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Distributed optimal control of a nonstandard system of phase field equations

Dedicated to Prof. Dr. Ingo Müller on the occasion of his 75th birthday

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Abstract

We investigate a distributed optimal control problem for a phase field model of Cahn-Hilliard type. The model describes two-species phase segregation on an atomic lattice under the presence of diffusion; it has been introduced recently in [4], on the basis of the theory developed in [15], and consists of a system of two highly nonlinearly coupled PDEs. For this reason, standard arguments of optimal control theory do not apply directly, although the control constraints and the cost functional are of standard type. We show that the problem admits a solution, and we derive the first-order necessary conditions of optimality.

1 Introduction

Let $\Omega \subset \mathbb{R}^3$ denote an open and bounded domain whose smooth boundary Γ has outward unit normal $\mathbf{n}$, let $T > 0$ be a given final time, and let $Q := \Omega \times (0,T)$, $\Sigma := \Gamma \times (0,T)$. In this paper, we study distributed optimal control problems of the following form:

(CP) Minimize the cost functional

$$\begin{aligned} J(u,\rho,\mu) \;=\; & \frac{1}{2}\int_\Omega |\rho(x,T)-\rho_T(x)|^2\,dx + \frac{\beta_1}{2}\int_0^T\!\!\int_\Omega |\mu(x,t)-\mu_T(x,t)|^2\,dx\,dt \\ & + \frac{\beta_2}{2}\int_0^T\!\!\int_\Omega |u(x,t)|^2\,dx\,dt \end{aligned} \tag{1.1}$$

subject to the state system

$$(\varepsilon + 2\,\rho)\mu_t + \mu\rho_t - \Delta\mu = u \quad \text{a.e. in } Q, \tag{1.2}$$

$$\delta\rho_t - \Delta\rho + f'(\rho) = \mu \quad \text{a.e. in } Q, \tag{1.3}$$

$$\frac{\partial\rho}{\partial\mathbf{n}} = \frac{\partial\mu}{\partial\mathbf{n}} = 0 \quad \text{a.e. on } \Sigma, \tag{1.4}$$

$$\rho(x,0) = \rho_0(x)\,, \quad \mu(x,0) = \mu_0(x)\,, \quad \text{a.e. in } \Omega, \tag{1.5}$$

and to the box control constraints

$$u \in U_{ad} = \{u \in L^\infty(Q)\,;\, 0 \le u \le U \quad \text{a.e. in } Q\}\,. \tag{1.6}$$

Here, $\beta_1 \ge 0$, $\beta_2 \ge 0$, $\varepsilon > 0$, and $\delta > 0$ are constants; $U \in L^\infty(Q)$ denotes a given bound, and $\rho_T \in L^2(\Omega)$ and $\mu_T \in L^2(Q)$ represent prescribed target functions of the tracking-type functional J. Although for large parts of the subsequent analysis much more general cost functionals could be admitted, we restrict ourselves to the above situation for the sake of a simpler exposition.

The state system (1.2)–(1.5) constitutes a phase field model of Cahn-Hilliard type that describes phase segregation of two species (atoms and vacancies, say) on a lattice in the presence of diffusion; it has been introduced recently in [15, 4]. The state variables are the *order parameter* ρ, interpreted as a volumetric density, and the *chemical potential* μ. For physical reasons, we must have $0 \le \rho \le 1$ and $\mu > 0$ almost everywhere in Q. The control function u on the right-hand side of (1.2) plays the role of a *microenergy source* (see below). Moreover, the nonlinearity f is a double-well potential defined in (0,1), whose derivative f' is singular at the endpoints $\rho = 0$ and $\rho = 1$: e. g., $f = f_1 + f_2$, with f_2 smooth and $f_1(\rho) = c\,(\rho\,\log(\rho) + (1-\rho)\,\log(1-\rho))$, with c a positive constant.

System (1.2)–(1.5) is singular, with highly nonlinear and nonstandard coupling. In particular, nasty nonlinear terms involving time derivatives occur in (1.2), and the expression $f'(\rho)$ in (1.3) may become singular. For the case $u = 0$ (no control), this system was analyzed in a recent paper [4]; the case $\varepsilon \searrow 0$ was studied in [5]. We also refer to the papers [2] and [3], where the corresponding Allen-Cahn model was discussed.

The mathematical literature on control problems for phase field systems is scarce and usually restricted to the so-called *Caginalp model* of phase transitions (see, e. g., [11], [9], [10], [17], and the references given there). More general, thermodynamically consistent phase field models were the subject of [13]. Control problems for the system (1.2)–(1.5) have never been studied before. We remark at this place that it would be a challenging task to study *boundary* control problems for the PDE system (1.2), (1.3) in place of distributed ones as in this paper; notice, however, that this would require to first establish appropriate well-posedness results for non-homogeneous Neumann boundary conditions or for non-homogeneous boundary conditions of third kind. Such results are presently not available.

The paper is organized as follows: below, we briefly recall the thermodynamic background of the state system (1.2)–(1.5). In Section 2, we establish the existence of a solution to the optimal control problem. First-order necessary optimality conditions, as usual given in terms of the adjoint system and a variational inequality, are derived in Section 3. A large part of this analysis is devoted to proving that the control-to-state mapping is directionally differentiable in appropriate function spaces.

1.1 Some thermodynamic background

The state equations (1.2), (1.3) result from the balances of microenergies and microforces postulated in a model for phase segregation and diffusion of atomic species on a lattice introduced in [15], a paper we refer the reader to for details. That model is a variation of the Cahn-Hilliard system

$$\rho_t - \kappa\,\Delta\mu = 0, \quad \mu = -\Delta\rho + f'(\rho), \tag{1.7}$$

when, for the sake of simplicity, the mobility coefficient $\kappa > 0$ is taken equal to one. Customarily, the equations in (1.7) are combined so as to get the well-known *Cahn-Hilliard equation*

$$\rho_t = \kappa\,\Delta(-\Delta\rho + f'(\rho)), \tag{1.8}$$

which describes diffusive phase separation processes in a two-phase material body.

A generalization of (1.8) was introduced by Fried and Gurtin in the papers [6] and [8]. Here is their line of reasoning:

(i) to regard the second equation in (1.7) as a *balance of microforces*:

$$\mathrm{div}\,\boldsymbol{\xi} + \pi + \gamma = 0, \tag{1.9}$$

where the distance microforce per unit volume is split into an internal part π and an external part γ, and where the contact microforce per unit area of a surface oriented by its normal $\boldsymbol{n}$ is measured by $\boldsymbol{\xi}\cdot\boldsymbol{n}$ in terms of the *microstress* vector $\boldsymbol{\xi}$;

(ii) to interpret the first equation in (1.7) as a *balance law for the order parameter*:

$$\rho_t = -\mathrm{div}\,\boldsymbol{h} + \sigma, \tag{1.10}$$

where the pair $(\boldsymbol{h},\sigma)$ is the *inflow* of ρ;

(iii) to restrict the admissible constitutive choices for $\pi, \boldsymbol{\xi}, \boldsymbol{h}$, and the *free energy density* ψ, to those consistent in the sense of Coleman and Noll [1], with an *ad hoc* version of the Second Law of Thermodynamics – namely, a postulated "dissipation inequality that accommodates diffusion" – given in the form

$$\psi_t + (\pi - \mu)\,\rho_t - \boldsymbol{\xi}\cdot\nabla\rho_t + \boldsymbol{h}\cdot\nabla\mu \le 0 \tag{1.11}$$

(cf., in particular, Eq. (3.6) of [8]). Within this framework, an admissible set of constitutive prescriptions turns out to be:

$$\psi = \widehat{\psi}(\rho,\nabla\rho), \quad \widehat{\pi}(\rho,\nabla\rho,\mu) = \mu - \partial_\rho\widehat{\psi}(\rho,\nabla\rho), \quad \widehat{\boldsymbol{\xi}}(\rho,\nabla\rho) = \partial_{\nabla\rho}\widehat{\psi}(\rho,\nabla\rho), \tag{1.12}$$

together with

$$\boldsymbol{h} = -\boldsymbol{M}\nabla\mu, \quad \text{where } \boldsymbol{M} = \widehat{\boldsymbol{M}}(\rho,\nabla\rho,\mu,\nabla\mu). \tag{1.13}$$

Moreover, it follows that the tensor-valued *mobility mapping* $\boldsymbol{M}$ must obey the inequality

$$\nabla\mu\cdot\widehat{\boldsymbol{M}}(\rho,\nabla\rho,\mu,\nabla\mu)\nabla\mu \ge 0.$$

It follows from (1.9), (1.10), (1.12), and $(1.13)_1$ that

$$\rho_t = \mathrm{div}\,\Big(\boldsymbol{M}\nabla\Big(\partial_\rho\widehat{\psi}(\rho,\nabla\rho) - \mathrm{div}\big(\partial_{\nabla\rho}\widehat{\psi}(\rho,\nabla\rho)\big) - \gamma\Big)\Big) + \sigma\,;$$

the Cahn-Hilliard equation (1.8) results for the special choice

$$\widehat{\psi}(\rho,\nabla\rho) = f(\rho) + \frac{1}{2}|\nabla\rho|^2, \quad \boldsymbol{M} = \kappa\mathbf{1}, \tag{1.14}$$

provided that the external distance microforce γ and the order parameter source term σ are taken identically zero.

