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Optimal boundary control of a nonstandard viscous Cahn–Hilliard system with dynamic boundary condition

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Abstract

In this paper, we study an optimal boundary control problem for a model for phase separation taking place in a spatial domain that was introduced by Podio-Guidugli in Ric. Mat. **55** (2006), pp. 105–118. The model consists of a strongly coupled system of nonlinear parabolic differential equations, in which products between the unknown functions and their time derivatives occur that are difficult to handle analytically. In contrast to the existing control literature about this PDE system, we consider here a dynamic boundary condition involving the Laplace–Beltrami operator for the order parameter of the system, which models an additional nonconserving phase transition occurring on the surface of the domain. We show the Fréchet differentiability of the associated control-to-state operator in appropriate Banach spaces and derive results on the existence of optimal controls and on first-order necessary optimality conditions in terms of a variational inequality and the adjoint state system.

1 Introduction

Let $\Omega \subset \mathbb{R}^3$ be an open, bounded and connected set with a smooth boundary Γ (since we aim to apply results from [24], we should at least have $\Gamma \in C^2$), and let $Q := \Omega \times (0,T)$ and $\Sigma := \Gamma \times (0,T)$. We denote by $\partial_{\mathbf{n}}$, ∇_Γ, Δ_Γ, the outward normal derivative, the tangential gradient, and the Laplace–Beltrami operator on Γ, in this order. We consider the following optimal boundary control problem:

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

$$
\begin{aligned}
&\mathcal{J}((\mu,\rho,\rho_\Gamma),\, u_\Gamma) \\
&:= \frac{\beta_1}{2}\,\|\mu-\hat\mu_Q\|^2_{L^2(Q)} + \frac{\beta_2}{2}\,\|\rho-\hat\rho_Q\|^2_{L^2(Q)} + \frac{\beta_3}{2}\,\|\rho_\Gamma-\hat\rho_\Sigma\|^2_{L^2(\Sigma)} \\
&+ \frac{\beta_4}{2}\,\|\rho(T)-\hat\rho_\Omega\|^2_{L^2(\Omega)} + \frac{\beta_5}{2}\,\|\rho_\Gamma(T)-\hat\rho_\Gamma\|^2_{L^2(\Gamma)} + \frac{\beta_6}{2}\,\|\,u_\Gamma\|^2_{L^2(\Sigma)}
\end{aligned}
\tag{1.1}
$$

over a suitable set $\mathcal{U}_{\rm ad} \subset (H^1(0,T;L^2(\Gamma)) \cap L^\infty(\Sigma))$ of admissible controls u_Γ (to be specified later), subject to the state system

$$\big(1+2g(\rho)\big)\,\partial_t\mu + \mu\, g'(\rho)\,\partial_t\rho - \Delta\mu = 0 \quad \text{and} \quad \mu \ge 0 \quad \text{in } Q, \tag{1.2}$$

$$\partial_{\mathbf{n}}\mu = 0 \quad \text{on } \Sigma, \tag{1.3}$$

$$\partial_t\rho - \Delta\rho + f'(\rho) + \pi(\rho) = \mu\, g'(\rho) \quad \text{in } Q, \tag{1.4}$$

$$\partial_{\mathbf{n}}\rho + \partial_t\rho_\Gamma + f_\Gamma'(\rho_\Gamma) + \pi_\Gamma(\rho_\Gamma) - \Delta_\Gamma\rho_\Gamma = u_\Gamma, \quad \rho_\Gamma = \rho_{|\Sigma}, \quad \text{on } \Sigma, \tag{1.5}$$

$$\mu(0) = \mu_0, \quad \rho(0) = \rho_0, \quad \text{in } \Omega, \quad \rho_\Gamma(0) = \rho_{0|\Gamma} \quad \text{on } \Gamma. \tag{1.6}$$

Here, β_i, $1 \le i \le 6$, are nonnegative weights, and $\hat\mu_Q, \hat\rho_Q \in L^2(Q)$, $\hat\rho_\Sigma \in L^2(\Sigma)$, $\hat\rho_\Omega \in L^2(\Omega)$, and $\hat\rho_\Gamma \in L^2(\Gamma)$ are prescribed target functions. Although more general cost functionals could be admitted for large parts of the subsequent analysis, we restrict ourselves to the above situation for the sake of a simpler exposition.

The physical background behind the control problem **(CP)** is the following: the state system (1.2)–(1.6) constitutes a model for phase separation taking place in the container Ω and originally introduced in [30]. In this connection, the unknowns μ and ρ denote the associated chemical potential, which in this particular model has to be nonnegative (see (1.2)), and the order parameter of the phase separation process, which is usually the volumetric density of one of the involved phases. We assume that ρ is normalized in such a way as to attain its values in the interval $(-1,1)$. The nonlinearities π, π_Γ, g are assumed to be smooth in $[-1,1]$, while f and f_Γ are double-well potentials defined in $(-1,1)$, whose derivatives f', f'_Γ are singular at the endpoints $r=-1$ and $r=1$. A typical case is given by the *logarithmic potential*

$$f(r) = f_\Gamma(r) = \hat{c}\,((1+r)\,\log(1+r) + (1-r)\,\log(1-r)), \text{ with a constant } \hat{c} > 0. \tag{1.7}$$

The state system (1.2)–(1.6) is singular, with highly nonlinear and nonstandard coupling. In particular, unpleasant nonlinear terms involving time derivatives occur in (1.2), and the expressions $f'(\rho)$ and $f'_\Gamma(\rho_\Gamma)$ in (1.4), (1.5) may become singular.

The state system has been the subject of intensive study in the past years for the case that (1.5) is replaced by a zero Neumann condition. In this connection, we refer the reader to [6–9,11–14]. In [10] an associated control problem with a distributed control in (1.2) was investigated for the special case $g(\rho)=\rho$, and in [16] the corresponding case of a boundary control in (1.3) was studied. A nonlocal version, in which the Laplacian $-\Delta\rho$ in (1.4) was replaced by a nonlocal operator, was discussed in the recent contributions [19–21].

In all of the works cited above a zero Neumann condition was assumed for the order parameter ρ. In contrast to this, we study in this paper the case of the dynamic boundary condition (1.5). It models a nonconserving phase transition taking place on the boundary, which could be, e. g., induced by an interaction between bulk and wall. The associated total free energy of the phase separation process is the sum of a bulk and a surface energy and has the form

$$\begin{aligned}
&\mathcal{F}_{\text{tot}}[\mu(t), \rho(t), \rho_\Gamma(t)] \\
&:= \int_\Omega \Big(f(\rho(x,t)) + \hat{\pi}(\rho(x,t)) \;-\; \mu(x,t)\, g(\rho(x,t)) \;+\; \frac{1}{2}|\nabla\rho(x,t)|^2 \Big)\, \mathrm{d}x \\
&\quad + \int_\Gamma \Big(f_\Gamma(\rho_\Gamma(x,t)) + \hat{\pi}_\Gamma(\rho_\Gamma(x,t)) \;-\; u_\Gamma(x,t)\,\rho_\Gamma(x,t) \;+\; \frac{1}{2}|\nabla_\Gamma\rho_\Gamma(x,t)|^2 \Big)\, \mathrm{d}\Gamma\,,
\end{aligned} \tag{1.8}$$

for $t \in [0,T]$, where $\hat{\pi}(r) = \int_0^r \pi(\xi)\mathrm{d}\xi$ and $\hat{\pi}_\Gamma(r) = \int_0^r \pi_\Gamma(\xi)\mathrm{d}\xi$.

In the recent contribution [22], the state system (1.2)–(1.6) was studied systematically concerning existence, uniqueness, and regularity. Notice that in [22] more general nonlinearities were admitted, including the case that f, f_Γ could be nondifferentiable indicator functions (in which case $f'(\rho)$ and $f'_\Gamma(\rho_\Gamma)$ have to be interpreted as elements of the (possibly multivalued) subdifferentials of f at ρ and of f_Γ at ρ_Γ, respectively, so that (1.4) and (1.5) have to be understood as differential inclusions).

The mathematical literature on control problems for phase field systems involving equations of viscous or nonviscous Cahn–Hilliard type is still scarce and quite recent. We refer in this connection to the works [3, 4, 17, 18, 27, 33]. Control problems for convective Cahn–Hilliard systems were studied in [31, 34, 35], and a few analytical contributions were made to the coupled Cahn–Hilliard/Navier–Stokes system (cf. [25, 26, 28, 29]). The contribution [15] dealt with the optimal control of a Cahn–Hilliard type system arising in the modeling of solid tumor growth. For the optimal control of Allen–Cahn equations with dynamic boundary conditions, we refer to [5, 23].

The paper is organized as follows: in Section 2, we formulate the relevant assumptions on the data of the control problem **(CP)**, and we prove a strong stability result for the state system (1.2)–(1.6). In Section 3, we prove the Fréchet differentiability of the control-to-state operator in appropriate Banach spaces. Section 4 then brings the main results of this paper, namely, the existence of optimal controls and the derivation of the first-order necessary conditions of optimality.

Throughout the paper, we denote for a general Banach space X by $\|\cdot\|_X$ its norm and by X' its dual space. The only exemption from this convention are the norms of the L^p spaces and of their powers, which we often denote by $\|\cdot\|_p$, for $1 \le p \le +\infty$. Moreover, we repeatedly utilize the continuity of the embedding $H^1(\Omega) \subset L^p(\Omega)$ for $1 \le p \le 6$ and the related Sobolev inequality

$$\|v\|_p \le C_\Omega \|v\|_{H^1(\Omega)} \quad \text{for every } v \in H^1(\Omega) \text{ and } 1 \le p \le 6, \tag{1.9}$$

where C_Ω depends only on Ω. Notice that these embeddings are compact for $1 \le p < 6$. We also recall that the embedding $H^2(\Omega) \subset C^0(\overline{\Omega})$ is compact. Furthermore, we make repeated use of Hölder's inequality and of the elementary Young inequality

$$|ab| \le \gamma\, |a|^2 + \tfrac{1}{4\gamma}\, |b|^2 \quad \text{for every } \ a, b \in \mathbb{R} \ \text{ and } \ \gamma > 0, \tag{1.10}$$

and we set

$$Q_t := \Omega \times (0,t), \quad \Sigma_t := \Gamma \times (0,t), \quad \text{for } \ t \in (0,T]. \tag{1.11}$$

About time derivatives of a time-dependent function v, we warn the reader that we will use both the notations $\partial_t v$, $\partial_t^2 v$ and the shorter ones v_t, v_{tt}.

2 General assumptions and results for the state system

In this section, we formulate the general assumptions for the data of the control problem **(CP)**, and we state some preparatory results for the state system (1.2)–(1.6). To begin with, we introduce some denotations. We set

$$\begin{aligned} &H := L^2(\Omega), \quad V := H^1(\Omega), \quad W := \{w \in H^2(\Omega) : \partial_{\mathbf{n}} w = 0 \ \text{ on } \ \Gamma\}, \\ &H_\Gamma := L^2(\Gamma), \quad V_\Gamma := H^1(\Gamma), \quad \mathcal{V} := \{v \in V : v_{|\Gamma} \in V_\Gamma\}, \end{aligned}$$

and endow these spaces with their standard norms. Notice that we have $V \subset H \subset V'$ and $V_\Gamma \subset H_\Gamma \subset V_\Gamma'$ with dense, continuous and compact embeddings.

We make the following general assumptions:

(A1) $\mu_0 \in W$, $\mu_0 \ge 0$ a.e. in Ω, $\rho_0 \in H^2(\Omega)$, $\rho_{0_\Gamma} := \rho_{0|\Gamma} \in H^2(\Gamma)$, and

$$-1 \;<\; \min_{x \in \overline{\Omega}} \rho_0(x), \quad \max_{x \in \overline{\Omega}} \rho_0(x) \;<\; +1. \tag{2.1}$$

(A2) $\pi, \pi_\Gamma \in C^2[-1,+1]$; $g \in C^3[-1,+1]$ is nonnegative and concave on $[-1,+1]$.

(A3) $f, f_\Gamma \in C^3(-1,+1)$ are nonnegative and convex, satisfy $f(0) = f_\Gamma(0) = 0$, and there are constants $\delta > 0$ and $C_\Gamma \geq 0$ such that

$$|f'(r)| \leq \delta\,|f_\Gamma'(r)| + C_\Gamma \quad \forall\, r \in (-1,+1). \tag{2.2}$$

Moreover, it holds that

$$\lim_{r\searrow -1} f'(r) = \lim_{r\searrow -1} f_\Gamma'(r) = -\infty, \quad \lim_{r\nearrow +1} f'(r) = \lim_{r\nearrow +1} f_\Gamma'(r) = +\infty. \tag{2.3}$$

(A4) $$\mathcal{U}_{\rm ad} = \Big\{ u_\Gamma \in H^1(0,T;H_\Gamma) \cap L^\infty(\Sigma) : \, u_* \leq u_\Gamma \leq u^* \text{ a.e. on } \Gamma \text{ and } \| u_\Gamma \|_{H^1(0,T;H_\Gamma)\cap L^\infty(\Sigma)} \leq R_0 \Big\},$$

where $u_*, u^* \in L^\infty(\Sigma)$ and $R_0 > 0$ are such that $\mathcal{U}_{\rm ad} \neq \emptyset$.

(A5) Let $R > 0$ be a constant such that $\mathcal{U}_{\rm ad} \subset \mathcal{U}_R$ with the open ball $\mathcal{U}_R := \big\{ u \in H^1(0,T;H_\Gamma) \cap L^\infty(\Sigma) : \|u\|_{H^1(0,T;H_\Gamma)\cap L^\infty(\Sigma)} < R \big\}$.

(A6) The constants β_i, $1 \leq i \leq 5$, are nonnegative, and we have that $\hat\mu_Q, \hat\rho_Q \in L^2(Q)$, $\hat\rho_\Sigma \in L^2(\Sigma)$, $\hat\rho_\Omega \in L^2(\Omega)$, and $\hat\rho_\Gamma \in L^2(\Gamma)$.

The assumption (A5) is rather a denotation. We also remark that (A3) entails, in particular, that $f'(0) = f_\Gamma'(0) = 0$, and it is easily seen that (A3) is fulfilled for the logarithmic potentials (1.7), even with different $\hat c$'s for f and f_Γ. In addition, if we assume that $u_\Gamma \in \mathcal{U}_R$, then it follows from the assumptions (A1)–(A3) that [22, Thm. 2.4] can be applied. In fact, a closer inspection of the proof of [22, Thm. 2.4] reveals that the following result holds true.

THEOREM 2.1: *Suppose that* (A1)–(A5) *are fulfilled. Then the state system* (1.2)–(1.6) *has for every* $u_\Gamma \in \mathcal{U}_R$ *a unique solution triple* (μ, ρ, ρ_Γ) *such that*

$$\mu \in H^1(0,T;H) \cap C^0([0,T];V) \cap L^2(0,T;W) \cap L^\infty(Q), \tag{2.4}$$
$$\rho \in W^{1,\infty}(0,T;H) \cap H^1(0,T;V) \cap L^\infty(0,T;H^2(\Omega)), \tag{2.5}$$
$$\rho_\Gamma \in W^{1,\infty}(0,T;H_\Gamma) \cap H^1(0,T;V_\Gamma) \cap L^\infty(0,T;H^2(\Gamma)). \tag{2.6}$$

Moreover, there is a constant $K_1^* > 0$, *which depends only on* R *and the data of the system, such that*

$$\begin{aligned} &\|\mu\|_{H^1(0,T;H)\cap C^0([0,T];V)\cap L^2(0,T;W)\cap L^\infty(Q)} + \|\rho\|_{W^{1,\infty}(0,T;H)\cap H^1(0,T;V)\cap L^\infty(0,T;H^2(\Omega))} \\ &+ \|\rho_\Gamma\|_{W^{1,\infty}(0,T;H_\Gamma)\cap H^1(0,T;V_\Gamma)\cap L^\infty(0,T;H^2(\Gamma))} \leq K_1^*, \end{aligned} \tag{2.7}$$

for every solution triple (μ, ρ, ρ_Γ) *corresponding to some* $u_\Gamma \in \mathcal{U}_R$. *In addition, there are constants* r_*, r^*, *which depend only on* R *and the data of the system, such that*

$$-1 < r_* \leq \rho(x,t) \leq r^* < +1 \quad \text{for every } (x,t) \in \overline{Q}, \tag{2.8}$$

for every solution triple (μ, ρ, ρ_Γ) *corresponding to some* $u_\Gamma \in \mathcal{U}_R$.

