^2(0,T;W)}+\|p\|_{H^1(0,T;V^*)\cap C^0([0,T];H)\cap L^2(0,T;V)}$$
$$+\|r\|_{H^1(0,T;V^*)\cap C^0([0,T];H)\cap L^2(0,T;V)}\le c \tag{4.24}$$

has been proved. The uniqueness part directly follows, since the system (2.16)–(2.20) is linear. □

Finally, we are left with the task of showing the necessary conditions for optimality. To this end, we begin by checking Theorem 2.7. Then, making use of the adjoint system, we simplify (2.15) and deduce a variational inequality which is more convenient for the applications.

Proof of Theorem 2.7 This result is a direct consequence of (1.12) and Theorem 2.6. Indeed, combining the Fréchet differentiability of $\mathcal{S}$ with the chain rule, we can exploit (1.12) to derive (2.15). □

We are now in the position to eliminate the solutions to the linearized system from the necessary condition (2.15). This procedure leads to (2.25) and thus to Theorem 2.9.

Proof of Theorem 2.9 Comparing the variational inequality (2.15) with (2.25), it becomes clear that we only need to ensure that

$$-\int_Q h(\overline{\varphi})qk + \int_Q rl = \gamma_1 \int_\Omega (\overline{\varphi}(T) - \varphi_\Omega)\xi(T) + \gamma_2 \int_Q (\overline{\varphi} - \varphi_Q)\xi$$
$$+ \gamma_3 \int_\Omega (\overline{\sigma}(T) - \sigma_\Omega)\zeta(T) \tag{4.25}$$

where ξ and ζ are the solution to the linearized system (2.8)–(2.12) corresponding to $k = u - \overline{u}$ and $l = w - \overline{w}$. In order to show (4.25), let us first point out that combining the Newton-Leibnitz formula with the initial and final conditions (2.12) and (2.20), respectively, we have that

$$\begin{aligned}
-\int_0^T \beta\langle\partial_t p(t), \xi(t)\rangle_V \, dt &= \beta \int_Q \partial_t\xi \, p - \int_0^T \frac{d}{dt}\Big(\int_\Omega \beta p\xi\Big)dt \\
&= \beta \int_Q \partial_t\xi \, p - \int_\Omega \gamma_1(\overline{\varphi}(T) - \varphi_\Omega)\xi(T), \\
-\int_0^T \langle\partial_t r(t), \zeta(t)\rangle_V \, dt &= \int_Q \partial_t\zeta \, r - \int_0^T \frac{d}{dt}\Big(\int_\Omega r\zeta\Big)dt \\
&= \int_Q \partial_t\zeta \, r - \int_\Omega \gamma_3(\overline{\sigma}(T) - \sigma_\Omega)\zeta(T).
\end{aligned}$$

Then, we consider the solution (η, ξ, ζ) to (2.8)–(2.12) corresponding to $k = u - \overline{u}$ and $l = w - \overline{w}$ as test functions in system (2.16)–(2.20). Namely, we test (2.16) by η, (2.17) by ξ, (2.18) by ζ, and integrate over $(0, T)$ to obtain that

$$\begin{aligned}
0 = &\int_Q \eta\,[-\alpha\partial_t q - \Delta q - p] \\
&- \int_Q \partial_t q\xi - \int_0^T \beta\langle\partial_t p(t), \xi(t)\rangle_V \, dt \\
&+ \int_Q \nabla p \cdot \nabla\xi - \chi \int_Q \nabla r \cdot \nabla\xi + \int_Q F''(\overline{\varphi})p\xi \\
&- \int_Q (P\overline{\sigma} - A - \overline{u})h'(\overline{\varphi})q\xi + \int_Q D\overline{\sigma}h'(\overline{\varphi})r\xi - \int_Q \gamma_2(\overline{\varphi} - \varphi_Q)\xi \\
&- \int_0^T \langle\partial_t r(t), \zeta(t)\rangle_V \, dt + \int_Q \nabla r \cdot \nabla\zeta + \int_Q Br\zeta + \int_Q Dh(\overline{\varphi})r\zeta - \int_Q \chi p\zeta \\
&- \int_Q Ph(\overline{\varphi})q\zeta - \int_Q \gamma_4(\overline{\sigma} - \sigma_Q)\zeta.
\end{aligned}$$

Hence, we integrate by parts making use of the boundary conditions, the initial data and the above identities. After rearrangements of the terms, we infer that

$$\begin{aligned}
&\int_\Omega \gamma_1(\overline{\varphi}(T)-\varphi_\Omega)\xi(T)+\int_Q \gamma_2(\overline{\varphi}-\varphi_Q)\xi+\int_\Omega \gamma_3(\overline{\sigma}(T)-\sigma_\Omega)\zeta(T)\\
&\quad+\int_Q \gamma_4(\overline{\sigma}-\sigma_Q)\zeta=\int_Q p\,[\beta\partial_t\xi-\Delta\xi+F''(\overline{\varphi})\xi-\chi\zeta-\eta]\\
&\quad+\int_Q q\,[\alpha\partial_t\eta+\partial_t\xi-\Delta\eta-P\zeta h(\overline{\varphi})-(P\overline{\sigma}-A-\overline{u})h'(\overline{\varphi})\xi]\\
&\quad+\int_Q r\,[\partial_t\zeta-\Delta\zeta+B\zeta+\chi\Delta\xi+D\zeta h(\overline{\varphi})+D\overline{\sigma}h'(\overline{\varphi})\xi].
\end{aligned}$$

Finally, we account for the equations of system (2.8)–(2.12) to realize that

$$\begin{aligned}
&\int_\Omega \gamma_1(\overline{\varphi}(T)-\varphi_\Omega)\xi(T)+\int_Q \gamma_2(\overline{\varphi}-\varphi_Q)\xi+\int_\Omega \gamma_3(\overline{\sigma}(T)-\sigma_\Omega)\zeta(T)\\
&\quad+\int_Q \gamma_4(\overline{\sigma}-\sigma_Q)\zeta=-\int_Q h(\overline{\varphi})q(u-\overline{u})+\int_Q r(w-\overline{w}),
\end{aligned}$$

that is (4.25), so that the variational inequality (2.25) has been shown.

Let us note, the last sentences in the statement of Theorem 2.9 straightforwardly follow by combining the fact that condition (2.25) can be decoupled by taking first $w=\overline{w}$ and then $u=\overline{u}$ and use the Hilbert projection theorem. □

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