In contrast to the theory developed by Fried and Gurtin, the approach taken in [15] was the following: while step (i) was retained, the order parameter balance (1.10) and the dissipation inequality (1.11) were replaced, respectively, by the *microenergy balance*

$$\varepsilon_t = e + w, \quad e := -\mathrm{div}\,\overline{\boldsymbol{h}} + \overline{\sigma}, \quad w := -\pi\,\rho_t + \boldsymbol{\xi}\cdot\nabla\rho_t, \tag{1.15}$$

and the *microentropy imbalance*

$$\eta_t \geq -\text{div}\, \boldsymbol{h} + \sigma, \quad \boldsymbol{h} := \mu \overline{\boldsymbol{h}}, \quad \sigma := \mu\, \overline{\sigma}. \tag{1.16}$$

The salient new feature of this approach to phase segregation modeling is that the *microentropy inflow* $(\boldsymbol{h}, \sigma)$ is deemed proportional to the *microenergy inflow* $(\overline{\boldsymbol{h}}, \overline{\sigma})$ through the *chemical potential* μ; consistently, the free energy is defined to be

$$\psi := \varepsilon - \mu^{-1}\eta, \tag{1.17}$$

where the chemical potential plays the same role as the *coldness* in the deduction of the heat equation. Just as the absolute temperature is a macroscopic measure of microscopic *agitation*, its inverse – the coldness – measures microscopic *quiet*. Likewise, as argued in [15], the chemical potential can be seen as a macroscopic measure of microscopic *organization*; and, just as is always done for coldness, one can provisionally assume that μ is positive almost everywhere in Q. This assumption, which is important to proving that the resulting system of field equations does have solutions, must be justified a posteriori. The requirement that μ be positive is also the reason why we cannot admit negative controls u in the control problem (1.1)–(1.6).

Combining (1.15)-(1.17), and assuming that $\mu > 0$, one finds that

$$\psi_t \leq -\eta\, \partial_t(\mu^{-1}) + \mu^{-1}\, \overline{\boldsymbol{h}} \cdot \nabla\mu - \pi\, \rho_t + \boldsymbol{\xi} \cdot \nabla\rho_t\,; \tag{1.18}$$

this reduced dissipation inequality replaces (1.11) in filtering out *à la* Coleman-Noll the inadmissible constitutive choices.

On taking all of the constitutive mappings delivering $\pi, \boldsymbol{\xi}, \eta$, and $\overline{\boldsymbol{h}}$, to depend in principle on the list of variables $\rho, \nabla\rho, \mu, \nabla\mu$, and on choosing

$$\psi = \widehat{\psi}(\rho, \nabla\rho, \mu) = -\mu\, \rho + f(\rho) + \frac{1}{2}|\nabla\rho|^2, \tag{1.19}$$

one sees that compatibility with (1.18) implies that

$$\begin{aligned}
\widehat{\pi}(\rho, \nabla\rho, \mu) &= -\partial_\rho \widehat{\psi}(\rho, \nabla\rho, \mu) = \mu - f'(\rho), \\
\widehat{\boldsymbol{\xi}}(\rho, \nabla\rho, \mu) &= \partial_{\nabla\rho} \widehat{\psi}(\rho, \nabla\rho, \mu) = \nabla\rho, \\
\widehat{\eta}(\rho, \nabla\rho, \mu) &= \mu^2 \partial_\mu \widehat{\psi}(\rho, \nabla\rho, \mu) = -\mu^2\rho,
\end{aligned} \tag{1.20}$$

together with

$$\widehat{\overline{\boldsymbol{h}}}(\rho, \nabla\rho, \mu, \nabla\mu) = \widehat{\boldsymbol{H}}(\rho, \nabla\rho, \mu, \nabla\mu)\nabla\mu, \quad \nabla\mu \cdot \widehat{\boldsymbol{H}}(\rho, \nabla\rho, \mu, \nabla\mu)\nabla\mu \geq 0.$$

If we now choose for $\widehat{\boldsymbol{H}}$ the simplest expression $\boldsymbol{H} = \kappa\mathbf{1}$, implying a constant and isotropic mobility, and if we once again assume that the external distance microforce γ and the source $\overline{\sigma}$ are null, then we can infer from (1.20) and (1.17) that the microforce balance (1.9) and the energy balance (1.15) become, respectively,

$$\text{div}(\nabla\rho) + \mu - f'(\rho) = 0, \tag{1.21}$$

$$2\rho\,\mu_t + \mu\,\rho_t - \kappa\,\Delta\mu = 0. \tag{1.22}$$

This is a nonlinear system for the unknowns ρ and μ, to be compared with system (1.7): while equations (1.21) and $(1.7)_2$ coincide, equation (1.22) is considerably more difficult to handle than $(1.7)_1$. Indeed, the latter is linear while the former is not; moreover, the time derivatives of ρ and μ are both present in (1.22), and there are nonconstant factors in front of both μ_t and ρ_t that should remain positive during the entire evolution. Note that, for nonzero microenergy source $\bar\sigma$, Eq. (1.22) becomes:

$$2\,\rho\,\mu_t \,+\, \mu\,\rho_t - \kappa\,\Delta\mu = -\bar\sigma. \tag{1.23}$$

In this sense, the control variable u in (1.2) is nothing but $-\bar\sigma$.

So far, it has not been possible to tackle the system (1.21), (1.22) (nor (1.21), (1.23)) mathematically. Not so for system (1.2), (1.3), a regularized version of (1.21), (1.23) (with $u = -\bar\sigma$) obtained by introducing the extra terms $\varepsilon\,\partial_t\mu$ in (1.23) and $\delta\,\partial_t\rho$ in (1.21), with small positive coefficients ε and δ (our motivations for including such terms have been proposed and emphasized in [4]).

2 Problem statement and existence

Consider the optimal control problem (1.2)–(1.6). For convenience, we introduce the abbreviated notation $H = L^2(\Omega)$, $V = H^1(\Omega)$, $W = \{w \in H^2(\Omega)\,;\, \partial w/\partial\mathbf{n} = 0 \ \text{ on } \Gamma\}$. We endow these spaces with their standard norms, for which we use self-explaining notation like $\|\cdot\|_V$; for simplicity, we also write $\|\cdot\|_H$ for the norm in the space $H\times H\times H$. Recall that the embeddings $W\subset V\subset H$ are compact. Moreover, since V is dense in H, we can identify H with a subspace of V^* in the usual way, i.e., by setting $\langle u, v\rangle_{V^*,V} = (u,v)_H$ for all $u\in H$ and $v\in V$, where $\langle\cdot\,,\,\cdot\rangle_{V^*,V}$ denotes the duality pairing between V^* and V. Then also the embedding $H\subset V^*$ is compact, and since $N\le 3$, we have the continuous Sobolev embeddings $W\subset C(\overline\Omega)$ and $V\subset L^6(\Omega)$.

We make the following assumptions on the data:

(A1) $f = f_1 + f_2$, where $f_1\in C^2(0,1)$ is convex, $f_2\in C^2[0,1]$, and

$$\lim_{r\searrow 0} f_1'(r) = -\infty, \quad \lim_{r\nearrow 1} f_1'(r) = +\infty. \tag{2.1}$$

(A2) $\rho_0\in W$, $f'(\rho_0)\in H$, $\mu_0\in V\cap L^\infty(\Omega)$, and

$$\inf\{\rho_0(x);\, x\in\Omega\} > 0, \quad \sup\{\rho_0(x);\, x\in\Omega\} < 1, \quad \mu_0\ge 0 \text{ a.e. in } \Omega. \tag{2.2}$$

Notice that (A2) implies that $\rho_0\in C(\overline\Omega)$, and that the convexity of f_1 implies that $f(\rho_0)\in H$.