Remark 2.2: It follows from well-known embedding results (cf. [32, Sect. 8, Cor. 4]) that $(H^1(0,T;V) \cap L^\infty(0,T;H^2(\Omega))) \subset C^0([0,T];H^s(\Omega))$, for $0 < s < 2$. Therefore, $\rho \in C^0(\overline{Q})$, and thus $\rho_\Gamma \in C^0(\overline{\Sigma})$. Moreover, there is a constant $K_2^* > 0$, which again depends only on R and the data, such that

$$\max_{0\le i\le 3}\left(\|f^{(i)}(\rho)\|_{C^0(\overline{Q})} + \|f_\Gamma^{(i)}(\rho_\Gamma)\|_{C^0(\overline{\Sigma})}\right) + \max_{0\le i\le 3}\|g^{(i)}(\rho)\|_{C^0(\overline{Q})}$$
$$+ \max_{0\le i\le 2}\left(\|\pi^{(i)}(\rho)\|_{C^0(\overline{Q})} + \|\pi_\Gamma^{(i)}(\rho_\Gamma)\|_{C^0(\overline{\Sigma})}\right) \le K_2^*\,, \tag{2.9}$$

for every solution triple (μ,ρ,ρ_Γ) corresponding to some $u_\Gamma \in \mathcal{U}_R$. In addition, we have that $1+2g(\rho) \in C^0(\overline{Q})$, where $1 \le 1+2g(\rho) \le 1+2\|g(\rho)\|_{C^0(\overline{Q})}$ on $\overline{Q}$. Hence, rewriting (1.2) as

$$\partial_t\mu - \tfrac{1}{1+2g(\rho)}\,\Delta\mu = z \quad \text{in } Q,$$

where it is easily seen that $z := -(1+2g(\rho))^{-1}\,\mu\,g'(\rho)\,\partial_t\rho \in L^\infty(0,T;H)\cap L^2(0,T;L^6(\Omega))$, we may thus infer from [24, Thm. 2.3] the additional regularity

$$\mu \in W^{1,p}(0,T;H) \cap H^1(0,T;L^6(\Omega)) \cap L^p(0,T;W) \cap L^2(0,T;W^{2,6}(\Omega))$$
$$\text{for every } p \in [1,+\infty). \tag{2.10}$$

Moreover, denoting by

$$\mathcal{X} := H^1(0,T;H_\Gamma) \cap L^\infty(\Sigma) \tag{2.11}$$

the control space for the remainder of this paper, we conclude from Theorem 2.1 that the control-to-state operator $\mathcal{S} : u_\Gamma \mapsto (\mu,\rho,\rho_\Gamma)$, where it is understood that $\rho_\Gamma = \rho_{|\Sigma}$ on Σ, is a well-defined mapping between $\mathcal{U}_R \subset \mathcal{X}$ and the space specified by the regularity properties (2.4)–(2.6).

For later use, we cite a known auxiliary result (cf. [23, Thm. 2.2]).

Lemma 2.3: *Suppose that functions $y_0 \in \mathcal{V}$, $a \in L^\infty(Q)$, $a_\Gamma \in L^\infty(\Sigma)$, $\sigma \in L^2(Q)$ and $\sigma_\Gamma \in L^2(\Sigma)$ are given. Then the linear initial-boundary value problem*

$$\partial_t y - \Delta y + a\,y = \sigma \quad \textit{a. e. in } Q, \tag{2.12}$$
$$\partial_{\mathbf{n}} y + \partial_t y_\Gamma - \Delta_\Gamma y_\Gamma + a_\Gamma\,y_\Gamma = \sigma_\Gamma, \quad y_\Gamma = y_{|\Sigma}, \quad \textit{a. e. on } \Sigma, \tag{2.13}$$
$$y(0) = y_0 \quad \textit{a. e. in } \Omega, \quad y_\Gamma(0) = y_{0|\Gamma} \quad \textit{a. e. on } \Gamma, \tag{2.14}$$

has a unique solution pair satisfying $y \in H^1(0,T;H) \cap C^0([0,T];V) \cap L^2(0,T;H^2(\Omega))$ and $y_\Gamma \in H^1(0,T;H_\Gamma) \cap C^0([0,T];V_\Gamma) \cap L^2(0,T;H^2(\Gamma))$. Moreover, there is a constant $C_L > 0$ such that the following holds true: whenever $y_0 = 0$ and (y,y_Γ) is the corresponding solution to (2.12)–(2.14), *then*

$$\|y\|_{H^1(0,t;H)\cap C^0([0,t];V)\cap L^2(0,t;H^2(\Omega))} + \|y_\Gamma\|_{H^1(0,t;H_\Gamma)\cap C^0([0,t];V_\Gamma)\cap L^2(0,t;H^2(\Gamma))}$$
$$\le C_L\left(\|\sigma\|_{L^2(Q_t)} + \|\sigma_\Gamma\|_{L^2(\Sigma_t)}\right) \quad \forall\, t \in (0,T]\,. \tag{2.15}$$

We are now going to investigate the stability properties of the state system (1.2)–(1.6). We have the following result.

THEOREM 2.4: *Suppose that the assumptions* (A1)–(A5) *are fulfilled, and assume that* $u_{\Gamma_1}, u_{\Gamma_2} \in \mathcal{U}_R$ *are given and that* $(\mu_i, \rho_i, \rho_{i_\Gamma}) = \mathcal{S}(u_{\Gamma_i})$, $i = 1, 2$, *are the corresponding unique solutions to* (1.2)–(1.6). *Then we have for every* $t \in (0, T]$ *the estimate*

$$\begin{aligned} & \|\mu_1 - \mu_2\|_{H^1(0,t;H)\cap C^0([0,t];V)\cap L^2(0,T;W)} + \|\rho_1 - \rho_2\|_{H^1(0,t;H)\cap C^0([0,t];V)\cap L^2(0,t;H^2(\Omega))} \\ & + \|\rho_{1_\Gamma} - \rho_{2_\Gamma}\|_{H^1(0,t;H_\Gamma)\cap C^0([0,t];V_\Gamma)\cap L^2(0,t;H^2(\Gamma))} \le K_3^* \|u_{\Gamma_1} - u_{\Gamma_2}\|_{L^2(\Sigma_t)}, \end{aligned} \tag{2.16}$$

with a constant $K_3^* > 0$ *that depends only on* R *and the data of the system.*

PROOF: Let $t \in (0, T]$ be fixed, and suppose that $u_{\Gamma_1}, u_{\Gamma_2} \in \mathcal{U}_R$ are given and that $(\mu_i, \rho_i, \rho_{i_\Gamma}) = \mathcal{S}(u_{\Gamma_i})$, $i = 1, 2$, are the corresponding unique solutions to (1.2)–(1.6) having the regularity properties (2.4)–(2.6) and (2.10). Observe that then the global bounds (2.7) and (2.9) hold true for both solutions. In the following, we will make repeated use of these bounds without further reference. We will also denote by $C > 0$ constants that depend only on the data, on $\|u_{\Gamma_i}\|_{\mathcal{X}}$, and on the norms of $(\mu_i, \rho_i, \rho_{i_\Gamma})$ in the spaces specified in (2.4)–(2.6) and (2.10). Now put

$$\begin{aligned} & \mu := \mu_1 - \mu_2, \quad \rho := \rho_1 - \rho_2, \quad \rho_\Gamma := \rho_{1_\Gamma} - \rho_{2_\Gamma}, \quad u_\Gamma := u_{\Gamma_1} - u_{\Gamma_2}, \\ & \psi := f' + \pi, \quad \psi_\Gamma := f'_\Gamma + \pi_\Gamma. \end{aligned}$$

Then the following system is satisfied:

$$\begin{aligned} & (1 + 2g(\rho_1))\,\partial_t\mu + g'(\rho_1)\,\partial_t\rho_1\,\mu - \Delta\mu + 2(g(\rho_1) - g(\rho_2))\,\partial_t\mu_2 \\ & \quad + \mu_2(g'(\rho_1) - g'(\rho_2))\,\partial_t\rho_1 + \mu_2\,g'(\rho_2)\,\partial_t\rho = 0 \quad \text{a.e. in } Q, \end{aligned} \tag{2.17}$$

$$\partial_{\mathbf{n}}\mu = 0 \quad \text{a.e. on } \Sigma, \quad \mu(0) = 0 \quad \text{a.e. in } \Omega, \tag{2.18}$$

$$\partial_t\rho - \Delta\rho = \psi(\rho_2) - \psi(\rho_1) + \mu\,g'(\rho_1) + \mu_2\,(g'(\rho_1) - g'(\rho_2)) \quad \text{a.e. in } Q, \tag{2.19}$$

$$\partial_{\mathbf{n}}\rho + \partial_t\rho_\Gamma - \Delta_\Gamma\rho_\Gamma = \psi_\Gamma(\rho_{2_\Gamma}) - \psi_\Gamma(\rho_{1_\Gamma}) + u_\Gamma, \quad \rho_\Gamma = \rho_{|\Sigma}, \quad \text{a.e. on } \Sigma, \tag{2.20}$$

$$\rho(0) = 0 \quad \text{a.e. in } \Omega, \quad \rho_\Gamma(0) = 0 \quad \text{a.e. on } \Sigma. \tag{2.21}$$

We will now prove a series of estimates in order to establish the validity of (2.16). At first, we observe that

$$\max_{0\le i\le 2} \left|g^{(i)}(\rho_1) - g^{(i)}(\rho_2)\right| + \max_{0\le i\le 1} \left|\psi^{(i)}(\rho_1) - \psi^{(i)}(\rho_2)\right| \le C\,|\rho| \quad \text{a.e. in } Q, \tag{2.22}$$

$$\max_{0\le i\le 1} \left|\psi_\Gamma^{(i)}(\rho_{1_\Gamma}) - \psi_\Gamma^{(i)}(\rho_{2_\Gamma})\right| \le C\,|\rho_\Gamma| \quad \text{a.e. on } \Sigma. \tag{2.23}$$

The first estimate can be inferred from the stability result of [22, Thm. 2.4], namely that

$$\begin{aligned} & \|\mu\|_{L^\infty(0,t;H)\cap L^2(0,t;V)} + \|\rho\|_{H^1(0,T;H)\cap C^0([0,t];V)\cap L^2(0,t;H^2(\Omega))} \\ & + \|\rho_\Gamma\|_{H^1(0,t;H_\Gamma)\cap C^0([0,t];V_\Gamma)\cap L^2(0,t;H^2(\Gamma))} \le C\,\|u_\Gamma\|_{L^2(0,t;H_\Gamma)}. \end{aligned} \tag{2.24}$$

Next, we add μ to both sides of (2.17), then multiply by $\partial_t\mu$ and integrate over Q_t to obtain that

$$\int_0^t\!\!\int_\Omega |\partial_t\mu|^2\,\mathrm{d}x\,\mathrm{d}s + \frac{1}{2}\,\|\mu(t)\|_V^2 \le I_1 + I_2 + I_3 + I_4, \tag{2.25}$$

where the quantities I_j, $1 \le j \le 4$, will be specified and estimated below. At first, we employ the continuity of the embeddings $V \subset L^4(\Omega) \subset L^2(\Omega)$, as well as Hölder's and Young's inequalities, to conclude that

$$\begin{aligned} I_1 :&= \int_0^t\!\!\int_\Omega \bigl(1 - g'(\rho_1)\,\partial_t\rho_1\bigr)\,\mu\,\partial_t\mu \,\mathrm{d}x\,\mathrm{d}s \\ &\le C \int_0^t \bigl(1 + \|\partial_t\rho_1(s)\|_4\bigr)\,\|\mu(s)\|_4\,\|\partial_t\mu(s)\|_2 \,\mathrm{d}s \\ &\le \frac{1}{6}\int_0^t\!\!\int_\Omega |\partial_t\mu|^2 \,\mathrm{d}x\,\mathrm{d}s \,+\, C\int_0^t \bigl(1 + \|\partial_t\rho_1(s)\|_V^2\bigr)\,\|\mu(s)\|_V^2 \,\mathrm{d}s\,. \end{aligned} \tag{2.26}$$

Similarly, by also using (2.22) and (2.24), we have that

$$\begin{aligned} I_3 :&= -\int_0^t\!\!\int_\Omega \mu_2\,(g'(\rho_1) - g'(\rho_2))\,\partial_t\rho_1\,\partial_t\mu \,\mathrm{d}x\,\mathrm{d}s \,\le\, C\int_0^t \|\partial_t\rho_1(s)\|_4\,\|\rho(s)\|_4\,\|\partial_t\mu(s)\|_2 \,\mathrm{d}s \\ &\le \frac{1}{6}\int_0^t\!\!\int_\Omega |\partial_t\mu|^2 \,\mathrm{d}x\,\mathrm{d}s \,+\, C \max_{0\le s\le t} \|\rho(s)\|_V^2 \int_0^t \|\partial_t\rho_1(s)\|_V^2 \,\mathrm{d}s \\ &\le \frac{1}{6}\int_0^t\!\!\int_\Omega |\partial_t\mu|^2 \,\mathrm{d}x\,\mathrm{d}s \,+\, C\int_0^t\!\!\int_\Gamma |\,u_\Gamma|^2 \,\mathrm{d}\Gamma\,\mathrm{d}s\,. \end{aligned} \tag{2.27}$$

Moreover, thanks to (2.24) and Young's inequality, we see that

$$\begin{aligned} I_4 :&= -\int_0^t\!\!\int_\Omega \mu_2\,g'(\rho_2)\,\partial_t\rho\,\partial_t\mu \,\mathrm{d}x\,\mathrm{d}s \,\le\, \frac{1}{6}\int_0^t\!\!\int_\Omega |\partial_t\mu|^2 \,\mathrm{d}x\,\mathrm{d}s \,+\, C\int_0^t\!\!\int_\Omega |\partial_t\rho|^2 \,\mathrm{d}x\,\mathrm{d}s \\ &\le \frac{1}{6}\int_0^t\!\!\int_\Omega |\partial_t\mu|^2 \,\mathrm{d}x\,\mathrm{d}s \,+\, C\,\|\,u_\Gamma\|_{L^2(0,t;H_\Gamma)}^2\,. \end{aligned} \tag{2.28}$$

Finally, we use (2.10), (2.22), (2.24), and Hölder's inequality to conclude that

$$\begin{aligned} I_2 :&= -2\int_0^t\!\!\int_\Omega (g(\rho_1) - g(\rho_2))\,\partial_t\mu_2\,\partial_t\mu \,\mathrm{d}x\,\mathrm{d}s \,\le\, C\int_0^t \|\partial_t\mu_2(s)\|_6\,\|\partial_t\mu(s)\|_2\,\|\rho(s)\|_3 \,\mathrm{d}s \\ &\le \frac{1}{6}\int_0^t\!\!\int_\Omega |\partial_t\mu|^2 \,\mathrm{d}x\,\mathrm{d}s \,+\, C\int_0^t \|\partial_t\mu_2(s)\|_6^2\,\|\rho(s)\|_V^2 \,\mathrm{d}s \\ &\le \frac{1}{6}\int_0^t\!\!\int_\Omega |\partial_t\mu|^2 \,\mathrm{d}x\,\mathrm{d}s \,+\, C \max_{0\le s\le t} \|\rho(s)\|_V^2 \int_0^t \|\partial_t\mu_2(s)\|_6^2 \,\mathrm{d}s \\ &\le \frac{1}{6}\int_0^t\!\!\int_\Omega |\partial_t\mu|^2 \,\mathrm{d}x\,\mathrm{d}s \,+\, C\,\|\,u_\Gamma\|_{L^2(0,t;H_\Gamma)}^2\,. \end{aligned} \tag{2.29}$$

Thus, combining (2.25) with (2.26)–(2.29), we have shown the estimate

$$\begin{aligned} &\frac{1}{3}\int_0^t\!\!\int_\Omega |\partial_t\mu|^2 \,\mathrm{d}x\,\mathrm{d}s \,+\, \frac{1}{2}\,\|\mu(t)\|_V^2 \\ &\le C\,\|\,u_\Gamma\|_{L^2(0,t;L^2(\Gamma))}^2 \,+\, C\int_0^t \bigl(1 + \|\partial_t\rho_1(s)\|_V^2\bigr)\,\|\mu(s)\|_V^2 \,\mathrm{d}s\,, \end{aligned} \tag{2.30}$$

where the mapping $s \mapsto \|\partial_t\rho_1(s)\|_V^2$ is known to belong to $L^1(0,T)$. We may therefore employ Gronwall's lemma to infer that

$$\|\mu\|_{H^1(0,t;H)\cap L^\infty(0,t;V)} \,\le\, C\,\|\,u_\Gamma\|_{L^2(0,t;H_\Gamma)}\,. \tag{2.31}$$

It then easily follows by comparison in (2.17) that also

$$\begin{aligned}\|\Delta\mu\|_{L^2(0,t;H)} &\le C\big(\|\partial_t\mu\|_{L^2(0,t;H)} + \|\mu\|_{L^\infty(0,t;V)} + \|\rho\|_{L^\infty(0,t;V)} + \|\partial_t\rho\|_{L^2(0,t;H)}\big)\\ &\le C\,\|\,u_\Gamma\|_{L^2(0,t;H_\Gamma)}\,, \end{aligned}\tag{2.32}$$

whence, by virtue of standard elliptic estimates,

$$\|\mu\|_{L^2(0,t;W)} \;\le\; C\,\|\,u_\Gamma\|_{L^2(0,t;H_\Gamma)}\,. \tag{2.33}$$

This concludes the proof of the assertion. $\square$

3 Fréchet differentiability of the control-to-state operator

In this section, we establish a differentiability result for the control-to-state operator $\mathcal{S}$. To this end, we fix some $\bar u_\Gamma \in \mathcal{U}_R$ and set $(\bar\mu,\bar\rho,\bar\rho_\Gamma) = \mathcal{S}(\bar u_\Gamma)$, which implies that $(\bar\mu,\bar\rho,\bar\rho_\Gamma)$ satisfies (2.7), (2.9), (2.10), and $\bar\rho_\Gamma = \bar\rho_{|\Sigma}$ a. e. on Σ. We then consider for a fixed perturbation $h\in\mathcal{X}$ (see (2.11)) the linearized system

$$\begin{aligned}&(1+2g(\bar\rho))\,\partial_t\eta \,+\, g'(\bar\rho)\partial_t\bar\rho\,\eta \,-\, \Delta\eta\\ &\quad=\, -\,2g'(\bar\rho)\,\partial_t\bar\mu\,\zeta \,-\, \bar\mu\, g''(\bar\rho)\,\partial_t\bar\rho\,\zeta \,-\, \bar\mu\, g'(\bar\rho)\,\partial_t\zeta \quad \text{a.e. in } Q, \end{aligned}\tag{3.1}$$

$$\partial_{\mathbf{n}}\eta \,=\, 0 \quad \text{a.e. on } \Sigma, \quad \eta(0)=0 \quad \text{a.e. in } \Omega, \tag{3.2}$$

$$\partial_t\zeta - \Delta\zeta + (f''(\bar\rho) + \pi'(\bar\rho) - \bar\mu\, g''(\bar\rho))\,\zeta \,=\, g'(\bar\rho)\,\eta \quad \text{a.e. in } Q, \tag{3.3}$$

$$\partial_{\mathbf{n}}\zeta + \partial_t\zeta_\Gamma - \Delta_\Gamma\zeta_\Gamma + (f_\Gamma''(\bar\rho_\Gamma) + \pi_\Gamma'(\bar\rho_\Gamma))\,\zeta_\Gamma = h, \quad \zeta_\Gamma = \zeta_{|\Sigma}, \quad \text{a.e. on } \Sigma, \tag{3.4}$$

$$\zeta(0)=0 \quad \text{a.e. in } \Omega, \quad \zeta_\Gamma(0)=0 \quad \text{a.e. on } \Gamma. \tag{3.5}$$

Provided that the system (3.1)–(3.5) has for every $h\in\mathcal{X}$ a unique solution triple $(\eta,\zeta,\zeta_\Gamma)$, we expect that the Fréchet derivative $D\mathcal{S}(\bar u_\Gamma)$ of $\mathcal{S}$ at $\bar u_\Gamma$ (if it exists) ought to be given by $D\mathcal{S}(\bar u_\Gamma)(h) = (\eta,\zeta,\zeta_\Gamma)$. In the following existence and uniqueness result, we show that the linearized problem is even solvable if only $h\in L^2(\Sigma)$.

Theorem 3.1: *Suppose that* (A1)–(A6) *are satisfied. Then the system* (3.1)–(3.5) *has for every $h\in L^2(\Sigma)$ a unique solution $(\eta,\zeta,\zeta_\Gamma)$ such that*

$$\eta \in H^1(0,T;H)\cap C^0([0,T];V)\cap L^2(0,T;W), \tag{3.6}$$

$$\zeta \in H^1(0,T;H)\cap C^0([0,T];V)\cap L^2(0,T;H^2(\Omega)), \tag{3.7}$$

$$\zeta_\Gamma \in H^1(0,T;H_\Gamma)\cap C^0([0,T];V_\Gamma)\cap L^2(0,T;H^2(\Gamma)). \tag{3.8}$$

Moreover, the linear mapping $h\mapsto(\eta,\zeta,\zeta_\Gamma)$ is continuous as a mapping from $L^2(\Sigma)$ into the Banach space

$$\begin{aligned}\mathcal{Z} := \big\{&(\mu,\rho,\rho_\Gamma)\in (H^1(0,T;H)\cap L^2(0,T;W))\times(H^1(0,T;H)\cap L^2(0,T;H^2(\Omega)))\\ &\times (H^1(0,T;H_\Gamma)\cap L^2(0,T;H^2(\Gamma)))\,:\ \rho_{|\Sigma} = \rho_\Gamma \ \text{ a.e. on } \Sigma\big\}\,.\end{aligned}$$

Proof: We use an approximation scheme based on a retarded argument method. To this end, we define for every $\tau \in (0,T)$ the translation operator $\mathcal{T}_\tau : C^0([0,T];H) \to C^0([0,T];H)$ by setting, for all $v \in C^0([0,T];H)$,

$$\mathcal{T}_\tau(v)(t) := v(t-\tau) \quad \text{if } t > \tau \quad \text{and } \mathcal{T}_\tau(v)(t) := v(0) \quad \text{if } t \le \tau. \tag{3.9}$$

Notice that for every $v \in H^1(0,T;H)$ it holds that

$$\|\mathcal{T}_\tau(v)\|^2_{L^2(Q_t)} \le \begin{cases} \|v\|^2_{L^2(Q_t)} + \tau\,\|v(0)\|^2_H & \text{for all } t \in [\tau,T], \\ t\,\|v(0)\|^2_H & \text{for all } t \in [0,\tau], \end{cases} \tag{3.10}$$

$$\|\partial_t\mathcal{T}_\tau(v)\|^2_{L^2(Q_t)} \le \|\partial_t v\|^2_{L^2(Q_t)} \quad \text{for a.e. } t \in (0,T), \tag{3.11}$$

while for every $v \in C^0([0,T];V)$ we have

$$\|\nabla\mathcal{T}_\tau(v)\|^2_{L^2(Q_t)} \le \begin{cases} \|\nabla v\|^2_{L^2(Q_t)} + \tau\,\|\nabla v(0)\|^2_H & \text{for all } t \in [\tau,T], \\ t\,\|\nabla v(0)\|^2_H & \text{for all } t \in [0,\tau]. \end{cases} \tag{3.12}$$

Now, let $N \in \mathbb{N}$ be fixed, $\tau_N := T/N$, as well as $t_n := n\tau_N$ and $I_n := (0,t_n)$, for $0 \le n \le N$. We then consider for every $n \in \{1,\dots,N\}$ the initial-boundary value problem

$$(1+2g(\bar\rho))\,\partial_t\eta_n - \Delta\eta_n = -\mathcal{T}_{\tau_N}(\eta_{n-1})\,g'(\bar\rho)\partial_t\bar\rho - 2g'(\bar\rho)\,\partial_t\bar\mu\,\zeta_n$$
$$- \bar\mu\,g''(\bar\rho)\,\partial_t\bar\rho\,\zeta_n - \bar\mu\,g'(\bar\rho)\,\partial_t\zeta_n \quad \text{a.e. in } \Omega\times I_n, \tag{3.13}$$

$$\partial_{\mathbf{n}}\eta_n = 0 \quad \text{a.e. on } \Gamma\times I_n, \quad \eta_n(0) = 0 \quad \text{a.e. in } \Omega, \tag{3.14}$$

$$\partial_t\zeta_n - \Delta\zeta_n + (f''(\bar\rho) + \pi'(\bar\rho) - \bar\mu\,g''(\bar\rho))\,\zeta_n = g'(\bar\rho)\,\mathcal{T}_{\tau_N}(\eta_{n-1}) \quad \text{a.e. in } \Omega\times I_n, \tag{3.15}$$

$$\partial_{\mathbf{n}}\zeta_n + \partial_t\zeta_{n_\Gamma} - \Delta_\Gamma\zeta_{n_\Gamma} + (f''_\Gamma(\bar\rho_\Gamma) + \pi'_\Gamma(\bar\rho_\Gamma))\,\zeta_{n_\Gamma} = h, \quad \zeta_{n_\Gamma} = \zeta_{n|\Gamma\times I_n}, \quad \text{a.e. on } \Gamma\times I_n, \tag{3.16}$$

$$\zeta_n(0) = 0 \quad \text{a.e. in } \Omega, \quad \zeta_{n_\Gamma}(0) = 0 \quad \text{a.e. on } \Gamma. \tag{3.17}$$

Here, we notice that the operator $\mathcal{T}_{\tau_N}$ acts on functions that are not defined on the whole of $\Omega\times(0,T)$; however, its meaning is still given by (3.9) if $n > 1$, while for $n = 1$ we simply set $\mathcal{T}_{\tau_N}(\eta_{n-1}) = 0$.

The plan of the upcoming proof is as follows: in the first step, we show that the above initial-boundary value problems have unique solutions $(\eta_n, \zeta_n, \zeta_{n_\Gamma})$ for $n = 1,\dots,N$ with the regularity as in (3.6)–(3.8). Once this will be shown, we can infer from the uniqueness that

$$\eta_{N|\Omega\times I_{N-1}} = \eta_{N-1}, \quad \zeta_{N|\Omega\times I_{N-1}} = \zeta_{N-1},$$

which then entails that, for almost every $(x,t) \in Q$,

$$\mathcal{T}_{\tau_N}(\eta_{N-1})(x,t) = \eta_{N-1}(x,t-\tau_N) = \eta_N(x,t-\tau_N) = \mathcal{T}_{\tau_N}(\eta_N)(x,t).$$

It then follows that $(\eta^\tau, \zeta^\tau, \zeta^\tau_\Gamma) := (\eta_N, \zeta_N, \zeta_{N_\Gamma})$ is for $\tau = \tau_N$ the unique solution to the retarded initial-boundary value problem

$$\begin{aligned}
&(1+2g(\bar\rho))\,\partial_t\eta^\tau \;+\; \mathcal{T}_\tau(\eta^\tau)\,g'(\bar\rho)\partial_t\bar\rho \;-\; \Delta\eta^\tau \\
&\quad =\; -\,2g'(\bar\rho)\,\partial_t\bar\mu\,\zeta^\tau \;-\; \bar\mu\,g''(\bar\rho)\,\partial_t\bar\rho\,\zeta^\tau \;-\; \bar\mu\,g'(\bar\rho)\,\partial_t\zeta^\tau \quad \text{a.e. in } Q, && (3.18)\\
&\partial_{\mathbf n}\eta^\tau \;=\; 0 \quad \text{a.e. on } \Sigma, \quad \eta^\tau(0)=0 \quad \text{a.e. in } \Omega, && (3.19)\\
&\partial_t\zeta^\tau - \Delta\zeta^\tau + (f''(\bar\rho)+\pi'(\bar\rho)-\bar\mu\,g''(\bar\rho))\,\zeta^\tau \;=\; g'(\bar\rho)\,\mathcal{T}_{\tau_N}(\eta^\tau) \quad \text{a.e. in } Q, && (3.20)\\
&\partial_{\mathbf n}\zeta^\tau + \partial_t\zeta^\tau_\Gamma - \Delta_\Gamma\zeta^\tau_\Gamma + (f''_\Gamma(\bar\rho_\Gamma)+\pi'_\Gamma(\bar\rho_\Gamma))\,\zeta^\tau_\Gamma = h, \quad \zeta^\tau_\Gamma = \zeta^\tau_{|\Sigma}, \quad \text{a.e. on } \Sigma, && (3.21)\\
&\zeta^\tau(0)=0 \quad \text{a.e. in } \Omega, \quad \zeta^\tau_\Gamma(0)=0 \quad \text{a.e. on } \Gamma. && (3.22)
\end{aligned}$$

Once the unique solvability of (3.18)–(3.22) will be shown for $\tau=\tau_N$, $N\in\mathbb N$, in the second step of this proof we will establish sufficiently strong a priori estimates, which are uniform with respect to $N\in\mathbb N$, and then pass to the limit as $N\to\infty$ by compactness arguments to show the existence of a solution $(\eta,\zeta,\zeta_\Gamma)$ having the required regularity properties. As a byproduct of our estimates, we will obtain the uniqueness of the solution and the continuity of the mapping $h\mapsto(\eta,\zeta,\zeta_\Gamma)$.

Pursuing our plan, we first establish the unique solvability of (3.13)–(3.17) for every $n\in\{1,\dots,N\}$. To this end, we argue by induction. Since the proof for $n=1$ is similar to that used in the induction step $n-1\longrightarrow n$, we may confine ourselves to just perform the latter.

So let $1<n\le N$, and assume that for $1\le k\le n-1$ unique solutions $(\eta_k,\zeta_k,\zeta_{k_\Gamma})$ to the system (3.13)–(3.17) have already been constructed that satisfy for $1\le k\le n-1$ the conditions

$$\begin{aligned}
&\eta_k \in H^1(I_k;H)\cap C^0(\bar I_k;V)\cap L^2(I_k;W),\\
&\zeta_k \in H^1(I_k;H)\cap C^0(\bar I_k;V)\cap L^2(I_k;H^2(\Omega)),\\
&\zeta_{k_\Gamma} \in H^1(I_k;H_\Gamma)\cap C^0(\bar I_k;V_\Gamma)\cap L^2(I_k;H^2(\Gamma)). && (3.23)
\end{aligned}$$

First, we apply Lemma 2.3 to infer that the initial-boundary value problem (3.15)–(3.17) has a unique solution pair with $\zeta_n\in H^1(I_n;H)\cap C^0(\bar I_n;V)\cap L^2(I_n;H^2(\Omega))$ and $\zeta_{n_\Gamma}\in H^1(I_n;H_\Gamma)\cap C^0(\bar I_n;V_\Gamma)\cap L^2(I_n;H^2(\Gamma))$. We then insert ζ_n in (3.13). Obviously, we can rewrite the resulting identity in the form

$$\partial_t\eta_n \;-\; \tfrac{1}{1+2g(\bar\rho)}\,\Delta\eta_n \;=\; z, \tag{3.24}$$

where $1+2g(\bar\rho)\in C^0(\overline Q)$, and where, owing to (2.4), (2.5), and (2.10), the right-hand side z is easily seen to belong to $L^2(\Omega\times(0,I_n))$. It thus follows from maximal parabolic regularity theory (see, e. g., [24, Thm. 2.1]) that the initial-boundary value problem (3.13)–(3.14) enjoys a unique solution $\eta_n\in H^1(I_n;H)\cap C^0(\bar I_n;V)\cap L^2(I_n;W)$.

Now that the unique solvability of the retarded problem (3.18)–(3.22) with the requested regularity is shown for every $\tau_N=T/N$, $N\in\mathbb N$, we aim to derive a number of a priori estimates that are uniform in $N\in\mathbb N$. In this process, we denote by $C>0$ constants that may depend on the data of the state system but not on $N\in\mathbb N$. For the sake of a better readability, we will suppress the superscript τ or τ_N during the estimations, writing it only at the very end of each step. We also make repeated use of the global estimates (2.7), (2.9) and of (2.10) without further reference.

<u>FIRST ESTIMATE:</u>

We add $\eta\, g'(\bar\rho)\,\partial_t\bar\rho$ to both sides of (3.18) and observe that we have $\partial_t((\frac12 + g(\bar\rho))\,\eta^2) = (1+2g(\bar\rho))\,\eta\,\partial_t\eta \,+\, g'(\bar\rho)\,\partial_t\bar\rho\,\eta^2$. Therefore, multiplying by η and integrating over Q_t, where $0<t\le T$, and recalling that g is nonnegative, we find that

$$\frac12\int_\Omega |\eta(t)|^2\,\mathrm{d}x \,+\, \int_0^t\!\!\int_\Omega |\nabla\eta|^2\,\mathrm{d}x\,\mathrm{d}s \,\le\, \sum_{j=1}^3 I_j\,, \tag{3.25}$$

where the expressions I_j, $1\le j\le 3$, will be specified end estimated below. At first, employing Hölder's inequality, (3.10), (3.12), and the continuity of the embedding $V\subset L^4(\Omega)$, we obtain from Young's inequality that

$$\begin{aligned} I_1 : &= \int_0^t\!\!\int_\Omega g'(\bar\rho)\,\partial_t\bar\rho\,(\eta - \mathcal{T}_{\tau_N}(\eta))\,\eta\,\mathrm{d}x\,\mathrm{d}s \\ &\le C\int_0^t \|\partial_t\bar\rho(s)\|_4\,(\|\eta(s)\|_4 + \|\mathcal{T}_{\tau_N}(\eta(s))\|_4)\,\|\eta(s)\|_2\,\mathrm{d}s \\ &\le \frac14\int_0^t \|\eta(s)\|_V^2\,\mathrm{d}s \,+\, C\int_0^t \|\partial_t\bar\rho(s)\|_V^2\,\|\eta(s)\|_H^2\,\mathrm{d}s\,. \end{aligned} \tag{3.26}$$

By the same token, we have that

$$\begin{aligned} I_2 : &= -\int_0^t\!\!\int_\Omega (2g'(\bar\rho)\,\partial_t\bar\mu \,+\, \bar\mu\, g''(\bar\rho)\,\partial_t\bar\rho)\,\zeta\,\eta\,\mathrm{d}x\,\mathrm{d}s \\ &\le C\int_0^t (\|\partial_t\bar\mu(s)\|_6 + \|\partial_t\bar\rho(s)\|_6)\,\|\zeta(s)\|_2\,\|\eta(s)\|_3\,\mathrm{d}s \\ &\le \frac14\int_0^t \|\eta(s)\|_V^2\,\mathrm{d}s \,+\, C\int_0^t \big(\|\partial_t\bar\mu(s)\|_6^2 + \|\partial_t\bar\rho(s)\|_V^2\big)\,\|\zeta(s)\|_H^2\,\mathrm{d}s\,. \end{aligned} \tag{3.27}$$

Moreover, from Young's inequality it follows that

$$I_3 := -\int_0^t\!\!\int_\Omega \bar\mu\, g'(\bar\rho)\,\partial_t\zeta\,\eta\,\mathrm{d}x\,\mathrm{d}s \,\le\, \frac14\int_0^t\!\!\int_\Omega |\partial_t\zeta|^2\,\mathrm{d}x\,\mathrm{d}s \,+\, C\int_0^t\!\!\int_\Omega |\eta|^2\,\mathrm{d}x\,\mathrm{d}s\,. \tag{3.28}$$

Hence, combining the estimates (3.25)–(3.28), we have shown that

$$\begin{aligned} \|\eta(t)\|_H^2 \,+\, \int_0^t \|\eta(s)\|_V^2\,\mathrm{d}s \,\le\, &\frac12\int_0^t\!\!\int_\Omega |\partial_t\zeta|^2\,\mathrm{d}x\,\mathrm{d}s \,+\, C\int_0^t \big(1 + \|\partial_t\bar\rho(s)\|_V^2\big)\,\|\eta(s)\|_H^2\,\mathrm{d}s \\ &+ C\int_0^t \big(\|\partial_t\bar\mu(s)\|_6^2 + \|\partial_t\bar\rho(s)\|_V^2\big)\,\|\zeta(s)\|_H^2\,\mathrm{d}s\,, \end{aligned} \tag{3.29}$$

where the mappings $s\mapsto \|\partial_t\bar\rho(s)\|_V^2$ and $s\mapsto\|\partial_t\bar\mu(s)\|_6^2$ are known to belong to $L^1(0,T)$.