An argumentation that parallels (and thus needs no repetition) the lines of the proofs of Theorem 2.2 and Theorem 2.3 of [4] (where we had $u = 0$) shows that the following well-posedness result holds for the state system (1.2)–(1.5):

Theorem 2.1 *Suppose that the hypotheses* (A1) *and* (A2) *are satisfied. Then we have:*

(i) *For every* $u \in U_{ad}$ *the state system* (1.2)–(1.5) *has a unique solution* (ρ, μ) *such that*

$$\rho \in W^{1,\infty}(0,T;H) \cap H^1(0,T;V) \cap L^\infty(0,T;W), \tag{2.3}$$

$$\mu \in H^1(0,T;H) \cap C^0([0,T];V) \cap L^2(0,T;W) \cap L^\infty(Q). \tag{2.4}$$

(ii) *There are constants* $0 < \rho_* < \rho^* < 1$, $\mu^* > 0$, *and* $K_1^* > 0$, *depending only on the data, such that for every* $u \in U_{ad}$ *the corresponding solution* (ρ, μ) *satisfies*

$$0 < \rho_* \le \rho \le \rho^* < 1, \quad 0 \le \mu \le \mu^*, \quad \text{a. e. in } Q, \tag{2.5}$$

$$\|\rho\|_{W^{1,\infty}(0,T;H)\cap H^1(0,T;V)\cap L^\infty(0,T;W)} + \|\mu\|_{H^1(0,T;H)\cap C^0([0,T];V)\cap L^2(0,T;W)\cap L^\infty(Q)} \le K_1^*. \tag{2.6}$$

(iii) *Let* $u_1, u_2 \in U_{ad}$, *and let* $(\rho_1, \mu_1), (\rho_2, \mu_2)$ *be the corresponding solutions to* (1.2)–(1.5). *Moreover, let* $u = u_1 - u_2$, $\rho = \rho_1 - \rho_2$, $\mu = \mu_1 - \mu_2$. *Then, for all* $t \in [0,T]$,

$$\max_{0 \le s \le t} \left(\|\mu(s)\|_H^2 + \|\rho(s)\|_V^2 \right) + \int_0^t \left(\|\mu(s)\|_V^2 + \|\rho_t(s)\|_H^2 \right) ds \le K_2^* \int_0^t \|u(s)\|_H^2 \, ds, \tag{2.7}$$

with a constant $K_2^* > 0$ *that may depend on the data, but not on* u_1, u_2.

Remarks: 1. Owing to (2.7), the solution operator $S : u \mapsto (\rho, \mu)$ is Lipschitz continuous as a mapping from U_{ad} (viewed as a subset of $L^2(Q)$) into $(H^1(0,T;H) \cap C^0([0,T];V)) \times (L^2(0,T;V) \cap C^0([0,T];H))$.

2. Thanks to (2.5) and to $f \in C^2(0,1)$, we have $f'(\rho) \in L^\infty(Q)$. Moreover, owing to (2.4) and to the embedding $V \subset L^6(\Omega)$, we have $\mu \in C^0([0,T];L^6(\Omega))$. Note that (2.3) implies, in particular, that ρ is continuous from $[0,T]$ to $H^s(\Omega)$ for all $s < 2$. Now, provided that s is sufficiently large, we have $H^s(\Omega) \subset C(\overline{\Omega})$; consequently, $\rho \in C(\overline{Q})$. Hence, without loss of generality (by possibly choosing a larger K_1^*), we may assume that also

$$\|\rho\|_{C(\overline{Q})} + \|\mu\|_{C^0([0,T];L^6(\Omega))} + \|\rho_t\|_{L^2(0,T;L^6(\Omega))} \le K_1^*. \tag{2.8}$$

We are now prepared to prove existence for the control problem **(CP)**:

Theorem 2.2 *Suppose that the conditions* (A1) *and* (A2) *are satisfied. Then the problem* **(CP)** *has a solution* $\overline{u} \in U_{ad}$.

Proof. Let $\{u_n\} \subset U_{ad}$ be a minimizing sequence for **(CP)**, and let $\{(\rho_n, \mu_n)\}$ be the sequence of the associated solutions to (1.2)–(1.5). We then can infer from (2.6) the existence of a triple $(\bar{u}, \bar{\rho}, \bar{\mu})$ such that, for a suitable subsequence again indexed by n, we have

$u_n \to \bar{u}$ weakly star in $L^\infty(Q)$,

$\rho_n \to \bar{\rho}$ weakly star in $W^{1,\infty}(0,T;H) \cap H^1(0,T;V) \cap L^\infty(0,T;W)$,

$\mu_n \to \bar{\mu}$ weakly star in $H^1(0,T;H) \cap L^\infty([0,T];V) \cap L^2(0,T;W)$.

Clearly, we have that $\bar{u} \in U_{ad}$. Moreover, by virtue of the Aubin-Lions lemma (cf. [14, Thm. 5.1, p. 58]) and similar compactness results (cf. [16, Sect. 8, Cor. 4]), we also have the strong convergences

$$\rho_n \to \bar{\rho} \quad \text{strongly in } C^0([0,T];H^s(\Omega)) \quad \text{for all } s<2, \tag{2.9}$$

$$\mu_n \to \bar{\mu} \quad \text{strongly in } C^0([0,T];H) \cap L^2(0,T;V). \tag{2.10}$$

From this we infer, possibly selecting another subsequence again indexed by n, that $\rho_n \to \bar{\rho}$ pointwise a. e. in Q. In particular, $\rho_* \le \bar{\rho} \le \rho^*$ a. e. in Q and, since $f \in C^2(0,1)$, also $f'(\rho_n) \to f'(\bar{\rho})$ strongly in $L^2(Q)$. Now notice that the above convergences imply, in particular, that

$$\rho_n \to \bar{\rho} \quad \text{strongly in } C^0([0,T];L^6(\Omega), \quad \partial_t\rho_n \to \partial_t\bar{\rho} \quad \text{weakly in } L^2(0,T;L^4(\Omega)),$$

$$\mu_n \to \bar{\mu} \quad \text{strongly in } L^2(0,T;L^4(\Omega)), \quad \partial_t\mu_n \to \partial_t\bar{\mu} \quad \text{weakly in } L^2(Q).$$

From this, it is easily verified that

$$\mu_n\,\partial_t\rho_n \to \bar{\mu}\,\partial_t\bar{\rho} \quad \text{weakly in } L^1(0,T;H),$$

$$\rho_n\,\partial_t\mu_n \to \bar{\rho}\,\partial_t\bar{\mu} \quad \text{weakly in } L^2(0,T;L^{3/2}(\Omega)).$$

In summary, if we pass to the limit as $n \to \infty$ in the state equations (1.2)–(1.5) written for the triple (u_n, ρ_n, μ_n), we find that $(\bar{\rho}, \bar{\mu}) = S(\bar{u})$, that is, the triple $(\bar{u}, \bar{\rho}, \bar{\mu})$ is admissible for the control problem **(CP)**. From the weak sequential lower semicontinuity of the cost functional J it finally follows that $\bar{u}$, together with $(\bar{\rho}, \bar{\mu}) = S(\bar{u})$, is a solution to **(CP)**. This concludes the proof. ∎

Remarks: 3. It can be shown that this existence result holds for much more general cost functionals. All we need is that J enjoy appropriate weak sequential lower semicontinuity properties that match the above weak convergences.

4. Since the state component ρ is continuous on $\overline{Q}$, the existence result remains valid if suitable pointwise state constraints for ρ are added (provided the admissible set is not empty). For instance, consider the case when the state has to obey the one-sided obstacle condition

$$\rho(x^*,t) \ge \frac{1}{2} \quad \forall\, t \in [0,T] \tag{2.11}$$

for some fixed $x^* \in \Omega$ (which of course requires that $\rho_0(x^*) \ge 1/2$). If the set of admissible controls in U_{ad} is not empty, i. e., if there is at least one $\hat{u} \in U_{ad}$ such that the corresponding state component $\hat{\rho}$ satisfies (2.11), then an optimal control exists. Indeed, we pick a minimizing sequence of admissible controls $\{u_n\} \subset U_{ad}$ with associated states (ρ_n, μ_n) obeying (2.11). Since Ω is a bounded three-dimensional domain, we can infer from (2.9) and Sobolev embeddings that $\rho_n \to \bar{\rho}$ uniformly in $\overline{Q}$, whence it follows that $\bar{\rho}$ satisfies (2.11).

3 Necessary optimality conditions

In this section, we derive the first-order necessary conditions of optimality for problem **(CP)**. In this whole section, we generally assume that the hypotheses (A1) and (A2) are satisfied and that

$\bar{u} \in U_{ad}$ is an optimal control with associated state $(\bar{\rho}, \bar{\mu})$, which has the properties (2.3)–(2.6) and (2.8); in particular, we have $\bar{\rho} \in C(\overline{Q})$. For technical reasons, we need to take a slightly smoother nonlinear term f; precisely, we take

(A3) $\quad f \in C^3(0,1)$.

With this assumption, we can improve the stability estimate (2.7). Before stating the result, let us observe that (2.3) implies, in particular, that the solution component ρ is weakly continuous from $[0,T]$ into W, which justifies the formulation of the next estimate (3.1).