Next, we observe that Lemma 2.3 can be applied to the system (3.20)–(3.22), with $a := f''(\bar\rho) + \pi'(\bar\rho) - \bar\mu\, g''(\bar\rho) \in L^\infty(Q)$, $a_\Gamma := f_\Gamma''(\bar\rho_\Gamma) + \pi_\Gamma'(\bar\rho_\Gamma)\in L^\infty(\Sigma)$, $\sigma := g'(\bar\rho)\,\mathcal{T}_{\tau_N}(\eta)$, and $\sigma_\Gamma := h$. We then obtain from (2.15) the estimate

$$\begin{aligned} &\|\zeta\|^2_{H^1(0,t;H)\cap C^0([0,t];V)\cap L^2(0,t;H^2(\Omega))} \,+\, \|\zeta_\Gamma\|^2_{H^1(0,t;H_\Gamma)\cap C^0([0,t];V_\Gamma)\cap L^2(0,t;H^2(\Gamma))} \\ &\le C\int_0^t \|\eta(s)\|_H^2\,\mathrm{d}s \,+\, C\int_0^t\!\!\int_\Gamma |h|^2\,\mathrm{d}\Gamma\,\mathrm{d}s\,. \end{aligned} \tag{3.30}$$

Combining this with (3.29), and invoking Gronwall's lemma, we have thus shown that, for every $t \in (0,T]$ and $N \in \mathbb{N}$,

$$\begin{aligned}
&\|\eta^{\tau_N}\|^2_{L^\infty(0,t;H)\cap L^2(0,t;V)} + \|\zeta^{\tau_N}\|^2_{H^1(0,t;H)\cap C^0([0,t];V)\cap L^2(0,t;H^2(\Omega))} \\
&\quad + \|\zeta_\Gamma^{\tau_N}\|^2_{H^1(0,t;H_\Gamma)\cap C^0([0,t];V_\Gamma)\cap L^2(0,t;H^2(\Gamma))} \le C\,\|h\|^2_{L^2(0,t;H_\Gamma)}\,.
\end{aligned} \tag{3.31}$$

<u>SECOND ESTIMATE:</u>

We now multiply (3.18) by $\partial_t\eta$ and integrate over Q_t, where $0 < t \le T$. Since g is nonnegative, we obtain

$$\int_0^t\!\!\int_\Omega |\partial_t\eta|^2\,\mathrm{d}x\,\mathrm{d}s + \frac{1}{2}\,\|\nabla\eta(t)\|^2_H \le \sum_{j=1}^4 J_j, \tag{3.32}$$

where the expressions J_j, $1 \le j \le 4$, will be specified and estimated below. At first, we invoke Hölder's and Young's inequalities to obtain that

$$\begin{aligned}
J_1 := -\int_0^t\!\!\int_\Omega g'(\bar\rho)\,\partial_t\bar\rho\,\mathcal{T}_{\tau_N}(\eta)\,\partial_t\eta\,\mathrm{d}x\,\mathrm{d}s &\le C\int_0^t \|\partial_t\bar\rho(s)\|_4\,\|\mathcal{T}_{\tau_N}(\eta(s))\|_4\,\|\partial_t\eta(s)\|_2\,\mathrm{d}x\,\mathrm{d}s \\
&\le \frac{1}{5}\int_0^t\!\!\int_\Omega |\partial_t\eta|^2\,\mathrm{d}x\,\mathrm{d}s + C\int_0^t \|\partial_t\bar\rho(s)\|_V^2\,\|\mathcal{T}_{\tau_N}(\eta(s))\|_V^2\,\mathrm{d}s\,,
\end{aligned} \tag{3.33}$$

where the second integral on the right-hand side, which we denote by $I(t)$, can be estimated as follows: by the definition of $\mathcal{T}_{\tau_N}$, and since $\eta(0) = 0$, we obviously have that $I(t) = 0$ if $0 \le t \le \tau_N$, while for $\tau_N < t \le T$ it holds that

$$I(t) = \int_{\tau_N}^t \|\partial_t\bar\rho(s)\|_V^2\,\|\eta(s-\tau_N)\|_V^2\,\mathrm{d}s = \int_0^{t-\tau_N} \|\partial_t\bar\rho(s+\tau_N)\|_V^2\,\|\eta(s)\|_V^2\,\mathrm{d}s\,. \tag{3.34}$$

Hence, it is clear that

$$I(t) = \int_0^t \varphi(s,t)\,\|\eta(s)\|_V^2\,\mathrm{d}s \quad \text{for every } t \in [0,T]$$

where the function $\varphi : [0,T]^2 \to \mathbb{R}$ is defined (almost everywhere with respect to s) by

$$\varphi(s,t) := \begin{cases} 0 & \text{if } t \le \tau_N \text{ and } s \in [0,T] \\ \|\partial_t\bar\rho(s+\tau_N)\|_V^2 & \text{if } t > \tau_N \text{ and } 0 \le s \le t-\tau_N \\ 0 & \text{if } t > \tau_N \text{ and } t-\tau_N < s \le T. \end{cases}$$

On the other hand, it holds that $\varphi(s,t) \le \overline{\varphi}(s)$ for every $(s,t) \in [0,T]^2$ where

$$\overline{\varphi}(s) := \begin{cases} \|\partial_t\bar\rho(s+\tau_N)\|_V^2 & \text{if } 0 \le s \le T-\tau_N \\ 0 & \text{if } T-\tau_N < s \le T. \end{cases}$$

Thus, we also have

$$I(t) \le \int_0^t \overline{\varphi}(s)\,\|\eta(s)\|_V^2\,\mathrm{d}s \quad \text{for every } t \in [0,T] \tag{3.35}$$

and $\overline{\varphi}$ is obviously bounded in $L^1(0,T)$, uniformly in $N \in \mathbb{N}$.

Next, owing to Hölder's and Young's inequalities, and invoking (3.31), we find that

$$\begin{aligned} J_2 :&= -2 \int_0^t\!\!\int_\Omega g'(\bar\rho)\,\partial_t\bar\mu\,\zeta\,\partial_t\eta \,\mathrm{d}x\,\mathrm{d}s \,\le\, C \int_0^t \|\partial_t\bar\mu(s)\|_6\,\|\zeta(s)\|_3\,\|\partial_t\eta(s)\|_2\,\mathrm{d}s \\ &\le \frac15 \int_0^t\!\!\int_\Omega |\partial_t\eta|^2\,\mathrm{d}x\,\mathrm{d}s \,+\, C \max_{0\le s\le t} \|\zeta(s)\|_V^2 \int_0^t \|\partial_t\bar\mu(s)\|_6^2\,\mathrm{d}s \\ &\le \frac15 \int_0^t\!\!\int_\Omega |\partial_t\eta|^2\,\mathrm{d}x\,\mathrm{d}s \,+\, C\,\|h\|^2_{L^2(0,t;H_\Gamma)}\,, \end{aligned} \tag{3.36}$$

as well as

$$\begin{aligned} J_3 :&= -\int_0^t\!\!\int_\Omega \bar\mu\, g''(\bar\rho)\,\partial_t\bar\rho\,\zeta\,\partial_t\eta\,\mathrm{d}x\,\mathrm{d}s \,\le\, C\int_0^t \|\partial_t\bar\rho(s)\|_6\,\|\zeta(s)\|_3\,\|\partial_t\eta(s)\|_2\,\mathrm{d}s \\ &\le \frac15 \int_0^t\!\!\int_\Omega |\partial_t\eta|^2\,\mathrm{d}x\,\mathrm{d}s \,+\, C\,\|h\|^2_{L^2(0,t;H_\Gamma)}\,. \end{aligned} \tag{3.37}$$

Finally, owing to (3.31) once more, we obtain that

$$\begin{aligned} J_4 :&= -\int_0^t\!\!\int_\Omega \bar\mu\, g'(\bar\rho)\,\partial_t\zeta\,\partial_t\eta\,\mathrm{d}x\,\mathrm{d}s \,\le\, \frac15\int_0^t\!\!\int_\Omega |\partial_t\eta|^2\,\mathrm{d}x\,\mathrm{d}s \,+\, C\int_0^t\!\!\int_\Omega |\partial_t\zeta|^2\,\mathrm{d}x\,\mathrm{d}s \\ &\le \frac15 \int_0^t\!\!\int_\Omega |\partial_t\eta|^2\,\mathrm{d}x\,\mathrm{d}s \,+\, C\,\|h\|^2_{L^2(0,t;H_\Gamma)}\,. \end{aligned} \tag{3.38}$$

Combining the estimates (3.32)–(3.38), we can infer from Gronwall's lemma that

$$\|\eta^{\tau_N}\|^2_{H^1(0,t;H)\cap L^\infty(0,t;V)} \,\le\, C\,\|h\|^2_{L^2(0,t;H_\Gamma)}\,. \tag{3.39}$$

Then, by comparing in (3.18) and using the full regularity of $(\bar\mu,\bar\rho)$ (in particular (2.10)), we easily check that also

$$\|\Delta\eta^{\tau_N}\|^2_{L^2(0,t;H)} \,\le\, C\,\|h\|^2_{L^2(0,t;H_\Gamma)}\,, \tag{3.40}$$

whence, by standard elliptic estimates,

$$\|\eta^{\tau_N}\|^2_{L^2(0,t;W)} \,\le\, C\,\|h\|^2_{L^2(0,t;H_\Gamma)}\,. \tag{3.41}$$

In conclusion, by virtue of (3.31), (3.39), (3.41), and since the embedding $(H^1(0,t;H)\cap L^2(0,t;H^2(\Omega)))\subset C^0([0,t];V)$ is continuous, we have shown the estimate

$$\begin{aligned} &\|\eta^{\tau_N}\|^2_{H^1(0,t;H)\cap C^0([0,t];V)\cap L^2(0,t;H^2(\Omega))} \,+\, \|\zeta^{\tau_N}\|^2_{H^1(0,t;H)\cap C^0([0,t];V)\cap L^2(0,t;H^2(\Omega))} \\ &\quad + \|\zeta_\Gamma^{\tau_N}\|^2_{H^1(0,t;H_\Gamma)\cap C^0([0,t];V_\Gamma)\cap L^2(0,t;H^2(\Gamma))} \,\le\, C\,\|h\|^2_{L^2(0,t;H_\Gamma)} \\ &\quad \text{for all } N\in\mathbb{N} \text{ and } t\in(0,T]. \end{aligned} \tag{3.42}$$

We are now in a position to show the existence of a solution to (3.1)–(3.5). Indeed, thanks to (3.42), there are functions $(\eta,\zeta,\zeta_\Gamma)$, such that, for a subsequence which is again indexed by N, we have for $N\to\infty$ that

$$\eta^{\tau_N} \to \eta \quad \text{weakly in } H^1(0,T;H)\cap C^0([0,T];V)\cap L^2(0,T;W)\,, \tag{3.43}$$

$$\zeta^{\tau_N} \to \zeta \quad \text{weakly in } H^1(0,T;H)\cap C^0([0,T];V)\cap L^2(0,T;H^2(\Omega))\,, \tag{3.44}$$

$$\zeta_\Gamma^{\tau_N} \to \zeta_\Gamma \quad \text{weakly in } H^1(0,T;H_\Gamma)\cap C^0([0,T];V_\Gamma)\cap L^2(0,T;H^2(\Gamma))\,. \tag{3.45}$$

This implies, in particular, that the initial and boundary conditions (3.2) and (3.5) are fulfilled, and, since $\zeta^{\tau_N}_{|\Sigma} \to \zeta_{|\Sigma}$ weakly in $L^2(0,T;H^{3/2}(\Gamma))$ by (3.44) and the trace theorem, we have that $\zeta_{|\Sigma} = \zeta_\Gamma$ almost everywhere on Σ.

Moreover, thanks to [32, Sect. 8, Cor. 4], we may without loss of generality assume that, for every $p \in [1,6)$,

$$\eta^{\tau_N} \to \eta \quad \text{ strongly in } C^0([0,T];L^p(\Omega))\,, \tag{3.46}$$

$$\zeta^{\tau_N} \to \zeta \quad \text{ strongly in } C^0([0,T];L^p(\Omega))\,, \tag{3.47}$$

$$\zeta^{\tau_N}_\Gamma \to \zeta_\Gamma \quad \text{ strongly in } C^0([0,T];L^p(\Gamma))\,. \tag{3.48}$$

In addition, it holds $\mathcal{T}_{\tau_N}(\eta^{\tau_N}) \to \eta$ strongly in $L^2(Q)$, and it is easily verified that

$$\begin{aligned}
&\mathcal{T}_{\tau_N}(\eta^{\tau_N})\, g'(\bar\rho)\,\partial_t\bar\rho \to \eta\, g'(\bar\rho)\,\partial_t\bar\rho, \;\; g'(\bar\rho)\,\partial_t\bar\mu\,\zeta^{\tau_N} \to g'(\bar\rho)\,\partial_t\bar\mu\,\zeta,\\
&\bar\mu\, g''(\bar\rho)\,\partial_t\bar\rho\,\zeta^{\tau_N} \to \bar\mu\, g''(\bar\rho)\,\partial_t\bar\rho\,\zeta, \;\; g'(\bar\rho)\,\mathcal{T}_{\tau_N}(\eta^{\tau_N}) \to g'(\bar\rho)\,\eta\,, \quad \text{all weakly in } L^1(Q)\,.
\end{aligned} \tag{3.49}$$

Therefore, we may pass to the limit as $N \to \infty$ in (3.18)–(3.22), written for $\tau = \tau_N$, to conclude that the triple $(\eta,\zeta,\zeta_\Gamma)$ is in fact a solution to the system (3.1)–(3.5) that enjoys the regularity properties (3.6)–(3.8). Moreover, passage to the limit as $N \to \infty$ in (3.42), using the weak sequential semicontinuity of norms, yields that

$$\begin{aligned}
&\|\eta\|^2_{H^1(0,t;H)\cap C^0([0,t];V)\cap L^2(0,t;H^2(\Omega))} + \|\zeta\|^2_{H^1(0,t;H)\cap C^0([0,t];V)\cap L^2(0,t;H^2(\Omega))}\\
&+ \|\zeta_\Gamma\|^2_{H^1(0,t;H_\Gamma)\cap C^0([0,t];V_\Gamma)\cap L^2(0,t;H^2(\Gamma))} \le C\,\|h\|^2_{L^2(0,t;H_\Gamma)} \quad \text{for all } t \in (0,T]\,.
\end{aligned} \tag{3.50}$$

It remains to show that the solution is unique, which, in view of (3.50), would entail that the linear mapping $h \mapsto (\eta,\zeta,\zeta_\Gamma)$ is continuous from $L^2(\Sigma)$ into $\mathcal{Z}$. So let us assume that two solutions $(\eta_i,\zeta_i,\zeta_{i_\Gamma})$, $i=1,2$, satisfying (3.6)–(3.8) are given. Then the triple $(\eta,\zeta,\zeta_\Gamma)$, where $\eta := \eta_1 - \eta_2$, $\zeta := \zeta_1 - \zeta_2$, $\zeta_\Gamma := \zeta_{1_\Gamma} - \zeta_{2_\Gamma}$, satisfies Eqs. (3.1)–(3.5) with $h = 0$.

At this point, we can repeat the estimations performed in the First estimate above, where the only difference (which even simplifies the analysis) is given by the fact that in Eq. (3.1) the term $\eta\, g'(\bar\rho)\,\partial_t\bar\rho$ appears in place of the expression $\mathcal{T}_\tau(\eta^\tau)\, g'(\bar\rho)\,\partial_t\bar\rho$ occurring in Eq. (3.18). We thus can claim that the estimate (3.31) is valid with $(\eta^{\tau_N},\zeta^{\tau_N},\zeta^{\tau_N}_\Gamma)$ replaced by $(\eta,\zeta,\zeta_\Gamma)$. Since $h = 0$ in the present situation, we obtain that $\eta = \zeta = 0$ almost everywhere in Q, and $\zeta_\Gamma = 0$ almost everywhere on Σ. This concludes the proof of the assertion. $\square$

We are now in a position to prove the Fréchet differentiability of the control-to-state operator. We recall the definition (2.11) of $\mathcal{X}$ and state the following result.