Lemma 3.1 *Suppose that* (A1)–(A3) *are satisfied, and let* $u_1, u_2 \in U_{ad}$ *be given and* $(\rho_1, \mu_1), (\rho_2, \mu_2)$ *be the corresponding solutions to* (1.2)–(1.5). *Moreover, let* $u = u_1 - u_2$, $\rho = \rho_1 - \rho_2$, $\mu = \mu_1 - \mu_2$. *Then, for all* $t \in [0,T]$,

$$\max_{0\le s\le t} \left(\|\rho_t(s)\|_V^2 + \|\mu(s)\|_V^2 + \|\rho(s)\|_W^2\right) + \int_0^t \left(\|\mu_t(s)\|_H^2 + \|\rho_t(s)\|_W^2\right) ds$$
$$\le K_3^* \int_0^t \|u(s)\|_H^2 \, ds\,, \tag{3.1}$$

with a constant $K_3^* > 0$ *that may depend on the data, but not on* u_1, u_2.

Proof. Obviously, the pair (ρ, μ) is a solution to the system

$$(\varepsilon + 2\rho_1)\mu_t + 2\,\rho\,\mu_{2,t} + \mu\,\rho_{1,t} + \mu_2\,\rho_t - \Delta\mu = u \quad \text{a.e. in } Q, \tag{3.2}$$
$$\delta\,\rho_t - \Delta\rho = \mu - (f'(\rho_1) - f'(\rho_2)) \quad \text{a.e. in } Q, \tag{3.3}$$
$$\frac{\partial\rho}{\partial\mathbf{n}} = \frac{\partial\mu}{\partial\mathbf{n}} = 0 \quad \text{a.e. on } \Sigma, \tag{3.4}$$
$$\rho(x,0) = \mu(x,0) = 0\,, \quad \text{a.e. in } \Omega. \tag{3.5}$$

We test Eq. (3.2) by μ_t. It then follows, with the use of Young's inequality, that

$$\frac{\varepsilon}{2}\int_0^t \|\mu_t(s)\|_H^2\,ds + \frac{1}{2}\|\nabla\mu(t)\|_H^2 \le \frac{1}{2}\int_0^t \|u(s)\|_H^2\,ds$$
$$+ \int_0^t \int_\Omega \left(2|\rho|\,|\mu_{2,t}| + |\mu|\,|\rho_{1,t}| + |\mu_2|\,|\rho_t|\right)|\mu_t|\,dx\,ds\,. \tag{3.6}$$

We estimate the terms on the right-hand side individually. In this process, C_i ($i \in \mathbb{N}$) denote positive constants that only depend on the constants $\varepsilon, \delta, \rho_*, \rho^*, \mu^*, T, K_1^*, K_2^*$. On using Hölder's and Young's inequalities, as well as the continuity of the embedding $H^1(\Omega) \subset L^4(\Omega)$, we have that

$$\int_0^t\int_\Omega |\mu|\,|\rho_{1,t}|\,|\mu_t|\,dx\,ds \le \int_0^t \|\mu_t(s)\|_H\,\|\mu(s)\|_{L^4(\Omega)}\,\|\rho_{1,t}(s)\|_{L^4(\Omega)}\,ds$$
$$\le \gamma\int_0^t \|\mu_t(s)\|_H^2\,ds + \frac{C_1}{\gamma}\int_0^t \|\rho_{1,t}(s)\|_V^2\|\mu(s)\|_V^2\,ds\,. \tag{3.7}$$

Observe that, owing to (2.6), the function $s \mapsto \|\rho_{1,t}(s)\|_V^2$ belongs to $L^1(0,T)$. Moreover, by (2.5) and Young's inequality,

$$\int_0^t\!\!\int_\Omega |\mu_2|\,|\rho_t|\,|\mu_t|\,dx\,ds \,\le\, \gamma\int_0^t \|\mu_t(s)\|_H^2\,ds \,+\, \frac{C_2}{\gamma}\int_0^t \|\rho_t(s)|_H^2\,ds\,, \tag{3.8}$$

where the second integral on the right-hand side can be estimated using (2.7). In addition, we have

$$I_1 := \int_0^t\!\!\int_\Omega 2\,|\rho|\,|\mu_{2,t}|\,|\mu_t|\,dx\,ds \le \gamma\int_0^t \|\mu_t(s)\|_H^2\,ds + \frac{C_3}{\gamma}\int_0^t \|\mu_{2,t}(s)\|_H^2\,\|\rho(s)\|_{L^\infty(\Omega)}^2\,ds\,. \tag{3.9}$$

Now, observe that the embedding $W \subset L^\infty(\Omega)$, in combination with standard elliptic estimates and (2.7), implies that

$$\|\rho(s)\|_{L^\infty(\Omega)}^2 \,\le\, C_4\int_0^s \|u(\tau)\|_H^2\,d\tau \,+\, C_5\,\|\Delta\rho(s)\|_H^2, \tag{3.10}$$

whence

$$I_1 \,\le\, \gamma\int_0^t \|\mu_t(s)\|_H^2\,ds \,+\, \frac{C_6}{\gamma}\Big(\int_0^t \|u(s)\|_H^2\,ds \,+\, \int_0^t \|\mu_{2,t}(s)\|_H^2\,\|\Delta\rho(s)\|_H^2\,ds\Big)\,, \tag{3.11}$$

where the mapping $s \mapsto \|\mu_{2,t}(s)\|_H^2$ belongs to $L^1(0,T)$.

Next, we formally test Eq. (3.3) by $-\Delta\rho_t$. On integrating by parts, we find that

$$\delta\int_0^t \|\nabla\rho_t(s)\|_H^2\,ds \,+\, \frac{1}{2}\,\|\Delta\rho(t)\|_H^2 \,\le\, \int_0^t\!\!\int_\Omega (-\mu + (f'(\rho_1) - f'(\rho_2))\,\,\Delta\rho_t\,dx\,ds\,. \tag{3.12}$$

After a further integration by parts, this time with respect to t, and invoking Young's inequality and (2.7), we find that

$$\begin{aligned}
-\int_0^t\!\!\int_\Omega \mu\,\Delta\rho_t\,dx\,ds \,&=\, -\int_\Omega \mu(t)\,\Delta\rho(t)\,dx \,+\, \int_0^t\!\!\int_\Omega \mu_t\,\Delta\rho\,dx\,ds \,\le\, \frac{1}{8}\,\|\Delta\rho(t)\|_H^2 \\
&+\gamma\int_0^t \|\mu_t(s)\|_H^2\,ds + \frac{C_7}{\gamma}\int_0^t \|\Delta\rho(s)\|_H^2\,ds \,+\, C_8\int_0^t \|u(s)\|_H^2\,ds\,.
\end{aligned} \tag{3.13}$$

Moreover, integration by parts with respect to t, with the help of Young's inequality, (2.6), and (2.7), yields:

$$\begin{aligned}
&\int_0^t\!\!\int_\Omega (f'(\rho_1) - f'(\rho_2))\,\Delta\rho_t\,dx\,ds \,\le\, \int_\Omega |f'(\rho_1(t)) - f'(\rho_2(t))|\,|\Delta\rho(t)|\,dx \\
&\quad+\, \int_0^t\!\!\int_\Omega (|f''(\rho_1)|\,|\rho_t| \,+\, |f''(\rho_1) - f''(\rho_2)|\,|\rho_{2,t}|)\,\,|\Delta\rho|\,dx\,ds \\
&\le\, \frac{1}{8}\,\|\Delta\rho(t)\|_H^2 \,+\, \int_0^t \|\Delta\rho(s)\|_H^2\,ds \,+\, C_9\int_0^t \|u(s)\|_H^2\,ds \,+\, I_2\,,
\end{aligned} \tag{3.14}$$

where

$$I_2 := \int_0^t\!\!\int_\Omega |f''(\rho_1) - f''(\rho_2)|\, |\rho_{2,t}|\, |\Delta\rho|\, dx\, ds\,.$$

From this inequality, on applying the mean value theorem, (2.6), (2.7), Young's inequality, and the continuity of the embedding $H^1(\Omega) \subset L^4(\Omega)$, we deduce the following estimate:

$$\begin{aligned}
I_2 \;&\le\; C_{10} \int_0^t \|\Delta\rho(s)\|_H \, \|\rho(s)\|_{L^4(\Omega)} \, \|\rho_{2,t}(s)\|_{L^4(\Omega)} \, ds \\
&\le\; C_{11} \max_{0\le s\le t} \|\rho(s)\|_V \int_0^t \|\rho_{2,t}(s)\|_V \, \|\Delta\rho(s)\|_H \, ds \\
&\le\; C_{12} \Big(\int_0^t \|\rho_{2,t}(s)\|_V^2 \, \|\Delta\rho(s)\|_H^2 \, ds \,+\, \int_0^t \|u(s)\|_H^2 \, ds \Big)\,. \qquad (3.15)
\end{aligned}$$

Observe that by (2.6) the mapping $s \mapsto \|\rho_{2,t}(s)\|_V^2$ belongs to $L^1(0,T)$.