Theorem 3.2: *Suppose that the conditions* (A1)–(A5) *are fulfilled. Then the control-to-state operator* $\mathcal{S} : u_\Gamma \mapsto (\mu,\rho,\rho_\Gamma)$ *is Fréchet differentiable as a mapping from* $\mathcal{U}_R \subset \mathcal{X}$ *into the Banach space*

$$\begin{aligned}
\mathcal{Y} := \big\{ &(\mu,\rho,\rho_\Gamma) \in (L^\infty(0,T;H)\cap L^2(0,T;V)) \times (H^1(0,T;H)\cap L^2(0,T;H^2(\Omega)))\\
&\times (H^1(0,T;H_\Gamma)\cap L^2(0,T;H^2(\Gamma))) : \; \rho_\Gamma = \rho_{|\Sigma} \;\text{ a.e. on } \Sigma \big\}\,.
\end{aligned}$$

Moreover, for every $\bar u_\Gamma \in \mathcal{U}_R$, the Fréchet derivative $D\mathcal{S}(\bar u_\Gamma) \in \mathcal{L}(\mathcal{X},\mathcal{Y})$ is evaluated at any $h \in \mathcal{X}$ by putting $D\mathcal{S}(\bar u_\Gamma)(h) := (\eta,\zeta,\zeta_\Gamma)$, where $(\eta,\zeta,\zeta_\Gamma)$ is the unique solution to the linearized system (3.1)–(3.5).

Proof: According to Theorem 3.1, the linear mapping $h \mapsto (\eta^h,\zeta^h,\zeta_\Gamma^h) := (\eta,\zeta,\zeta_\Gamma)$ is continuous from $L^2(\Sigma)$ into $\mathcal{Z}$ and thus, a fortiori, also from $\mathcal{X}$ into $\mathcal{Y}$. Hence, if the derivative $D\mathcal{S}(\bar u_\Gamma)$ exists and has the asserted form, then it belongs to $\mathcal{L}(\mathcal{X},\mathcal{Y})$.

Now notice that $\mathcal{U}_R$ is open in $\mathcal{X}$, and thus there is some $\Lambda > 0$ such that $\bar u_\Gamma + h \in \mathcal{U}_R$ whenever $\|h\|_{\mathcal{X}} \le \Lambda$. In the following, we consider only such perturbations h. We then put, for any such h,

$$(\mu^h,\rho^h,\rho_\Gamma^h) := \mathcal{S}(\bar u_\Gamma + h), \quad z^h := \mu^h - \bar\mu - \eta^h, \quad y^h := \rho^h - \bar\rho - \zeta^h, \quad y_\Gamma^h := \rho_\Gamma^h - \bar\rho_\Gamma - \zeta_\Gamma^h,$$

where $(\bar\mu,\bar\rho,\bar\rho_\Gamma) := \mathcal{S}(\bar u_\Gamma)$ and $(\eta^h,\zeta^h,\zeta_\Gamma^h)$ denotes the unique solution $(\eta,\zeta,\zeta_\Gamma)$ to the linearized system (3.1)–(3.5). Notice that we have $y_\Gamma^h = y^h_{|\Sigma}$, as well as

$$z^h \in H^1(0,T;H) \cap C^0([0,T];V) \cap L^2(0,T;W), \tag{3.51}$$
$$y^h \in H^1(0,T;H) \cap C^0([0,T];V) \cap L^2(0,T;H^2(\Omega)), \tag{3.52}$$
$$y_\Gamma^h \in H^1(0,T;H_\Gamma) \cap C^0([0,T];V_\Gamma) \cap L^2(0,T;H^2(\Gamma)). \tag{3.53}$$

We also notice that the global bounds (2.7) and (2.9) are satisfied for $(\mu^h,\rho^h,\rho_\Gamma^h)$, and, owing to Theorem 2.4, we have the global stability estimate

$$\begin{aligned}&\|\mu^h - \bar\mu\|_{H^1(0,t;H)\cap C^0([0,t];V)\cap L^2(0,t;W)} + \|\rho^h - \bar\rho\|_{H^1(0,t;H)\cap C^0([0,t];V)\cap L^2(0,t;H^2(\Omega))}\\ &+ \|\rho_\Gamma^h - \bar\rho_\Gamma\|_{H^1(0,t;H_\Gamma)\cap C^0([0,t];V_\Gamma)\cap L^2(0,t;H^2(\Gamma))} \le K_3^* \|h\|_{L^2(0,t;H_\Gamma)} \quad \forall\, t \in (0,T).\end{aligned} \tag{3.54}$$

Moreover, by Taylor's theorem and (2.9), it holds that

$$\begin{aligned}&\left|f'(\rho^h) - f'(\bar\rho) - f''(\bar\rho)\,\zeta^h\right| + \left|g(\rho^h) - g(\bar\rho) - g'(\bar\rho)\,\zeta^h\right| + \left|g'(\rho^h) - g'(\bar\rho) - g''(\bar\rho)\,\zeta^h\right|\\ &+ \left|\pi(\rho^h) - \pi(\bar\rho) - \pi'(\bar\rho)\,\zeta^h\right| \le C\left(|y^h| + |\rho^h - \bar\rho|^2\right) \quad \text{a.e. in } Q,\end{aligned} \tag{3.55}$$

$$\begin{aligned}&\left|f_\Gamma'(\rho_\Gamma^h) - f_\Gamma'(\bar\rho_\Gamma) - f_\Gamma''(\bar\rho_\Gamma)\,\zeta_\Gamma^h\right| + \left|\pi_\Gamma(\rho_\Gamma^h) - \pi_\Gamma(\bar\rho_\Gamma) - \pi_\Gamma'(\bar\rho_\Gamma)\,\zeta_\Gamma^h\right|\\ &\le C\left(|y_\Gamma^h| + |\rho_\Gamma^h - \bar\rho_\Gamma|^2\right) \quad \text{a.e. on } \Sigma,\end{aligned} \tag{3.56}$$

where, here and in the remainder of the proof, we denote by $C > 0$ constants that may depend on the data of the system but not on the special choice of h with $\|h\|_{\mathcal{X}} \le \Lambda$. The actual value of C may change between lines and even within formulas.

According to the definition of the notion of Fréchet differentiability, we need to show that

$$\lim_{\|h\|_{\mathcal{X}}\to 0} \frac{\left\|\mathcal{S}(\bar u_\Gamma + h) - \mathcal{S}(\bar u_\Gamma) - (\eta^h,\zeta^h,\zeta_\Gamma^h)\right\|_{\mathcal{Y}}}{\|h\|_{\mathcal{X}}} = 0\,. \tag{3.57}$$

It thus suffices to prove the existence of an increasing function $Z : (0,\Lambda) \to (0,+\infty)$ such that $\lim_{\lambda\searrow 0} \frac{Z(\lambda)}{\lambda^2} = 0$ and

$$\begin{aligned}&\|z^h\|^2_{L^\infty(0,T;H)\cap L^2(0,T;V)} + \|y^h\|^2_{H^1(0,T;H)\cap L^2(0,T;H^2(\Omega))} + \|y_\Gamma^h\|^2_{H^1(0,T;H_\Gamma)\cap L^2(0,T;H^2(\Gamma))}\\ &\le Z\big(\|h\|_{H^1(0,T;H_\Gamma)}\big)\,.\end{aligned} \tag{3.58}$$

To begin with, using the state system (1.2)–(1.6) and the linearized system (3.1)–(3.5), we easily verify that the triple (z^h, y^h, y_Γ^h) is a strong solution to the system

$$\begin{aligned}
&(1+2g(\bar\rho))\, z_t^h \;+\; g'(\bar\rho)\bar\rho_t\, z^h \;+\; \bar\mu\, g'(\bar\rho)\, y_t^h - \Delta z^h \\
&= -\,2\left(g(\rho^h)-g(\bar\rho)\right)\left(\mu_t^h-\bar\mu_t\right) \;-\; 2\,\bar\mu_t\left(g(\rho^h)-g(\bar\rho)-g'(\bar\rho)\zeta^h\right) \\
&\quad -\;\bar\mu\,\bar\rho_t\left(g'(\rho^h)-g'(\bar\rho)-g''(\bar\rho)\zeta^h\right) \;-\; \bar\mu\left(g'(\rho^h)-g'(\bar\rho)\right)\left(\rho_t^h-\bar\rho_t\right) \\
&\quad -\left(\mu^h-\bar\mu\right)\left[\left(g'(\rho^h)-g'(\bar\rho)\right)\bar\rho_t + g'(\rho^h)\left(\rho_t^h-\bar\rho_t\right)\right] \quad \text{a.e. in } Q,
\end{aligned} \tag{3.59}$$

$$\partial_{\mathbf n} z^h = 0 \quad \text{a.e. on } \Sigma, \quad z^h(0)=0 \quad \text{a.e. in } \Omega, \tag{3.60}$$

$$\begin{aligned}
y_t^h - \Delta y^h &= -\left(f'(\rho^h)-f'(\bar\rho)-f''(\bar\rho)\zeta^h\right) - \left(\pi(\rho^h)-\pi(\bar\rho)-\pi'(\bar\rho)\,\zeta^h\right) \\
&\quad + g'(\bar\rho)\, z^h \;+\; \bar\mu\left(g'(\rho^h)-g'(\bar\rho)-g''(\bar\rho)\zeta^h\right) \\
&\quad + \left(\mu^h-\bar\mu\right)\left(g'(\rho^h)-g'(\bar\rho)\right) \quad \text{a.e. in}\, Q,
\end{aligned} \tag{3.61}$$

$$\begin{aligned}
&\partial_{\mathbf n} y^h \;+\; \partial_t y_\Gamma^h \;-\; \Delta_\Gamma y_\Gamma^h \;=\; -\left(f_\Gamma'(\rho_\Gamma^h)-f_\Gamma'(\bar\rho_\Gamma)-f_\Gamma''(\bar\rho_\Gamma)\,\zeta_\Gamma^h\right) \\
&\quad -\;\left(\pi_\Gamma(\rho_\Gamma^h)-\pi_\Gamma(\bar\rho_\Gamma)-\pi_\Gamma'(\bar\rho_\Gamma)\zeta_\Gamma^h\right), \quad y_\Gamma^h = y^h_{|\Sigma}, \quad \text{a.e. on } \Sigma,
\end{aligned} \tag{3.62}$$

$$y^h(0)=0 \quad \text{a.e. in } \Omega, \quad y_\Gamma^h(0)=0 \quad \text{a.e. on } \Gamma. \tag{3.63}$$

In the following, we make repeated use of the mean value theorem and of the global estimates (2.7), (2.9), and (3.54), without further reference. For the sake of a better readability, we will omit the superscript h of the quantities z^h, y^h, y_Γ^h during the estimations, writing it only at the end of the respective estimates.

<u>FIRST ESTIMATE:</u>

Let an arbitrary $t \in (0,T]$ be fixed. First, let us observe that $\partial_t\left((\frac12 + g(\bar\rho))z^2\right) = (1+2\,g(\bar\rho))\, z\, z_t \;+\; g'(\bar\rho)\,\bar\rho_t\, z^2$. Hence, adding the same term z to both sides of (3.59) for convenience, multiplication by z and integration over Q_t yield the estimate

$$\int_\Omega \left(\tfrac12 + g(\bar\rho(t))\right) z^2(t)\,\mathrm{d}x + \int_0^t \|z(s)\|_V^2\,\mathrm{d}s \le \int_0^t \|z(s)\|_H^2\,\mathrm{d}s + C\sum_{j=1}^7 |I_j|\,, \tag{3.64}$$

where the quantities I_j, $1 \le j \le 7$, are specified and estimated as follows: at first, Young's inequality shows that, for every $\gamma > 0$ (to be chosen later),

$$I_1 := -\int_0^t\!\!\int_\Omega \bar\mu\, g'(\bar\rho)\, y_t\, z\,\mathrm{d}x\,\mathrm{d}s \;\le\; \gamma \int_0^t\!\!\int_\Omega y_t^2\,\mathrm{d}x\,\mathrm{d}s \;+\; \frac{C}{\gamma}\int_0^t\!\!\int_\Omega z^2\,\mathrm{d}x\,\mathrm{d}s\,. \tag{3.65}$$

Moreover, we have, by Hölder's and Young's inequalities and (3.54),

$$\begin{aligned}
I_2 :&= \;-2\int_0^t\!\!\int_\Omega \left(g(\rho^h)-g(\bar\rho)\right)\left(\mu_t^h-\bar\mu_t\right) z\,\mathrm{d}x\,\mathrm{d}s \\
&\le\; C\int_0^t \|\rho^h(s)-\bar\rho(s)\|_6\,\|\mu_t^h(s)-\bar\mu_t(s)\|_2\,\|z(s)\|_3\,\mathrm{d}s \\
&\le\; C\,\|\rho^h-\bar\rho\|_{C^0([0,t];V)}\,\|\mu^h-\bar\mu\|_{H^1(0,t;H)}\,\|z\|_{L^2(0,t;V)} \\
&\le\; \gamma\,\|z\|_{L^2(0,t;V)}^2 \;+\; \frac{C}{\gamma}\,\|h\|_{L^2(0,t;H_\Gamma)}^4\,.
\end{aligned} \tag{3.66}$$

Next, we employ (3.55), the Hölder and Young inequalities, and (3.54), to infer that

$$
\begin{aligned}
I_3 :=\ & -2 \int_0^t\!\!\int_\Omega \bar\mu_t \left(g(\rho^h) - g(\bar\rho) - g'(\bar\rho)\zeta^h\right) z \,\mathrm{d}x\,\mathrm{d}s \\
\le\ & C \int_0^t\!\!\int_\Omega |\bar\mu_t| \left(|y| \,+\, |\rho^h - \bar\rho|^2\right) |z| \,\mathrm{d}x\,\mathrm{d}s \\
\le\ & C \int_0^t \|\bar\mu_t(s)\|_6 \left(\|y(s)\|_3 \,\|z(s)\|_2 \,+\, \|\rho^h(s) - \bar\rho(s)\|_6^2 \,\|z(s)\|_2\right) \mathrm{d}s \\
\le\ & C \int_0^t \|\bar\mu_t(s)\|_6^2 \,\|z(s)\|_H^2 \,\mathrm{d}s \,+\, C \int_0^t \|y(s)\|_V^2 \,\mathrm{d}s \,+\, C \int_0^t \|\rho^h(s) - \bar\rho(s)\|_V^4 \,\mathrm{d}s \\
\le\ & C \int_0^t \left(1 + \|\bar\mu_t(s)\|_6^2\right) \left(\|y(s)\|_V^2 \,+\, \|z(s)\|_H^2\right) ds \,+\, C\,\|h\|^4_{L^2(0,t;H_\Gamma)} \,.
\end{aligned}
\tag{3.67}
$$

Likewise, with (2.9), (3.55), (2.16), and the Hölder and Young inequalities, we find that

$$
\begin{aligned}
I_4 :=\ & -\int_0^t\!\!\int_\Omega \bar\mu\,\bar\rho_t \,(g'(\rho^h) - g'(\bar\rho) - g''(\bar\rho)\zeta^h)\, z \,\mathrm{d}x\,\mathrm{d}s \le C \int_0^t\!\!\int_\Omega |\bar\rho_t|(|y| + |\rho^h - \bar\rho|^2)|z| \,\mathrm{d}x\,\mathrm{d}s \\
\le\ & C \int_0^t \|\bar\rho_t(s)\|_6 \left(\|y(s)\|_3 \,+\, \|\rho^h(s) - \bar\rho(s)\|_6^2\right) \|z(s)\|_2 \,\mathrm{d}x\,\mathrm{d}s \\
\le\ & C \int_0^t \|y(s)\|_V^2 \,\mathrm{d}s \,+\, C \int_0^t \|\bar\rho_t(s)\|_V^2 \,\|z(s)\|_H^2 \,\mathrm{d}s \,+\, C \max_{0\le s\le t} \|\rho^h(s) - \bar\rho(s)\|_V^4 \\
\le\ & C \int_0^t \|y(s)\|_V^2 \,\mathrm{d}s \,+\, C \int_0^t \|\bar\rho_t(s)\|_V^2 \,\|z(s)\|_H^2 \,\mathrm{d}s \,+\, C\,\|h\|^4_{L^2(0,t;H_\Gamma)} \,.
\end{aligned}
\tag{3.68}
$$

In addition, arguing similarly, we have

$$
\begin{aligned}
I_5 :=\ & -\int_0^t\!\!\int_\Omega \bar\mu \left(g'(\rho^h) - g'(\bar\rho)\right) \left(\rho^h_t - \bar\rho_t\right) z \,\mathrm{d}x\,\mathrm{d}s \\
\le\ & C \int_0^t \|\rho^h(s) - \bar\rho(s)\|_6 \,\|\rho^h_t(s) - \bar\rho_t(s)\|_2 \,\|z(s)\|_3 \,\mathrm{d}s \\
\le\ & C\,\|\rho^h - \bar\rho\|_{C^0([0,t];V)} \,\|\rho^h - \bar\rho\|_{H^1(0,t;H)} \,\|z\|_{L^2(0,t;V)} \\
\le\ & \gamma \int_0^t \|z(s)\|_V^2 \,\mathrm{d}s \,+\, \frac{C}{\gamma}\,\|h\|^4_{L^2(0,t;H_\Gamma)} \,,
\end{aligned}
\tag{3.69}
$$

as well as

$$
\begin{aligned}
I_6 :=\ & -\int_0^t\!\!\int_\Omega \bar\rho_t \left(\mu^h - \bar\mu\right) \left(g'(\rho^h) - g'(\bar\rho)\right) z \,\mathrm{d}x\,\mathrm{d}s \\
\le\ & C \int_0^t \|\bar\rho_t(s)\|_6 \left\|\mu^h(s) - \bar\mu(s)\right\|_6 \left\|\rho^h(s) - \bar\rho(s)\right\|_6 \,\|z(s)\|_2 \,\mathrm{d}x\,\mathrm{d}s \\
\le\ & C \int_0^t \|\bar\rho_t(s)\|_V^2 \,\|z(s)\|_H^2 \,\mathrm{d}s \,+\, C\,\|\mu^h - \bar\mu\|^2_{C^0([0,t];V)} \,\|\rho^h - \bar\rho\|^2_{C^0([0,t];V)} \\
\le\ & C \int_0^t \|\bar\rho_t(s)\|_V^2 \,\|z(s)\|_H^2 \,\mathrm{d}s \,+\, C\,\|h\|^4_{L^2(0,t;H_\Gamma)} \,.
\end{aligned}
\tag{3.70}
$$

Finally, we find that

$$
\begin{aligned}
I_7 := &- \int_0^t\!\!\int_\Omega \left(\mu^h - \bar\mu\right) g'(\rho^h) \left(\rho_t^h - \bar\rho_t\right) z \,\mathrm{d}x\,\mathrm{d}s \\
&\le C \int_0^t \|\mu^h(s) - \bar\mu(s)\|_6 \, \|\rho_t^h(s) - \bar\rho_t(s)\|_2 \, \|z(s)\|_3 \,\mathrm{d}s \\
&\le C \, \|\mu^h - \bar\mu\|_{C^0([0,t];V)} \, \|\rho^h - \bar\rho\|_{H^1(0,t;H)} \, \|z\|_{L^2(0,t;V)} \\
&\le \gamma \int_0^t \|z(s)\|_V^2 \,\mathrm{d}s + \frac{C}{\gamma} \, \|h\|^4_{L^2(0,t;H_\Gamma)} \,.
\end{aligned} \tag{3.71}
$$

In conclusion, combining the estimates (3.64)–(3.71), and choosing $\gamma = \frac{1}{8}$, we have shown that

$$
\begin{aligned}
&\frac12 \left\|z^h(t)\right\|_H^2 + \frac12 \int_0^t \left\|z^h(s)\right\|_V^2 ds \le \frac18 \int_0^t\!\!\int_\Omega \left|y_t^h\right|^2 dx\,\mathrm{d}s + C\,\|h\|^4_{L^2(0,t;H_\Gamma)} \\
&\quad + C \int_0^t \left(1 + \|\bar\mu_t(s)\|_6^2 + \|\bar\rho_t(s)\|_V^2\right) \left(\left\|y^h(s)\right\|_V^2 + \left\|z^h(s)\right\|_H^2\right) \mathrm{d}s \,,
\end{aligned} \tag{3.72}
$$

where we observe that, in view of (2.4) and (2.10), the mapping $s \mapsto \|\bar\mu_t(s)\|_6^2 + \|\bar\rho_t(s)\|_V^2$ belongs to $L^1(0,T)$.