At this point, we may combine the estimates (3.6)–(3.15): in fact, choosing $\gamma > 0$ appropriately small, and invoking Gronwall's lemma, we find the estimate:

$$\begin{aligned}
&\int_0^t \Big(\|\mu_t(s)\|_H^2 \,+\, \|\nabla\rho_t(s)\|_H^2 \Big)\, ds \,+\, \max_{0\le s\le t} \big(\|\mu(s)\|_V^2 \,+\, \|\rho(s)\|_W^2 \big) \\
&\le\; C_{13} \int_0^t \|u(s)\|_H^2 \, ds\,, \qquad (3.16)
\end{aligned}$$

for all $t \in [0,T]$. Next, we formally differentiate Eq. (3.3) with respect to t, and obtain

$$\delta\rho_{tt} - \Delta\rho_t = \mu_t \,-\, f''(\rho_1)\,\rho_t - (f''(\rho_1) - f''(\rho_2))\,\rho_{2,t}\,, \qquad (3.17)$$

with zero initial and Neumann boundary conditions for ρ_t (cf. (3.4), (3.5), and (1.5)). Hence, testing (3.17) by ρ_t, invoking Young's inequality, and recalling (2.7), and (3.16), we find that

$$\begin{aligned}
\frac{\delta}{2}\, \|\rho_t(t)\|_H^2 \,+\, \int_0^t \|\nabla\rho_t(s)\|_H^2 \, ds \;&\le\; C_{14} \int_0^t \|u(s)\|_H^2 \, ds \\
&\quad +\, \int_0^t\!\!\int_\Omega |\rho_{2,t}|\, |f''(\rho_1) - f''(\rho_2)|\, |\rho_t|\, dx\, ds\,. \qquad (3.18)
\end{aligned}$$

Moreover, using Hölder's and Young's inequalities, (A3), (2.6), and (2.7), we see that

$$\begin{aligned}
&\int_0^t\!\!\int_\Omega |\rho_{2,t}|\, |f''(\rho_1) - f''(\rho_2)|\, |\rho_t|\, dx\, ds \\
&\le\; C_{15} \int_0^t \|\rho_{2,t}(s)\|_{L^4(\Omega)} \, \|\rho(s)\|_{L^4(\Omega)} \|\rho_t(s)\|_H \, ds \\
&\le\; C_{16} \Big(\int_0^t \|\rho_t(s)\|_H^2 \, ds \,+\, \max_{0\le s\le t} \|\rho(s)\|_V^2 \int_0^t \|\rho_{2,t}(s)\|_V^2 \, ds \Big) \\
&\le\; C_{17} \int_0^t \|u(s)\|_H^2 \, ds\,. \qquad (3.19)
\end{aligned}$$

Finally, we test (3.17) by $-\Delta\rho_t$. Using Young's inequality and (3.16), we find that

$$
\begin{aligned}
&\frac{\delta}{2}\,\|\nabla\rho_t(t)\|_H^2 \,+\, \int_0^t \|\Delta\rho_t(s)\|_H^2\,ds \,\le\, \gamma\int_0^t \|\Delta\rho_t(s)\|_H^2\,ds \\
&\quad + \frac{C_{18}}{\gamma}\int_0^t \|u(s)\|_H^2\,ds \,+\, \int_0^t\!\!\int_\Omega |\rho_{2,t}|\,|f''(\rho_1)-f''(\rho_2)|\,|\Delta\rho_t|\,dx\,ds \\
&\le\, 2\gamma\int_0^t \|\Delta\rho_t(s)\|_H^2\,ds \,+\, \frac{C_{19}}{\gamma}\Big(\int_0^t \|u(s)\|_H^2\,ds \,+\, \max_{0\le s\le t}\|\rho(s)\|_V^2\int_0^t \|\rho_{2,t}(s)\|_V^2\,ds\Big) \\
&\le\, 2\gamma\int_0^t \|\Delta\rho_t(s)\|_H^2\,ds \,+\, \frac{C_{20}}{\gamma}\int_0^t \|u(s)\|_H^2\,ds\,.
\end{aligned}
\tag{3.20}
$$

Choosing $\gamma > 0$ appropriately small, we can infer that the estimate (3.1) is in fact true. This concludes the proof. ∎

3.1 The linearized system

Suppose that $h \in L^\infty(Q)$ is an admissible variation with respect to $\bar u$, i. e., that there exists $\bar\lambda > 0$ such that $\bar u + \lambda h \in U_{ad}$ whenever $0 < \lambda \le \bar\lambda$. We have to determine the directional derivative $DJ_{\rm red}(\bar u)h$ of the "reduced" cost functional $J_{\rm red}(u) := J(u, Su)$ at $\bar u$ in the direction h. This requires to find the directional derivative $DS(\bar u)h$ of the solution operator S at $\bar u$ in the direction h. To this end, we consider the following system, which is obtained by linearizing the system (1.2)–(1.5) at $(\bar\rho,\bar\mu)$:

$$(\varepsilon + 2\bar\rho)\,\eta_t - \Delta\eta + 2\,\bar\mu_t\,\xi + \bar\mu\,\xi_t + \bar\rho_t\,\eta = h \quad \text{a. e. in } Q, \tag{3.21}$$

$$\delta\,\xi_t - \Delta\xi = -f''(\bar\rho)\,\xi \,+\, \eta \quad \text{a. e. in } Q, \tag{3.22}$$

$$\frac{\partial\xi}{\partial\mathbf{n}} = \frac{\partial\eta}{\partial\mathbf{n}} = 0 \quad \text{a. e. on } \Sigma, \tag{3.23}$$

$$\xi(x,0) = \eta(x,0) = 0 \quad \text{a. e. in } \Omega. \tag{3.24}$$

We expect that $(\xi,\eta) = DS(\bar u)h$, provided that (3.21)–(3.24) admits a unique solution (ξ,η). In view of (2.3) and (2.4), we can guess the regularity of ξ and η :

$$\xi \in H^1(0,T;H)\cap C^0([0,T];V)\cap L^2(0,T;W)\cap L^\infty(Q), \tag{3.25}$$

$$\eta \in H^1(0,T;H)\cap C^0([0,T];V)\cap L^2(0,T;W). \tag{3.26}$$

Indeed, if (3.25) and (3.26) hold then the collection of source terms in (3.21), i. e., the part $h - 2\,\bar\mu_t\,\xi - \bar\mu\,\xi_t - \bar\rho_t\,\eta$, belongs to $L^2(Q)$ (as it should for a solution η satisfying (3.26)), whereas the regularity (3.26) for η allows us to conclude from (3.22) that also $\xi \in C(\overline{Q})$ (by applying maximal parabolic regularity theory, see, e. g., [7, Thm. 6.8] or [17, Lemma 7.12]).

In fact, as to ξ, we can count on an even better regularity. Indeed, we may differentiate (3.22) with respect to t to find that

$$\delta\xi_{tt} - \Delta\xi_t = -f'''(\bar\rho)\,\bar\rho_t\,\xi - f''(\bar\rho)\,\xi_t + \eta_t\,, \tag{3.27}$$

with zero initial and Neumann boundary conditions for ξ_t. Since the right-hand side of (3.27) belongs to $L^2(Q)$, we may test by any of the functions ξ_t, ξ_{tt}, and $-\Delta\xi_t$, to obtain that even

$$\xi \in H^2(0,T;H) \cap C^1([0,T];V) \cap H^1(0,T;W). \tag{3.28}$$

Notice, however, that this fact has no bearing on the regularity of η, since the coefficient $\bar{\mu}_t$ in (3.21) only belongs to $L^2(Q)$.

We first prove the well-posedness of the linear system (3.21)–(3.24).

Proposition 3.2 *Suppose that* (A1)–(A3) *are fulfilled. Then the system* (3.21)–(3.24) *has a unique solution* (ξ,η) *satisfying* (3.26) *and* (3.28).

Proof. We proceed in series of steps.

Step 1: Approximation. Following the lines of our approach in [4], we use an approximation technique based on a delay in the right-hand side of (3.22). To this end, we define for $\tau>0$ the translation operator $\mathcal{T}_\tau:\ L^1(0,T;H)\ \to L^1(0,T;H)$ by putting, for every $v\in L^1(0,T;H)$ and almost every $t\in(0,T)$,

$$(\mathcal{T}_\tau v)(t) = v(t-\tau) \ \text{ if } t\ge\tau, \quad \text{and} \quad (\mathcal{T}_\tau v)(t)=0 \ \text{ if } t<\tau. \tag{3.29}$$

Notice that, for any $v\in L^2(Q)$ and any $\tau>0$, we obviously have $\|\mathcal{T}_\tau v\|_{L^2(Q)} \le \|v\|_{L^2(Q)}$. Then, for any fixed $\tau>0$, we look for functions (ξ^τ,η^τ), which satisfy (3.25) and (3.26) and the system:

$$(\varepsilon+2\bar{\rho})\,\eta^\tau_t - \Delta\eta^\tau + 2\,\bar{\mu}_t\,\xi^\tau + \bar{\mu}\,\xi^\tau_t + \bar{\rho}_t\,\eta^\tau = h \quad \text{a.e. in } Q, \tag{3.30}$$

$$\delta\,\xi^\tau_t - \Delta\xi^\tau + f''(\bar{\rho})\,\xi^\tau = \mathcal{T}_\tau\eta^\tau \quad \text{a.e. in } Q, \tag{3.31}$$

$$\frac{\partial\xi^\tau}{\partial\mathbf{n}} = \frac{\partial\eta^\tau}{\partial\mathbf{n}} = 0 \quad \text{a.e. on } \Sigma, \tag{3.32}$$

$$\xi^\tau(x,0) = \eta^\tau(x,0) = 0 \quad \text{a.e. in } \Omega. \tag{3.33}$$

Precisely, we choose for $\tau>0$ the discrete values $\tau=T/N$, where $N\in\mathbb{N}$ is arbitrary, and put $t_n = n\,\tau$, $0\le n\le N$, and $I_n=(0,t_n)$. For $1\le n\le N$, we solve the problem

$$(\varepsilon+2\bar{\rho})\,\eta_{n,t} - \Delta\eta_n + 2\,\bar{\mu}_t\,\xi_n + \bar{\mu}\,\xi_{n,t} + \bar{\rho}_t\,\eta_n = h \quad \text{a.e. in } \Omega\times I_n, \tag{3.34}$$

$$\frac{\partial\eta_n}{\partial\mathbf{n}} = 0 \quad \text{a.e. on } \Gamma\times I_n, \qquad \eta_n(x,0)=0 \quad \text{a.e. in } \Omega, \tag{3.35}$$

$$\delta\,\xi_{n,t} - \Delta\xi_n + f''(\bar{\rho})\,\xi_n = \mathcal{T}_\tau\eta_n \quad \text{a.e. in } \Omega\times I_n, \tag{3.36}$$

$$\frac{\partial\xi_n}{\partial\mathbf{n}} = 0 \quad \text{a.e. on } \Gamma\times I_n, \qquad \xi_n(x,0)=0 \quad \text{a.e. in } \Omega, \tag{3.37}$$

where the variables η_n and ξ_n, defined on I_n, have obvious meaning. Here, $\mathcal{T}_\tau$ acts on functions that are not defined on the entire interval $(0,T)$; however, for $n>1$ it is still defined by (3.29), while for $n = 1$ we simply put $\mathcal{T}_\tau \eta_n = 0$. Notice that whenever the pairs (ξ_k, η_k) with

$$\xi_k \in H^1(I_k; H) \cap C^0(\bar{I}_k; V) \cap L^2(I_k; W) \cap C(\overline{\Omega \times I_k}), \tag{3.38}$$

$$\eta_k \in H^1(I_k; H) \cap C^0(\bar{I}_k; V) \cap L^2(I_k; W), \tag{3.39}$$

have been constructed for $1 \le k \le n < N$, then we look for the pair (ξ_{n+1}, η_{n+1}) that coincides with (ξ_n, η_n) in I_n, and note that the linear parabolic problem (3.36), (3.37) has a unique solution ξ_{n+1} on $\Omega \times I_{n+1}$ that satisfies (3.38) for $k = n + 1$. Inserting ξ_{n+1} in (3.34) (where n is replaced by $n + 1$), we then find that the linear parabolic problem (3.34), (3.35) admits a unique solution η_{n+1} that fulfills (3.39) for $k = n + 1$. Hence, we conclude that $(\xi^\tau, \eta^\tau) = (\xi_N, \eta_N)$ satisfies (3.30)–(3.33), and (3.25), (3.26).

Step 2: A priori estimates. We now prove a series of a priori estimates for the functions (ξ^τ, η^τ). In the following, we denote by C_i $(i \in \mathbb{N})$ some generic positive constants, which may depend on $\varepsilon, \delta, \rho_*, \rho^*, \mu^*, T, K_1^*, K_2^*$, but not on τ (i.e., not on N). For the sake of simplicity, we omit the superscript τ and simply write (ξ, η). We recall the continuity of the embedding $H^1(\Omega) \subset L^6(\Omega)$.

First a priori estimate. Observe that $2\,\bar{\rho}\,\eta\,\eta_t = (\bar{\rho}\,\eta^2)_t - \bar{\rho}_t\,\eta^2$. Hence, testing (3.30) by η, we have, for $0 \le t \le T$,

$$\int_\Omega \Big(\frac{\varepsilon}{2} + \bar{\rho}\Big)\,\eta(t)^2\,dx + \int_0^t \|\nabla\eta(s)\|_H^2\,ds \le \frac{1}{2}\int_0^t \big(\|\eta(s)\|_H^2 + \|h(s)\|_H^2\big)\,ds$$
$$+\,2\int_0^t\int_\Omega |\bar{\mu}_t|\,|\xi|\,|\eta|\,dx\,ds + \int_0^t\int_\Omega |\bar{\mu}|\,|\xi_t|\,|\eta|\,dx\,ds\,. \tag{3.40}$$

For any $\gamma > 0$, we have by Young's inequality that

$$\int_0^t\int_\Omega |\bar{\mu}|\,|\xi_t|\,|\eta|\,dx\,ds \;\le\; \|\bar{\mu}\|_{L^\infty(Q)}\int_0^t \|\eta(s)\|_H\,\|\xi_t(s)\|_H\,ds$$
$$\le\; \gamma\int_0^t \|\xi_t(s)\|_H^2\,ds \;+\; \frac{C_1}{\gamma}\int_0^t \|\eta(s)\|_H^2\,ds\,. \tag{3.41}$$

Moreover,

$$\int_0^t\int_\Omega |\bar{\mu}_t|\,|\xi|\,|\eta|\,dx\,ds \le \int_0^t \|\bar{\mu}_t(s)\|_H\,\|\xi(s)\|_{L^4(\Omega)}\,\|\eta(s)\|_{L^4(\Omega)}\,ds$$
$$\le\; \gamma\int_0^t \|\eta(s)\|_V^2\,ds \;+\; \frac{C_2}{\gamma}\int_0^t \|\bar{\mu}_t(s)\|_H^2\,\|\xi(s)\|_V^2\,ds\,. \tag{3.42}$$

Notice that, by virtue of (2.6), the mapping $s \mapsto \|\bar{\mu}_t(s)\|_H^2$ belongs to $L^1(0,T)$.

Next, we add ξ on both sides of Eq. (3.31) and test the resulting equation by ξ_t. On using Young's inequality again, we obtain:

$$\frac{\delta}{4}\int_0^t \|\xi_t(s)\|_H^2\,ds \;+\; \frac{1}{2}\big(\|\xi(t)\|_H^2 + \|\nabla\xi(t)\|_H^2\big)$$
$$\le\; C_3\Big(\int_0^t \|\eta(s)\|_H^2\,ds \;+\; \int_0^t \|\xi(s)\|_H^2\,ds\Big)\,. \tag{3.43}$$

Adding the inequalities (3.40) and (3.43), and choosing $\gamma > 0$ sufficiently small, we conclude from the above estimates and Gronwall's lemma that

$$\int_0^T \big(\|\xi_t(t)\|_H^2 + \|\eta(t)\|_V^2\big)\,dt \,+\, \max_{0\le t\le T}\big(\|\xi(t)\|_V^2 \,+\, \|\eta(t)\|_H^2\big) \le C_4 \int_0^T \|h(t)\|_H^2\,dt. \tag{3.44}$$

By comparison in (3.31), and thanks to (3.32), we may also infer (possibly by choosing a larger C_4) that

$$\int_0^T \|\xi(t)\|_W^2\,dt \,\le\, C_4 \int_0^T \|h(t)\|_H^2\,dt\,. \tag{3.45}$$

<ins>Second a priori estimate.</ins> We test (3.30) by η_t and apply Young's inequality in order to obtain

$$\begin{aligned}&\frac{\varepsilon}{2}\int_0^t \|\eta_t(s)\|_H^2\,ds \,+\, \frac12\,\|\nabla\eta(t)\|_H^2\\ &\quad\le\, \frac{1}{2\varepsilon}\int_0^t \|h(s)\|_H^2\,ds \,+\, \int_0^t\!\!\int_\Omega (2\,|\bar\mu_t|\,|\xi| \,+\, |\bar\mu|\,|\xi_t| \,+\, |\bar\rho_t|\,|\eta|\,)\;|\eta_t|\,dx\,ds\,. \end{aligned}\tag{3.46}$$

Since $\bar\mu \in L^\infty(Q)$, we can infer from Young's inequality that

$$\int_0^t \int_\Omega |\bar\mu|\,|\xi_t|\,|\eta_t|\,dx\,ds \,\le\, \gamma\int_0^t \|\eta_t(s)\|_H^2\,ds \,+\, \frac{C_5}{\gamma}\int_0^t \|\xi_t(s)\|_H^2\,ds\,. \tag{3.47}$$

Moreover, by virtue of Hölder's and Young's inequalities,

$$\begin{aligned}&\int_0^t \int_\Omega |\bar\rho_t|\,|\eta|\,|\eta_t|\,dx\,ds \,\le\, \gamma\int_0^t \|\eta_t(s)\|_H^2\,ds \,+\, \frac{C_6}{\gamma}\int_0^t \|\bar\rho_t(s)\|_{L^4(\Omega)}^2\,\|\eta(s)\|_{L^4(\Omega)}^2\,ds\\ &\quad\le \gamma\int_0^t \|\eta_t(s)\|_H^2\,ds \,+\, \frac{C_7}{\gamma}\int_0^t \|\bar\rho_t(s)\|_V^2\,\|\eta(s)\|_V^2\,ds\,. \end{aligned}\tag{3.48}$$

Observe that by (2.6) the mapping $s \mapsto \|\bar\rho_t(s)\|_V^2$ belongs to $L^1(0,T)$.