<u>SECOND ESTIMATE:</u> We now observe that y^h satisfies a linear problem of the form (2.12)–(2.14), where in this case $a = 0$ and $a_\Gamma = 0$, and where σ and σ_Γ are equal to the right-hand sides of (3.61) and (3.62), respectively. We therefore have, with this choice of σ, σ_Γ,

$$
\begin{aligned}
&\|y^h\|_{H^1(0,t;H)\cap C^0([0,t];V)\cap L^2(0,t;H^2(\Omega))} + \|y_\Gamma^h\|_{H^1(0,t;H_\Gamma)\cap C^0([0,t];V_\Gamma)\cap L^2(0,t;H^2(\Gamma))} \\
&\le C_L \left(\|\sigma\|_{L^2(Q_t)} + \|\sigma_\Gamma\|_{L^2(\Sigma_t)}\right) \quad \forall\, t \in (0,T]\,.
\end{aligned} \tag{3.73}
$$

Now, using (3.55), (3.56), and the stability estimate (2.16), we easily conclude that

$$
\begin{aligned}
\|\sigma\|^2_{L^2(Q_t)} &\le C \int_0^t\!\!\int_\Omega \left(|y^h|^2 + |z^h|^2 + |\rho^h - \bar\rho|^4 + |\mu^h - \bar\mu|^2 \, |\rho^h - \bar\rho|^2\right) \mathrm{d}x\,\mathrm{d}s \\
&\le C \int_0^t\!\!\int_\Omega \left(|y^h|^2 + |z^h|^2\right) \mathrm{d}x\,\mathrm{d}s + C\,\|h\|^4_{L^2(0,t;H_\Gamma)} \,,
\end{aligned} \tag{3.74}
$$

$$
\begin{aligned}
\|\sigma_\Gamma\|^2_{L^2(\Sigma_t)} &\le C \int_0^t\!\!\int_\Gamma \left|y_\Gamma^h\right|^2 \mathrm{d}\Gamma\,\mathrm{d}s + C \int_0^t\!\!\int_\Gamma \left|\rho_\Gamma^h - \bar\rho_\Gamma\right|^4 \mathrm{d}\Gamma\,\mathrm{d}s \\
&\le C \int_0^t\!\!\int_\Gamma \left|y_\Gamma^h\right|^2 \mathrm{d}\Gamma\,\mathrm{d}s + C\,\|h\|^4_{L^2(0,t;H_\Gamma)} \,.
\end{aligned} \tag{3.75}
$$

Thus, combining the estimates (3.72)–(3.75) and invoking Gronwall's lemma, we have proved the estimate

$$
\begin{aligned}
&\|z^h\|^2_{C^0([0,t];H)\cap L^2(0,t;V)} + \|y^h\|^2_{H^1(0,t;H)\cap C^0([0,t];V)\cap L^2(0,t;H^2(\Omega))} \\
&+ \|y_\Gamma^h\|^2_{H^1(0,t;H_\Gamma)\cap C^0([0,t];V_\Gamma)\cap L^2(0,t;H^2(\Gamma))} \le \widetilde{C}\,\|h\|^4_{L^2(0,t;H_\Gamma)}
\end{aligned} \tag{3.76}
$$

where $\widetilde{C}$ is a sufficiently large constant. Therefore, the condition (3.58) is satisfied for the function $Z(\lambda) = \widetilde{C}\,\lambda^4$. This concludes the proof of the assertion. $\square$

We are now in the position to state the following necessary optimality condition, which is a simple standard application of the chain rule and of the fact that $\mathcal{U}_{\rm ad}$ is a convex set. We thus may leave its proof to the reader.

Corollary 3.3: *Let the general hypotheses* (A1)–(A6) *be fulfilled, and assume that* $\bar u_\Gamma \in \mathcal{U}_{\rm ad}$ *is a solution to the control problem* **(CP)** *with associated state* $(\bar\mu, \bar\rho, \bar\rho_\Gamma) = \mathcal{S}(\bar u_\Gamma)$. *Then we have, for every* $v_\Gamma \in \mathcal{U}_{\rm ad}$,

$$\beta_1 \int_0^T\!\!\int_\Omega (\bar\mu - \hat\mu_Q)\,\eta\,{\rm d}x\,{\rm d}t \,+\, \beta_2 \int_0^T\!\!\int_\Omega (\bar\rho - \hat\rho_Q)\,\zeta\,{\rm d}x\,{\rm d}t \,+\, \beta_3 \int_0^T\!\!\int_\Gamma (\bar\rho_\Gamma - \hat\rho_\Sigma)\,\zeta_\Gamma\,{\rm d}\Gamma\,{\rm d}t$$
$$+\, \beta_4 \int_\Omega (\bar\rho(T) - \hat\rho_\Omega)\,\zeta(T)\,{\rm d}x \,+\, \beta_5 \int_\Gamma (\bar\rho_\Gamma(T) - \hat\rho_\Gamma)\,\zeta_\Gamma(T)\,{\rm d}\Gamma$$
$$+\, \beta_6 \int_0^T\!\!\int_\Gamma \bar u_\Gamma\,(v_\Gamma - \bar u_\Gamma)\,{\rm d}\Gamma\,{\rm d}t \,\ge\, 0\,, \tag{3.77}$$

where $(\eta, \zeta, \zeta_\Gamma)$ *denotes the (unique) solution to the linearized system* (3.1)–(3.5) *associated with* $h = v_\Gamma - \bar u_\Gamma$.

4 Existence and necessary optimality conditions

In this section, we state and prove the main results of this paper. We begin with an existence result.

Theorem 4.1: *Suppose that the conditions* (A1)–(A6) *are fulfilled. Then the optimal control problem* **(CP)** *admits a solution* $u_\Gamma \in \mathcal{U}_{\rm ad}$.

Proof: Since $\mathcal{U}_{\rm ad} \ne \emptyset$, we may pick a minimizing sequence $\{u_{\Gamma,n}\}_{n\in\mathbb{N}} \subset \mathcal{U}_{\rm ad}$ for the control problem. Now put $(\mu_n, \rho_n, \rho_{n_\Gamma}) := \mathcal{S}(u_{\Gamma,n})$, where $\rho_{n_\Gamma} = \rho_{n|\Sigma}$, for $n \in \mathbb{N}$. By virtue of the global estimates (2.7), (2.9) and of the separation property (2.8), and invoking [32, Sect. 8, Cor. 4], we may without loss of generality assume that there exist some $\bar u_\Gamma \in \mathcal{U}_{\rm ad}$ and functions $\bar\mu, \bar\rho, \bar\rho_\Gamma$ such that, as $n \to \infty$,

$$u_{\Gamma,n} \to \bar u_\Gamma \quad \text{weakly-star in } H^1(0,T;H_\Gamma) \cap L^\infty(\Sigma), \tag{4.1}$$
$$\mu_n \to \bar\mu \quad \text{weakly star in } H^1(0,T;H) \cap L^\infty(0,T;V) \cap L^2(0,T;W) \cap L^\infty(Q)$$
$$\text{and strongly in } C^0([0,T];H) \cap L^2(0,T;L^\infty(\Omega)), \tag{4.2}$$
$$\rho_n \to \bar\rho \quad \text{weakly-star in } W^{1,\infty}(0,T;H) \cap H^1(0,T;V) \cap L^\infty(0,T;H^2(\Omega))$$
$$\text{and strongly in } C^0(\overline{Q}), \tag{4.3}$$
$$\rho_{n_\Gamma} \to \bar\rho_\Gamma \quad \text{weakly-star in } W^{1,\infty}(0,T;H_\Gamma) \cap H^1(0,T;V_\Gamma) \cap L^\infty(0,T;H^2(\Gamma)), \tag{4.4}$$
$$-1 < r_* \le \rho_n(x,t) \le r^* < +1 \quad \forall\,(x,t) \in \overline{Q}\,. \tag{4.5}$$

In particular, it holds $\rho_{n_\Gamma} = \rho_{n_{|\Sigma}} \to \bar\rho_{|\Sigma}$ strongly in $C^0(\overline{\Sigma})$, which entails that $\bar\rho_\Gamma = \bar\rho_{|\Sigma}$ on $\overline{\Sigma}$ and, thanks to the assumptions (A2) and (A3), that

$$\Phi(\rho_n) \to \Phi(\bar\rho) \quad \text{strongly in } C^0(\overline{Q}) \text{ for } \Phi \in \{g, g', f', \pi\}, \tag{4.6}$$

$$\Phi_\Gamma(\rho_{n_\Gamma}) \to \Phi_\Gamma(\bar\rho_\Gamma) \quad \text{strongly in } C^0(\overline{\Sigma}) \text{ for } \Phi_\Gamma \in \{f'_\Gamma, \pi_\Gamma\}. \tag{4.7}$$

Moreover, owing to the trace theorem,

$$\partial_{\mathbf{n}}\mu_n \to \partial_{\mathbf{n}}\bar\mu, \quad \partial_{\mathbf{n}}\rho_n \to \partial_{\mathbf{n}}\bar\rho, \quad \text{both weakly in } L^2(0,T;H^{1/2}(\Gamma)), \tag{4.8}$$

and it obviously holds $\bar\mu(0) = \mu_0$, $\bar\rho(0) = \rho_0$, and $\bar\rho_\Gamma(0) = \rho_{0_{|\Gamma}}$. In addition, it is easily verified that

$$\mu_n\, g'(\rho_n) \to \bar\mu\, g'(\bar\rho), \quad \mu_n\, g'(\rho_n)\,\partial_t\rho_n \to \bar\mu\, g'(\bar\rho)\,\partial_t\bar\rho, \quad \text{both weakly in } L^2(Q). \tag{4.9}$$

Now, we let $n \to \infty$ in the system (1.2)–(1.6), written for $(\mu_n, \rho_n, \rho_{n_\Gamma})$ and the right-hand side $u_{\Gamma,n}$. It then follows from the above convergence results that $(\bar\mu, \bar\rho, \bar\rho_\Gamma)$ solves (1.2)-(1.6) with the right-hand side $\bar u_\Gamma$, that is, we have $(\bar\mu, \bar\rho, \bar\rho_\Gamma) = \mathcal{S}(\bar u_\Gamma)$, whence we infer that the pair $((\bar\mu, \bar\rho, \bar\rho_\Gamma), \bar u_\Gamma)$ is admissible for **(CP)**. Its optimality is then a simple consequence of the weak sequential semicontinuity properties of the cost functional $\mathcal{J}$. $\square$

We now turn our interest to the derivation of first-order necessary optimality conditions for problem **(CP)**. For this purpose, we generally assume that the hypotheses (A1)–(A6) are fulfilled and that $\bar u_\Gamma \in \mathcal{U}_{\mathrm{ad}}$ is an optimal control with associated state $(\bar\mu, \bar\rho, \bar\rho_\Gamma) = \mathcal{S}(\bar u_\Gamma)$ having the properties (2.4)–(2.6) and (2.8). We aim to eliminate the quantities $\eta, \zeta, \zeta_\Gamma$ from the variational inequality (3.77). To this end, we invoke the adjoint state system associated with (1.2)–(1.6) for $\bar u_\Gamma$, which is formally given by:

$$-\,(1 + 2g(\bar\rho))\, p_t - g'(\bar\rho)\,\bar\rho_t\, p - \Delta p \;=\; g'(\bar\rho)\, q + \beta_1(\bar\mu - \hat\mu_Q) \quad \text{in } Q, \tag{4.10}$$

$$\partial_{\mathbf{n}} p = 0 \quad \text{on } \Sigma, \quad p(T) = 0 \quad \text{in } \Omega, \tag{4.11}$$

$$\begin{aligned} &-\,q_t - \Delta q \;+\; (f''(\bar\rho) + \pi'(\bar\rho) - \bar\mu\, g''(\bar\rho))\, q \\ &\quad = g'(\bar\rho)\,(\bar\mu\, p_t - \bar\mu_t\, p) + \beta_2(\bar\rho - \hat\rho_Q) \quad \text{in } Q, \end{aligned} \tag{4.12}$$

$$\partial_{\mathbf{n}} q - \partial_t q_\Gamma - \Delta_\Gamma q_\Gamma + (f''_\Gamma(\bar\rho_\Gamma) + \pi'_\Gamma(\bar\rho_\Gamma))\, q_\Gamma \;=\; \beta_3(\bar\rho_\Gamma - \hat\rho_\Sigma), \quad q_\Gamma = q_{|\Sigma}, \quad \text{on } \Sigma, \tag{4.13}$$

$$q(T) = \beta_4(\bar\rho(T) - \hat\rho_\Omega) \quad \text{in } \Omega, \quad q_\Gamma(T) = \beta_5(\bar\rho_\Gamma(T) - \hat\rho_\Gamma) \quad \text{on } \Gamma. \tag{4.14}$$

At this point, we simplify the problem somewhat by imposing the following additional condition:

(A7) It holds that $(\beta_4(\bar\rho(T) - \hat\rho_\Omega), \beta_5(\bar\rho_\Gamma(T) - \hat\rho_\Gamma)) \in \mathcal{V}$.

Observe that (A7) is obviously satisfied if $\beta_4 = \beta_5 = 0$. Another situation, in which (A7) is fulfilled, is given in the case when we have $\beta_4 = \beta_5$, $\hat\rho_\Omega \in V$, $\hat\rho_\Gamma \in V_\Gamma$, and $\hat\rho_\Gamma = \hat\rho_{\Omega_{|\Gamma}}$. In view of the fact that always $\bar\rho(T) \in \mathcal{V}$, these conditions for the target functions $\hat\rho_\Omega$ and $\hat\rho_\Gamma$ seem to be quite natural.

We have the following result.