Finally, we have, owing to the continuity of the embedding $W \subset L^\infty(\Omega)$ and (3.44),

$$\begin{aligned}&\int_0^t \int_\Omega 2\,|\bar\mu_t|\,|\xi|\,|\eta_t|\,dx\,ds \,\le\, \gamma\int_0^t \|\eta_t(s)\|_H^2\,ds \,+\, \frac{C_8}{\gamma}\int_0^t \|\bar\mu_t(s)\|_H^2\,\|\xi(s)\|_{L^\infty(\Omega)}^2 ds\\ &\le\, \gamma\int_0^t \|\eta_t(s)\|_H^2\,ds \,+\, \frac{C_9}{\gamma}\Big(\int_0^T \|h(s)\|_H^2\,ds \,+\, \int_0^t \|\bar\mu_t(s)\|_H^2\,\|\Delta\xi(s)\|_H^2\,ds\Big)\,, \end{aligned}\tag{3.49}$$

where, owing to (2.6), the mapping $s \mapsto \|\bar\mu_t(s)\|_H^2$ belongs to $L^1(0,T)$.

Next, we test (3.31) by $-\Delta\xi_t$ to obtain, for every $t \in [0,T]$,

$$\delta\int_0^t \|\nabla\xi_t(s)\|_H^2\,ds \,+\, \frac12\,\|\Delta\xi(t)\|_H^2 \,=\, \int_0^t\!\!\int_\Omega (-\,(\mathcal{T}_\tau\eta) \,+\, f''(\bar\rho)\,\xi)\;\Delta\xi_t\,dx\,ds\,. \tag{3.50}$$

Now, by virtue of (3.44) and (3.45), and invoking Young's inequality, we have

$$\Big|\int_0^t\!\!\int_\Omega (\mathcal{T}_\tau\eta)\,\Delta\xi_t\,dx\,ds\Big| \;\le\; \int_\Omega\!|(\mathcal{T}_\tau\eta)\,(t)|\;|\Delta\xi(t)|\,dx \;+\int_0^t\!\!\int_\Omega |\partial_t\,(\mathcal{T}_\tau\eta)|\;|\Delta\xi|\,dx\,ds$$
$$\le\;\frac{1}{8}\,\|\Delta\xi(t)\|_H^2\;+\;\gamma\int_0^t\|\eta_t(s)\|_H^2\,ds\;+\;C_{10}\left(1+\frac{1}{\gamma}\right)\int_0^T\|h(s)\|_H^2\,ds. \tag{3.51}$$

Moreover, it turns out that

$$\Big|\int_0^t\!\!\int_\Omega f''(\bar\rho)\,\xi\,\Delta\xi_t\,dx\,ds\Big| \;\le\; \int_\Omega\!|f''(\bar\rho(t))|\,|\xi(t)|\,|\Delta\xi(t)|\,dx$$
$$+\int_0^t\!\!\int_\Omega |f'''(\bar\rho)\,\bar\rho_t\,\xi+f''(\bar\rho)\,\xi_t|\;|\Delta\xi|\,dx\,ds\,. \tag{3.52}$$

We have, owing to (2.5) and (3.44),

$$\int_\Omega\!|f''(\bar\rho(t))|\,|\xi(t)|\,|\Delta\xi(t)|\,dx\;\le\;\frac{1}{8}\,\|\Delta\xi(t)\|_H^2\;+\;C_{11}\int_0^T\|h(s)\|_H^2\,ds\,. \tag{3.53}$$

Also the second integral on the right-hand side of (3.52) is bounded, since (2.5), (2.6), (3.44), and (3.45) imply that

$$\begin{aligned}
&\int_0^t\!\!\int_\Omega |f'''(\bar\rho)\,\bar\rho_t\,\xi+f''(\bar\rho)\,\xi_t|\;|\Delta\xi|\,dx\,ds\\
&\le\;C_{12}\int_0^t\|\bar\rho_t(s)\|_{L^4(\Omega)}^2\,\|\xi(s)\|_{L^4(\Omega)}^2ds\;+\;\int_0^t\|\Delta\xi(s)\|_H^2\,ds\\
&\le\;C_{13}\max_{0\le t\le T}\,\|\xi(t)\|_V^2\int_0^t\|\bar\rho_t(s)\|_V^2\,ds\;+\;\int_0^t\|\Delta\xi(s)\|_H^2\,ds\\
&\le\;C_{14}\int_0^T\,\|h(s)\|_H^2\,ds\,,
\end{aligned} \tag{3.54}$$

thanks to the continuity of the embedding $V\subset L^4(\Omega)$. Thus, combining the estimates (3.46) –(3.54), choosing $\gamma>0$ sufficiently small, and invoking Gronwall's inequality, we can infer that

$$\int_0^T\!\Big(\|\eta_t(t)\|_H^2\;+\;\|\xi_t(t)\|_V^2\Big)\,dt\;+\;\max_{0\le t\le T}\,\big(\|\eta(t)\|_V^2\;+\;\|\xi(t)\|_W^2\big)\;\le\;C_{15}\int_0^T\,\|h(t)\|_H^2\,dt\,. \tag{3.55}$$

Now, testing (3.30) by $-\Delta\eta$, and arguing as for (3.46)–(3.49), we find that

$$\int_0^T\,\|\eta(t)\|_W^2\,dt\;\le\;C_{16}\int_0^T\,\|h(t)\|_H^2\,dt\,.$$

Next, we differentiate Eq. (3.31) with respect to t. We obtain:

$$\delta\,\xi_{tt}-\Delta\xi_t=\partial_t(\mathcal{T}_\tau\eta)-f'''(\bar\rho)\,\bar\rho_t\,\xi-f''(\bar\rho)\,\xi_t\quad\text{a. e. in } Q. \tag{3.56}$$

From (2.5), (2.6), (3.44), and (3.55), we can infer that the expression on the right-hand side of (3.56) is bounded in $L^2(Q)$. Therefore, we may test (3.56) by any of the functions ξ_t, $-\Delta\xi_t$, and ξ_{tt}, in order to find that

$$\int_0^T \Big(\|\xi_{tt}(t)\|_H^2 \,+\, \|\Delta\xi_t(t)\|_H^2 \Big)\,dt \,+\, \max_{0\le t\le T}\,\|\xi_t(t)\|_V^2 \,\le\, C_{17}\int_0^T \|h(t)\|_H^2\,dt\,. \tag{3.57}$$

Step 3: Passage to the limit. Let (ξ_N,η_N) denote the solution to the system (3.30)–(3.33) associated with $\tau_N = T/N$, for $N\in\mathbb{N}$. In Step 2, we have shown that there is some $C>0$, which does not depend on N, such that

$$\|\xi_N\|_{H^2(0,T;H)\cap C^1([0,T];V)\cap H^1(0,T;W)\cap C(\overline{Q})} \,+\, \|\eta_N\|_{H^1(0,T;H)\cap C^0([0,T];V)\cap L^2(0,T;W)} \,\le\, C. \tag{3.58}$$

Hence, there is a subsequence, which is again indexed by N, such that

$$\xi_N\to\xi \qquad \text{weakly star in} \quad H^2(0,T;H)\cap W^{1,\infty}(0,T;V)\cap H^1(0,T;W),$$

$$\eta_N\to\eta \qquad \text{weakly star in} \quad H^1(0,T;H)\cap L^\infty(0,T;V)\cap L^2(0,T;W). \tag{3.59}$$

By compact embedding, we also have, in particular,

$$\xi_N\to\xi \quad \text{strongly in } C(\overline{Q}), \qquad \eta_N\to\eta \quad \text{strongly in } L^2(Q), \tag{3.60}$$

so that $\bar\rho\,\eta_{N,t}\,\to\,\bar\rho\,\eta_t$ and $\bar\mu\,\xi_{N,t}\,\to\,\bar\mu\,\xi_t$, both weakly in $L^2(Q)$, $f''(\bar\rho)\,\xi_N\,\to\,f''(\bar\rho)\,\xi$ strongly in $L^2(Q)$, as well as $\bar\mu_t\,\xi_{N,t}\to\bar\mu_t\,\xi_t$ and $\bar\rho_t\,\eta_N\,\to\,\bar\rho_t\,\eta$, both strongly in $L^1(Q)$. Finally, it is easily verified that $\{\mathcal{T}_{T/N}\eta_N\}$ converges strongly in $L^2(Q)$ to η. In conclusion, we may pass to the limit as $N\to\infty$ in the system (3.30)–(3.33) (written for $\tau=T/N$) to find that the pair (ξ,η) is in fact a strong solution to the linearized system (3.21)–(3.24).