THEOREM 4.2: *Suppose that* (A1)–(A6) *hold true and that* $\bar{u}_\Gamma \in \mathcal{U}_{\rm ad}$ *is an optimal control whose associated state* $(\bar{\mu}, \bar{\rho}, \bar{\rho}_\Gamma) = \mathcal{S}(\bar{u}_\Gamma)$ *fulfills* (A7). *Then the adjoint state system* (4.10)–(4.14) *has a unique solution* (p, q, q_Γ) *such that*

$$p \in H^1(0,T;H) \cap C^0([0,T];V) \cap L^2(0,T;W), \tag{4.15}$$
$$q \in H^1(0,T;H) \cap C^0([0,T];V) \cap L^2(0,T;H^2(\Omega)), \tag{4.16}$$
$$q_\Gamma \in H^1(0,T;H_\Gamma) \cap C^0([0,T];V_\Gamma) \cap L^2(0,T;H^2(\Gamma)). \tag{4.17}$$

PROOF: First, we rewrite the backward-in-time system (4.10)–(4.14). To this end, we define the functions

$$\tilde{\mu}(x,t) := \bar{\mu}(x,T-t), \quad \tilde{\rho}(x,t) := \bar{\rho}(x,T-t), \quad \tilde{\rho}_\Gamma(x,t) := \bar{\rho}_\Gamma(x,T-t),$$
$$\tilde{\mu}_Q(x,t) := \hat{\mu}_Q(x,T-t), \quad \tilde{\rho}_Q := \hat{\rho}_Q(x,T-t), \quad \tilde{\rho}_\Sigma(x,t) := \hat{\rho}_\Sigma(x,T-t),$$

and consider the initial-boundary value problem

$$(1 + 2g(\tilde{\rho}))\,\partial_t y + g'(\tilde{\rho})\,\partial_t\tilde{\rho}\,y - \Delta y \;=\; g'(\tilde{\rho})\,z + \beta_1(\tilde{\mu} - \tilde{\mu}_Q) \quad \text{a.e. in } Q, \tag{4.18}$$
$$\partial_{\mathbf{n}} y = 0 \quad \text{a.e. on } \Sigma, \quad y(0) = 0 \quad \text{a.e. in } \Omega, \tag{4.19}$$

$$\begin{aligned}&\partial_t z - \Delta z + (f''(\tilde{\rho}) + \pi'(\tilde{\rho}) - \tilde{\mu}\,g''(\tilde{\rho}))\,z\\ &\quad = g'(\tilde{\rho})(\partial_t\tilde{\mu}\,y - \tilde{\mu}\,\partial_t y) + \beta_2(\tilde{\rho} - \tilde{\rho}_Q) \quad \text{a.e. in } Q,\end{aligned} \tag{4.20}$$
$$\begin{aligned}&\partial_{\mathbf{n}} z + \partial_t z_\Gamma - \Delta_\Gamma z_\Gamma + (f''_\Gamma(\tilde{\rho}_\Gamma) + \pi'_\Gamma(\tilde{\rho}_\Gamma))\,z_\Gamma \;=\; \beta_3(\tilde{\rho}_\Gamma - \tilde{\rho}_\Sigma)\\ &\quad \text{and} \quad z_\Gamma = z_{|\Sigma}, \quad \text{a.e. on } \Sigma,\end{aligned} \tag{4.21}$$
$$z(0) = \beta_4(\tilde{\rho}(0) - \hat{\rho}_\Omega) \quad \text{a.e. in } \Omega, \quad z_\Gamma(0) = \beta_5(\tilde{\rho}_\Gamma(0) - \hat{\rho}_\Gamma) \quad \text{a.e. on } \Gamma. \tag{4.22}$$

Obviously, any sufficiently smooth solution (y, z, z_Γ) to (4.18)–(4.22) induces a solution (p, q, q_Γ) to the adjoint system (4.10)–(4.14) (and vice versa) by putting

$$p(x,t) := y(x,T-t), \quad q(x,t) := z(x,T-t), \quad q_\Gamma(x,t) = z_\Gamma(x,T-t). \tag{4.23}$$

Observe that, thanks to assumption (A7), we have $(z(0), z_\Gamma(0)) \in \mathcal{V}$. In addition, we recall the global bounds (2.7), (2.9), and the regularity result (2.10), which yield, in particular, that

$$\begin{aligned}&a := f''(\tilde{\rho}) + \pi'(\tilde{\rho}) - \tilde{\mu}\,g''(\tilde{\rho}) \in L^\infty(Q), \quad a_\Gamma := f''_\Gamma(\tilde{\rho}_\Gamma) + \pi'_\Gamma(\tilde{\rho}_\Gamma) \in L^\infty(\Sigma),\\ &\partial_t\tilde{\mu} \in L^2(0,T;L^6(\Omega)), \quad \partial_t\tilde{\rho} \in L^2(0,T;V).\end{aligned} \tag{4.24}$$

We aim to show that the system (4.18)–(4.22) has a unique solution triple (y, z, z_Γ) having the same regularity as requested for (p, q, q_Γ) in (4.15)–(4.17). We divide the proof of this claim into several steps.

<u>STEP 1:</u>

We first prove uniqueness. To this end, suppose that two solutions (y_i, z_i, z_{i_Γ}), $i = 1, 2$, with the asserted regularity are given. Then the triple (y, z, z_Γ), where $y := y_1 - y_2$, $z := z_1 - z_2$, $z_\Gamma := z_{1_\Gamma} - z_{2_\Gamma}$, satisfies the system that results if in (4.18)–(4.22) the terms containing the factors β_i, $1 \le i \le 5$, are omitted. In particular, $z(0) = 0$ and $z_\Gamma(0) = 0$. We then can infer from Lemma 2.3 that, for every $t \in (0, T]$,

$$
\begin{aligned}
&\|z\|^2_{H^1(0,t;H)\cap C^0([0,t];V)\cap L^2(0,t;H^2(\Omega))} + \|z_\Gamma\|^2_{H^1(0,t;H_\Gamma)\cap C^0([0,t];V_\Gamma)\cap L^2(0,t;H^2(\Gamma))} \\
&\le C_1 \|\sigma\|^2_{L^2(Q_t)}, \quad \text{with } \sigma := g'(\tilde\rho)\,(\partial_t\tilde\mu\, y - \tilde\mu\, \partial_t y),
\end{aligned}
\tag{4.25}
$$

where, here and in the remainder of the uniqueness proof, we denote by C_i, $i \in \mathbb{N}$, positive constants that depend only on the data of the system and on norms of the solutions. Now, by Hölder's and Young's inequalities, we have that

$$
\begin{aligned}
\|\sigma\|^2_{L^2(Q_t)} &\le C_2 \int_0^t\!\!\int_\Omega |\partial_t\tilde\mu\, y - \tilde\mu\, \partial_t y|^2 \,\mathrm{d}x\,\mathrm{d}s \\
&\le C_3 \int_0^t\!\!\int_\Omega |\partial_t y|^2 \,\mathrm{d}x\,\mathrm{d}s + C_4 \int_0^t \|\partial_t\tilde\mu(s)\|_4^2\, \|y(s)\|_4^2 \,\mathrm{d}s \\
&\le C_3 \int_0^t\!\!\int_\Omega |\partial_t y|^2 \,\mathrm{d}x\,\mathrm{d}s + C_5 \int_0^t \|\partial_t\tilde\mu(s)\|_6^2\, \|y(s)\|_V^2 \,\mathrm{d}s,
\end{aligned}
\tag{4.26}
$$

where the mapping $s \mapsto \|\partial_t\tilde\mu(s)\|_6^2$ belongs to $L^1(0, T)$.

Next, we add y on both sides of the equation resulting from (4.18), multiply by $\partial_t y$, and integrate over Q_t, where $t \in (0, T]$. Since $g(\tilde\rho) \ge 0$, we obtain from Hölder's and Young's inequalities that

$$
\begin{aligned}
&\int_0^t\!\!\int_\Omega |\partial_t y|^2 \,\mathrm{d}x\,\mathrm{d}s + \frac12 \|y(t)\|_V^2 \le C_6 \int_0^t\!\!\int_\Omega |\partial_t y|\,(|z| + (1 + |\partial_t\tilde\rho|)\,|y|) \,\mathrm{d}x\,\mathrm{d}s \\
&\le \frac14 \int_0^t\!\!\int_\Omega |\partial_t y|^2 \,\mathrm{d}x\,\mathrm{d}s + C_7 \int_0^t\!\!\int_\Omega (y^2 + z^2) \,\mathrm{d}x\,\mathrm{d}s + C_8 \int_0^t \|\partial_t\tilde\rho(s)\|_4\, \|y(s)\|_4\, \|\partial_t y(s)\|_2 \,\mathrm{d}s \\
&\le \frac12 \int_0^t\!\!\int_\Omega |\partial_t y|^2 \,\mathrm{d}x\,\mathrm{d}s + C_7 \int_0^t\!\!\int_\Omega (y^2 + z^2) \,\mathrm{d}x\,\mathrm{d}s + C_9 \int_0^t \|\partial_t\tilde\rho(s)\|_V^2\, \|y(s)\|_V^2 \,\mathrm{d}s\,,
\end{aligned}
\tag{4.27}
$$

where the mapping $s \mapsto \|\partial_t\tilde\rho(s)\|_V^2$ belongs to $L^1(0, T)$.

Now, we multiply the inequality (4.27) by $4\,C_1\,C_3$ and add the result to the inequality (4.25). Taking (4.26) into account, we then conclude from Gronwall's lemma that $y = z = 0$ in Q and $z_\Gamma = 0$ on Σ, whence the uniqueness is proved.

Step 2:

We now approximate the system (4.18)–(4.22), where we employ a similar approach as in the proof of Theorem 3.1. To this end, we consider for $\tau = \tau_N := T/N$, $N \in \mathbb{N}$, the retarded system

$$
\begin{aligned}
&(1 + 2g(\tilde\rho))\,\partial_t y^\tau + g'(\tilde\rho)\,\partial_t\tilde\rho\,\mathcal{T}_\tau(y^\tau) - \Delta y^\tau \\
&\quad = g'(\tilde\rho)\,\mathcal{T}_\tau(z^\tau) + \beta_1(\tilde\mu - \tilde\mu_Q) \quad \text{a.e. in } Q,
\end{aligned}
\tag{4.28}
$$

$$\partial_{\mathbf{n}} y^\tau = 0 \quad \text{a.e. on } \Sigma, \quad y^\tau(0) = 0 \quad \text{a.e. in } \Omega, \tag{4.29}$$

$$\partial_t z^\tau - \Delta z^\tau + a\, z^\tau = g'(\tilde\rho)(\partial_t\tilde\mu\, y^\tau - \tilde\mu\,\partial_t y^\tau) + \beta_2(\tilde\rho - \tilde\rho_Q) \quad \text{a.e. in } Q, \tag{4.30}$$

$$\partial_{\mathbf{n}} z^\tau + \partial_t z^\tau_\Gamma - \Delta_\Gamma z^\tau_\Gamma + a_\Gamma\, z^\tau_\Gamma = \beta_3(\tilde\rho_\Gamma - \tilde\rho_\Sigma), \quad z^\tau_{|\Sigma} = z^\tau_\Gamma \quad \text{a.e. on } \Sigma, \tag{4.31}$$

$$z^\tau(0) = \beta_4(\tilde\rho(0) - \hat\rho_\Omega) \quad \text{a.e. in } \Omega, \quad z^\tau_\Gamma(0) = \beta_5(\tilde\rho_\Gamma(0) - \hat\rho_\Gamma) \quad \text{a.e. on } \Gamma, \tag{4.32}$$

with the translation operator $\mathcal{T}_\tau$ introduced in (3.9), and where a, a_Γ are defined in (4.24). Putting again $\tau_N := T/N$, $t_n := n\tau_N$, and $I_n := (0, t_n)$, $1 \le n \le N$, for fixed $N \in \mathbb{N}$, we then consider for every $n \in \{1, \dots, N\}$ the initial-boundary value problem

$$\begin{aligned} &(1 + 2g(\tilde\rho))\, \partial_t y_n + g'(\tilde\rho)\, \partial_t\tilde\rho\, \mathcal{T}_{\tau_N}(y_{n-1}) - \Delta y_n \\ &\quad = g'(\tilde\rho)\, \mathcal{T}_{\tau_N}(z_{n-1}) + \beta_1(\tilde\mu - \tilde\mu_Q) \quad \text{a.e. in } \Omega \times I_n, \qquad (4.33)\\ &\partial_{\mathbf{n}} y_n = 0 \quad \text{a.e. on } \Gamma \times I_n, \quad y_n(0) = 0 \quad \text{a.e. in } \Omega, \qquad (4.34)\\ &\partial_t z_n - \Delta z_n + a\, z_n = g'(\tilde\rho)(\partial_t\tilde\mu\, y_n - \tilde\mu\, \partial_t y_n) + \beta_2(\tilde\rho - \tilde\rho_Q) \quad \text{a.e. in } \Omega \times I_n, \qquad (4.35)\\ &\partial_{\mathbf{n}} z_n + \partial_t z_{n_\Gamma} - \Delta_\Gamma z_{n_\Gamma} + a_\Gamma\, z_{n_\Gamma} = \beta_3(\tilde\rho_\Gamma - \tilde\rho_\Sigma), \quad z_{n|\Sigma} = z_{n_\Gamma} \quad \text{a.e. on } \Gamma \times I_n, \qquad (4.36)\\ &z_n(0) = \beta_4(\tilde\rho(0) - \hat\rho_\Omega) \quad \text{a.e. in } \Omega, \quad z_{n_\Gamma}(0) = \beta_5(\tilde\rho_\Gamma(0) - \hat\rho_\Gamma) \quad \text{a.e. on } \Gamma. \qquad (4.37) \end{aligned}$$

Here, it is understood that $\mathcal{T}_{\tau_N}(y_{n-1}) = 0$ and $\mathcal{T}_{\tau_N}(z_{n-1}) = \beta_4(\tilde\rho(0) - \hat\rho_\Omega)$ for $n = 1$. Using induction with respect to n, we again find that (4.33)–(4.37) has for every $n \in \{1, \dots, N\}$ a unique solution with the requested regularity. Once more, we confine ourselves to show the induction step $n-1 \longrightarrow n$. So, let $1 < n \le N$, and assume that for $1 \le k \le n-1$ the unique solutions (y_k, z_k, z_{k_Γ}) have already been constructed that satisfy the conditions

$$\begin{aligned} &y_k \in H^1(I_k; H) \cap C^0(\bar I_k; V) \cap L^2(I_k; W),\\ &z_k \in H^1(I_k; H) \cap C^0(\bar I_k; V) \cap L^2(I_k; H^2(\Omega)),\\ &z_{k_\Gamma} \in H^1(I_k; H_\Gamma) \cap C^0(\bar I_k; V_\Gamma) \cap L^2(I_k; H^2(\Gamma)). \qquad (4.38) \end{aligned}$$

Since $\tilde\rho \in C^0(\overline{Q})$ and $\partial_t\tilde\rho \in L^2(0, T; V)$, we obviously have that

$$1 + 2g(\tilde\rho) \in C^0(\overline{Q}), \quad g'(\tilde\rho)\, \mathcal{T}_{\tau_N}(z_{n-1}) - g'(\tilde\rho)\, \partial_t\tilde\rho\, \mathcal{T}_{\tau_N}(y_{n-1}) + \beta_1(\tilde\mu - \tilde\mu_Q) \in L^2(I_n; H).$$

We thus can infer from, e.g., [24, Thm. 2.1] that the initial-boundary value problem (4.33)–(4.34) enjoys a unique solution $y_n \in H^1(I_n; H) \cap C^0(\bar I_n; V) \cap L^2(I_n; W)$. We then substitute y_n in (4.35), recalling that $(z_n(0), z_{n_\Gamma}(0)) \in \mathcal{V}$. Moreover, we readily verify that

$$g'(\tilde\rho)(\partial_t\tilde\mu\, y_n - \tilde\mu\, \partial_t y_n) + \beta_2(\tilde\rho - \tilde\rho_Q) \in L^2(I_n; H), \quad \beta_3(\tilde\rho_\Gamma - \tilde\rho_\Sigma) \in L^2(I_n; H_\Gamma).$$

Hence, we can infer from Lemma 2.3 the existence of a unique solution pair (z_n, z_{n_Γ}) with

$$\begin{aligned} &z_n \in H^1(I_n; H) \cap C^0(\bar I_n; V) \cap L^2(I_n; H^2(\Omega)),\\ &z_{n_\Gamma} \in H^1(I_n; H_\Gamma) \cap C^0(\bar I_n; V_\Gamma) \cap L^2(I_n; H^2(\Gamma)). \end{aligned}$$

Arguing as in the proof of Theorem 3.1, we then conclude that (y_N, z_N, z_{N_Γ}) is the unique solution to the retarded problem (4.28)–(4.32) for $\tau = \tau_N$.

<u>STEP 3:</u>

In this part of the existence proof, we derive a priori estimates for the approximations (y_N, z_N, z_{N_Γ}), $N \in \mathbb{N}$, where we denote by C_i, $i \in \mathbb{N}$, positive constants that may depend on the data but not on $N \in \mathbb{N}$. For the sake of a better readability, we omit the superscript τ_N in the estimates, writing it only at the end of each estimation step.

FIRST ESTIMATE:

We add y on both sides of (4.28), multiply the resulting identity by $\partial_t y$, and integrate over Q_t, where $0 < t \le T$. Since $g(\tilde\rho) \ge 0$, we then find that

$$\int_0^t\!\!\int_\Omega |\partial_t y|^2 \,\mathrm{d}x\,\mathrm{d}s \,+\, \frac12\,\|y(t)\|_V^2 \,\le\, \sum_{j=1}^4 I_j, \tag{4.39}$$

where the quantities I_j, $1 \le j \le 4$, are specified and estimated below. Clearly, by Young's inequality and (A6) we infer that

$$I_1 := \int_0^t\!\!\int_\Omega y\,\partial_t y \,\mathrm{d}x\,\mathrm{d}s \,\le\, \frac15 \int_0^t\!\!\int_\Omega |\partial_t y|^2 \,\mathrm{d}x\,\mathrm{d}s \,+\, C_1 \int_0^t\!\!\int_\Omega |y|^2 \,\mathrm{d}x\,\mathrm{d}s, \tag{4.40}$$

$$I_4 := \beta_1 \int_0^t\!\!\int_\Omega (\tilde\mu - \tilde\mu_Q)\,\partial_t y \,\mathrm{d}x\,\mathrm{d}s \,\le\, \frac15 \int_0^t\!\!\int_\Omega |\partial_t y|^2 \,\mathrm{d}x\,\mathrm{d}s \,+\, C_2\,, \tag{4.41}$$

$$\begin{aligned} I_3 &:= \int_0^t\!\!\int_\Omega g'(\tilde\rho)\,\mathcal{T}_{\tau_N}(z)\,\partial_t y \,\mathrm{d}x\,\mathrm{d}s \,\le\, \frac15 \int_0^t\!\!\int_\Omega |\partial_t y|^2 \,\mathrm{d}x\,\mathrm{d}s \,+\, C_3 \int_0^t\!\!\int_\Omega |\mathcal{T}_{\tau_N}(z)|^2 \,\mathrm{d}x\,\mathrm{d}s \\ &\le\, \frac15 \int_0^t\!\!\int_\Omega |\partial_t y|^2 \,\mathrm{d}x\,\mathrm{d}s \,+\, C_4 \int_0^t\!\!\int_\Omega |z|^2 \,\mathrm{d}x\,\mathrm{d}s \,+\, C_5, \end{aligned} \tag{4.42}$$

where in the last estimate we have employed (3.10). Finally, we argue as in the estimates (3.33)–(3.35) to conclude that

$$\begin{aligned} I_2 :&= -\int_0^t\!\!\int_\Omega g'(\tilde\rho)\partial_t\tilde\rho\,\mathcal{T}_{\tau_N}(y)\,\partial_t y \,\mathrm{d}x\,\mathrm{d}s \\ &\le\, \frac15 \int_0^t\!\!\int_\Omega |\partial_t y|^2 \,\mathrm{d}x\,\mathrm{d}s \,+\, C_6 \int_0^t \psi(s)\|y(s)\|_V^2 \,\mathrm{d}s, \end{aligned} \tag{4.43}$$

where the function

$$s \mapsto \psi(s) := \begin{cases} \|\partial_t\tilde\rho(s+\tau_N)\|_V^2 & \text{if } 0 \le s \le T-\tau_N \\ 0 & \text{if } T-\tau_N < s \le T \end{cases}$$

is bounded in $L^1(0,T)$, uniformly in $N \in \mathbb{N}$. Combining (4.39)–(4.43), we have thus shown the estimate

$$\frac15\,\|\partial_t y\|_{L^2(Q_t)}^2 \,+\, \frac12\,\|y(t)\|_V^2 \,\le\, C_7 \,+\, C_8\,\|z\|_{L^2(Q_t)}^2 \,+\, C_9 \int_0^t (1+\psi(s))\|y(s)\|_V^2 \,\mathrm{d}s\,. \tag{4.44}$$

SECOND ESTIMATE:

Next, we add z on both sides of (4.30), and z_Γ on both sides of (4.31), and multiply the first resulting equation by $\partial_t z$. Integrating over Q_t, where $0 < t \le T$, we find the inequality

$$\begin{aligned}
&\int_0^t\!\!\int_\Omega |\partial_t z|^2 \,\mathrm{d}x\,\mathrm{d}s \,+\, \int_0^t\!\!\int_\Gamma |\partial_t z_\Gamma|^2 \,\mathrm{d}\Gamma\,\mathrm{d}s \,+\, \frac{1}{2}\left(\|z(t)\|_V^2 + \|z_\Gamma(t)\|_{V_\Gamma}^2\right) \\
&\le \int_0^t\!\!\int_\Omega \left(1 + \|a\|_{L^\infty(Q)}\right) |z|\,|\partial_t z| \,\mathrm{d}x\,\mathrm{d}s \,+\, \int_0^t\!\!\int_\Omega \left(1 + \|a_\Gamma\|_{L^\infty(\Sigma)}\right) |z_\Gamma|\,|\partial_t z_\Gamma| \,\mathrm{d}\Gamma\,\mathrm{d}s \\
&\quad + \beta_2 \int_0^t\!\!\int_\Omega (\tilde\rho - \tilde\rho_Q)\,\partial_t z \,\mathrm{d}x\,\mathrm{d}s \,+\, \beta_3 \int_0^t\!\!\int_\Omega (\tilde\rho_\Gamma - \tilde\rho_\Sigma)\,\partial_t z_\Gamma \,\mathrm{d}\Gamma\,\mathrm{d}s \\
&\quad + C_{10} \int_0^t\!\!\int_\Omega \left(|\partial_t\tilde\mu|\,|y| + |\tilde\mu|\,|\partial_t y|\right)\,|\partial_t z| \,\mathrm{d}x\,\mathrm{d}s \\
&\quad + \frac{1}{2}\left(\|\beta_4(\tilde\rho(0) - \hat\rho_\Omega)\|_V^2 + \|\beta_5(\tilde\rho_\Gamma(0) - \hat\rho_\Gamma)\|_{V_\Gamma}^2\right)
\end{aligned} \tag{4.45}$$

and observe that the terms in the last line are finite by assumption (A7). Thanks to (A6) and Young's inequality, the first four summands on the right-hand side are bounded by an expression of the form

$$\frac{1}{4}\left(\|\partial_t z\|_{L^2(Q_t)}^2 + \|\partial_t z_\Gamma\|_{L^2(\Sigma_t)}^2\right) + C_{11}\left(1 \,+\, \|z\|_{L^2(Q_t)}^2 \,+\, \|z_\Gamma\|_{L^2(\Sigma_t)}^2\right). \tag{4.46}$$

Moreover, since $\tilde\mu \in L^\infty(Q)$, we have

$$C_{10} \int_0^t\!\!\int_\Omega |\tilde\mu|\,|\partial_t y|\,|\partial_t z| \,\mathrm{d}x\,\mathrm{d}s \,\le\, \frac{1}{4}\|\partial_t z\|_{L^2(Q_t)}^2 \,+\, C_{12}\,\|\partial_t y\|_{L^2(Q_t)}^2 . \tag{4.47}$$

In addition, by also using Hölder's inequality,

$$\begin{aligned}
&C_{10} \int_0^t\!\!\int_\Omega |\partial_t\tilde\mu|\,|y|\,|\partial_t z| \,\mathrm{d}x\,\mathrm{d}s \,\le\, C_{13} \int_0^t \|\partial_t\tilde\mu(s)\|_6\,\|y(s)\|_3\,\|\partial_t z(s)\|_2 \,\mathrm{d}s \\
&\le\, \frac{1}{4}\|\partial_t z\|_{L^2(Q_t)}^2 \,+\, C_{14} \int_0^t \|\partial_t\tilde\mu(s)\|_6^2\,\|y(s)\|_V^2 \,\mathrm{d}s .
\end{aligned} \tag{4.48}$$

Combining the estimates (4.45)–(4.48), we have thus shown that

$$\begin{aligned}
&\frac{1}{4}\,\|\partial_t z\|_{L^2(Q_t)}^2 \,+\, \frac{3}{4}\,\|\partial_t z_\Gamma\|_{L^2(\Sigma_t)}^2 \,+\, \frac{1}{2}\left(\|z(t)\|_V^2 + \|z_\Gamma(t)\|_{V_\Gamma}^2\right) \\
&\le\, C_{11}\left(1 \,+\, \|z\|_{L^2(Q_t)}^2 \,+\, \|z_\Gamma\|_{L^2(\Sigma_t)}^2\right) \,+\, C_{12}\,\|\partial_t y\|_{L^2(Q_t)}^2 \\
&\quad + C_{14} \int_0^t \|\partial_t\tilde\mu(s)\|_6^2\,\|y(s)\|_V^2 \,\mathrm{d}s + C_{15} ,
\end{aligned} \tag{4.49}$$

where the mapping $s \mapsto \|\partial_t\tilde\mu(s)\|_6^2$ belongs to $L^1(0,T)$.

Now, we multiply (4.44) by $10\,C_{12}$ and add the resulting inequality to (4.49). It then follows from Gronwall's lemma that, for all $t \in (0,T]$ and $N \in \mathbb{N}$,

$$\begin{aligned}
&\|y^{\tau_N}\|_{H^1(0,t;H)\cap L^\infty(0,t;V)} \,+\, \|z^{\tau_N}\|_{H^1(0,t;H)\cap L^\infty(0,t;V)} \\
&\quad + \|z_\Gamma^{\tau_N}\|_{H^1(0,t;H_\Gamma)\cap L^\infty(0,t;V_\Gamma)} \,\le\, C_{16} .
\end{aligned} \tag{4.50}$$

Third estimate:

Now that the basic estimate (4.50) is shown, we can easily conclude from comparison in (4.28) and (4.30), respectively, that

$$\|\Delta y\|_{L^2(Q)} + \|\Delta z\|_{L^2(Q)} \leq C_{17}, \tag{4.51}$$

whence, using the boundary condition in (4.29) and standard elliptic estimates, we deduce that

$$\|y\|_{L^2(0,T;W)} \leq C_{18}\,. \tag{4.52}$$

Moreover, we invoke [1, Thm. 3.2, p. 1.79] to conclude that

$$\int_0^T \|z(t)\|^2_{H^{3/2}(\Omega)}\,\mathrm{d}t \leq C_{19}\int_0^T \Big(\|\Delta z(t)\|^2_H + \|z_\Gamma(t)\|^2_{H^1(\Gamma)}\Big)\,\mathrm{d}t,$$

which entails that

$$\|z\|_{L^2(0,T;H^{3/2}(\Omega))} \leq C_{20}\,. \tag{4.53}$$

Hence, by the trace theorem (cf. [1, Thm. 2.27, p. 1.64]), we have that

$$\|\partial_{\mathbf{n}} z\|_{L^2(0,T;H_\Gamma)} \leq C_{21}\,. \tag{4.54}$$

Comparison in (4.31) then yields that

$$\|\Delta_\Gamma z_\Gamma\|_{L^2(0,T;H_\Gamma)} \leq C_{22}\,, \tag{4.55}$$

and it follows from the boundary version of the elliptic estimates that

$$\|z_\Gamma\|_{L^2(0,T;H^2(\Gamma))} \leq C_{23}\,. \tag{4.56}$$

At this point, (4.50), (4.51), (4.56) allow us to improve (4.53) as

$$\|z\|_{L^2(0,T;H^2(\Omega))} \leq C_{24}\,. \tag{4.57}$$

Recalling that the embeddings $(H^1(0,T;H) \cap L^2(0,T;H^2(\Omega))) \subset C^0([0,T];V)$ and $(H^1(0,T;H_\Gamma) \cap L^2(0,T;H^2(\Gamma)) \subset C^0([0,T];V_\Gamma)$ are continuous, we have finally shown the estimate

$$\begin{aligned}&\|y^{\tau_N}\|_{H^1(0,T;H)\cap C^0([0,T];V)\cap L^2(0,T;W)} + \|z^{\tau_N}\|_{H^1(0,T;H)\cap C^0([0,T];V)\cap L^2(0,T;H^2(\Omega))}\\ &+ \|z_\Gamma^{\tau_N}\|_{H^1(0,T;H_\Gamma)\cap C^0([0,T];V_\Gamma)\cap L^2(0,T;H^2(\Gamma))} \leq C_{25}\,.\end{aligned} \tag{4.58}$$

Step 4:

We now conclude the existence part of the proof. To this end, we observe that (4.58) yields the existence of a triple (y, z, z_Γ) such that, at least for a subsequence which is again indexed by N, we have that

$$y^{\tau_N} \to y \quad \text{weakly in } H^1(0,T;H)\cap C^0([0,T];V)\cap L^2(0,T;W)\,, \tag{4.59}$$

$$z^{\tau_N} \to z \quad \text{weakly in } H^1(0,T;H)\cap C^0([0,T];V)\cap L^2(0,T;H^2(\Omega))\,, \tag{4.60}$$

$$z_\Gamma^{\tau_N} \to z_\Gamma \quad \text{weakly in } H^1(0,T;H_\Gamma)\cap C^0([0,T];V_\Gamma)\cap L^2(0,T;H^2(\Gamma)) \tag{4.61}$$

as $N \to \infty$. We are now in a similar situation as in the proof of Theorem 3.1 after showing the corresponding convergence results (3.43)–(3.45). Adapting the arguments used there (with obvious modifications) to our situation, we can conclude that (y, z, z_Γ) is in fact a solution to the transformed system (4.18)–(4.22) having the asserted regularity properties. As this is a rather straightforward repetition of the argumentation utilized there, we may allow ourselves to leave it to the reader to work out the details. Since, as it was shown in Step 1, such a solution is uniquely determined, we can conclude that the adjoint state system (4.10)–(4.14) has indeed a unique solution satisfying (4.15)–(4.17). The assertion is thus completely proved. $\square$

We now can eliminate the functions $(\eta, \zeta, \zeta_\Gamma)$ from the variational inequality (3.77). We have the following result.

Corollary 4.3: *Suppose that* (A1)–(A6) *are satisfied, assume that* $\bar u_\Gamma \in \mathcal{U}_{\rm ad}$ *is an optimal control whose associated state* $(\bar\mu, \bar\rho, \bar\rho_\Gamma) = \mathcal{S}(\bar u_\Gamma)$ *fulfills* (A7), *and let* (p, q, q_Γ) *be the corresponding unique solution to the adjoint state system* (4.10)–(4.14) *established in Theorem 4.2. Then there holds the variational inequality*

$$\int_0^T\!\!\int_\Gamma (q_\Gamma + \beta_6\,\bar u_\Gamma)\,(v_\Gamma - \bar u_\Gamma)\,{\rm d}\Gamma\,{\rm d}t \,\geq\, 0 \qquad \forall\, v_\Gamma \in \mathcal{U}_{\rm ad}. \tag{4.62}$$

Proof: Let $v_\Gamma \in \mathcal{U}_{\rm ad}$ be arbitrary, and let $h := v_\Gamma - \bar u_\Gamma$. We multiply (3.1) by p, (3.3) by q, (4.10) by $-\eta$, (4.12) by $-\zeta$, add the resulting equations and integrate over Q and by parts. A straightforward calculation, in which many terms cancel out, leads to the identity

$$\begin{aligned}
&\int_0^T\!\!\int_\Omega \partial_t\big((1+2g(\bar\rho))\,p\,\eta + q\,\zeta\big)\,{\rm d}x\,{\rm d}t \,+\, \int_0^T\!\!\int_\Gamma (\zeta_\Gamma\,\partial_{\mathbf n} q - q_\Gamma\,\partial_{\mathbf n}\zeta)\,{\rm d}\Gamma\,{\rm d}t \\
&+ \int_0^T\!\!\int_\Omega \{\partial_t\bar\mu\, g'(\bar\rho)\,\zeta\,p + \bar\mu\, g''(\bar\rho)\,\partial_t\bar\rho\,\zeta\,p + \bar\mu\, g'(\bar\rho)\,\partial_t\zeta\,p + \bar\mu\, g'(\bar\rho)\,\zeta\,\partial_t p\}\,{\rm d}x\,{\rm d}t \\
&= -\,\beta_1 \int_0^T\!\!\int_\Omega (\bar\mu - \hat\mu_Q)\,\eta\,{\rm d}x\,{\rm d}t \,-\, \beta_2 \int_0^T\!\!\int_\Omega (\bar\rho - \hat\rho_Q)\,\zeta\,{\rm d}x\,{\rm d}t\,.
\end{aligned} \tag{4.63}$$

Clearly, the integrand in the curly brackets equals $\partial_t(\bar\mu\, g'(\bar\rho)\,\zeta\,p)$, whence the corresponding integral vanishes since $\zeta(0) = p(T) = 0$. Moreover, owing to (3.4) and (4.13),

$$\int_0^T\!\!\int_\Gamma (\zeta_\Gamma\,\partial_{\mathbf n} q - q_\Gamma\,\partial_{\mathbf n}\zeta)\,{\rm d}\Gamma\,{\rm d}t \,=\, \int_0^T\!\!\int_\Gamma \big(\partial_t(q_\Gamma\,\zeta_\Gamma) + \beta_3\,(\bar\rho_\Gamma - \hat\rho_\Sigma)\zeta_\Gamma - q_\Gamma(v_\Gamma - \bar u_\Gamma)\big)\,{\rm d}\Gamma\,{\rm d}t\,, \tag{4.64}$$

because the terms involving the Laplace-Beltrami operator cancel each other. Recalling that $\eta(0) = \zeta(0) = p(T) = 0$ in Ω and $\zeta_\Gamma(0) = 0$ on Γ, invoking the end point conditions (4.14), and rearranging terms, we finally arrive at the identity

$$\begin{aligned}
&\beta_1 \int_0^T\!\!\int_\Omega (\bar\mu - \hat\mu_Q)\,\eta\,{\rm d}x\,{\rm d}t \,+\, \beta_2 \int_0^T\!\!\int_\Omega (\bar\rho - \hat\rho_Q)\,\zeta\,{\rm d}x\,{\rm d}t \,+\, \beta_3 \int_0^T\!\!\int_\Gamma (\bar\rho_\Gamma - \hat\rho_\Sigma)\,\zeta_\Gamma\,{\rm d}\Gamma\,{\rm d}t \\
&+\, \beta_4 \int_\Omega (\bar\rho(T) - \hat\rho_\Omega)\,\zeta(T)\,{\rm d}x \,+\, \beta_5 \int_\Gamma (\bar\rho_\Gamma(T) - \hat\rho_\Gamma)\,\zeta_\Gamma(T)\,{\rm d}\Gamma \\
&= \int_0^T\!\!\int_\Gamma q_\Gamma\,(v_\Gamma - \bar u_\Gamma)\,{\rm d}\Gamma\,{\rm d}t\,.
\end{aligned} \tag{4.65}$$

The assertion then follows from insertion of this identity in (3.77). □

REMARK 4.4: If $\beta_6 > 0$, then (4.62) implies that $\bar{u}_\Gamma$ is nothing but the $L^2(\Sigma)$-orthogonal projection of $-\beta_6^{-1} q_\Gamma$ onto $\mathcal{U}_{\mathrm{ad}}$.

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