It remains to show the uniqueness. But if (ξ_1,η_1), (ξ_2,η_2) are two solutions having the above properties, then the pair (ξ,η), where $\xi=\xi_1-\xi_2$ and $\eta=\eta_1-\eta_2$, satisfies (3.21)–(3.24) with $h=0$. We thus may repeat the first a priori estimate in Step 2 to conclude that $\xi=\eta=0$. This concludes the proof. ∎

3.2 Directional differentiability of the control-to-state mapping

In this section, we prove the following result.

Proposition 3.3 *Suppose that the assumptions* (A1)–(A3) *are satisfied. Then the solution operator S, viewed as a mapping from U_{ad}, subset of $L^2(Q)$, into*

$$\big(H^1(0,T;H)\cap C^0([0,T];V)\cap L^2(0,T;W)\big)\times\big(C^0([0,T];H)\cap L^2(0,T;V)\big)\,,$$

is directionally differentiable at $\bar u$ in the direction h. The directional derivative $(\xi,\eta)=DS(\bar u)h$ is given by the unique solution (ξ,η) to the linearized system (3.21)–(3.24).

Proof. Let $\bar\lambda>0$ be such that $\bar u+\lambda h\in U_{ad}$ for $0<\lambda\le\bar\lambda$. We put

$$u^\lambda=\bar u+\lambda h,\quad (\rho^\lambda,\mu^\lambda)=S(u^\lambda),\quad y^\lambda=\rho^\lambda-\bar\rho-\lambda\xi,\quad z^\lambda=\mu^\lambda-\bar\mu-\lambda\eta.$$

We have to show that there is a function $Z : [0, \bar{\lambda}] \to [0, +\infty)$ with $\lim_{\lambda \searrow 0} Z(\lambda)/\lambda^2 = 0$ such that

$$\|y^\lambda\|^2_{H^1(0,T;H) \cap C^0([0,T];V) \cap L^2(0,T;W)} + \|z^\lambda\|^2_{C^0([0,T];H) \cap L^2(0,T;V)} \le Z(\lambda). \tag{3.61}$$

Using the state system (1.2)–(1.5) and the linearized system (3.21)–(3.24), we easily verify that for $0 < \lambda \le \bar{\lambda}$ the pair (y^λ, z^λ) is a strong solution to the system

$$\begin{aligned}
&(\varepsilon + 2\bar{\rho})\, z^\lambda_t + \bar{\rho}_t\, z^\lambda + \bar{\mu}\, y^\lambda_t + 2\bar{\mu}_t\, y^\lambda - \Delta z^\lambda \\
&\quad = -2\left(\mu^\lambda_t - \bar{\mu}_t\right)\left(\rho^\lambda - \bar{\rho}\right) - \left(\rho^\lambda_t - \bar{\rho}_t\right)\left(\mu^\lambda - \bar{\mu}\right) \quad \text{a.e. in } Q,
\end{aligned} \tag{3.62}$$

$$\delta y^\lambda_t - \Delta y^\lambda + f'(\rho^\lambda) - f'(\bar{\rho}) - \lambda\, f''(\bar{\rho})\, \xi = z^\lambda, \quad \text{a.e. in } Q, \tag{3.63}$$

$$\frac{\partial y^\lambda}{\partial \mathbf{n}} = \frac{\partial z^\lambda}{\partial \mathbf{n}} = 0, \quad \text{a.e. on } \Sigma, \tag{3.64}$$

$$y^\lambda(x, 0) = z^\lambda(x, 0) = 0 \quad \text{a.e. in } \Omega. \tag{3.65}$$

Notice that

$$\begin{aligned}
&y^\lambda \in H^1(0,T;H) \cap C^0([0,T];V) \cap L^2(0,T;W) \cap C(\bar{Q}), \\
&z^\lambda \in H^1(0,T;H) \cap C^0([0,T];V) \cap L^2(0,T;W).
\end{aligned}$$

For the sake of a better readability, in the following estimates we omit the superscript λ of y^λ and z^λ. As before, we denote by C_i $(i \in \mathbb{N})$ certain positive constants that only depend on $\varepsilon, \delta, \rho_*, \rho^*, \mu^*, T, K_1^*, K_2^*, K_3^*$, but not on λ.

We now add y on both sides of Eq. (3.63) and test the resulting equation by y_t. Using Young's inequality, we find that for all $t \in [0, T]$ it holds

$$\begin{aligned}
&\frac{\delta}{2} \int_0^t \|y_t(s)\|^2_H \, ds + \frac{1}{2}\left(\|\nabla y(t)\|^2_H + \|y(t)\|^2_H\right) \le \frac{2}{\delta} \int_0^t \|z(s)\|^2_H \, ds \\
&\quad + C_1 \int_0^t \|y(s)\|^2_H \, ds + C_2 \int_0^t \|(f'(\rho^\lambda) - f'(\bar{\rho}) - \lambda f''(\bar{\rho})\, \xi)(s)\|^2_H \, ds\,.
\end{aligned} \tag{3.66}$$

In order to handle the third term on the right-hand side of (3.66), we note that the stability estimate (3.1) implies, in particular, that

$$\|\rho^\lambda - \bar{\rho}\|^2_{L^\infty(Q)} \le K_3^* \, \lambda^2 \, \|h\|^2_{L^2(Q)}\,, \tag{3.67}$$

that is, $\rho^\lambda \to \bar{\rho}$ uniformly on $\overline{Q}$ as $\lambda \searrow 0$. Since $f \in C^3(0,1)$, we can infer from Taylor's theorem that

$$\left|f'(\rho^\lambda) - f'(\bar{\rho}) - \lambda\, f''(\bar{\rho})\, \xi\right| \le \frac{1}{2} \max_{\rho_* \le \sigma \le \rho^*} |f'''(\sigma)| \left|\rho^\lambda - \bar{\rho}\right|^2 + |f''(\bar{\rho})|\, |y| \quad \text{on } \overline{Q}. \tag{3.68}$$

It then follows from the estimates (3.1) and (3.66) that

$$\frac{\delta}{2} \int_0^t \|y_t(s)\|^2_H \, ds + \frac{1}{2}\|y(t)\|^2_V \le \frac{2}{\delta} \int_0^t \|z(s)\|^2_H \, ds + C_3 \int_0^t \|y(s)\|^2_H \, ds + C_4 \lambda^4, \tag{3.69}$$

since we can assume that $\|h\|_{L^2(Q)} \le 1$. Next, observe that $2\,\bar\rho\, z\, z_t = (\bar\rho\, z^2)_t - \bar\rho_t\, z^2$. Therefore, testing (3.62) by z yields for every $t \in [0,T]$ that

$$\int_\Omega \Big(\frac{\varepsilon}{2} + \bar\rho(t)\Big)\, z^2(t)\, dx \,+\, \int_0^t \|\nabla z(s)\|_H^2\, ds \,=\, -\int_0^t\!\!\int_\Omega (\bar\mu\, y_t \,+\, 2\,\bar\mu_t\, y)\, z\, dx\, ds$$
$$-\,2\int_0^t\!\!\int_\Omega \big(\mu_t^\lambda - \bar\mu_t\big)\,\big(\rho^\lambda - \bar\rho\big)\; z\, dx\, ds - \int_0^t\!\!\int_\Omega \big(\rho_t^\lambda - \bar\rho_t\big)\,\big(\mu^\lambda - \bar\mu\big)\; z\, dx\, ds\,. \quad (3.70)$$

We estimate the terms on the right-hand side of (3.70) individually. At first, using (2.6) and Young's inequality, we find that

$$\int_0^t\!\!\int_\Omega |\bar\mu|\, |y_t|\, |z|\, dx\, ds \,\le\, \gamma \int_0^t \|y_t(s)\|_H^2\, ds \,+\, \frac{C_5}{\gamma}\int_0^t \|z(s)\|_H^2\, ds. \quad (3.71)$$

Moreover, using the continuity of the embedding $H^1(\Omega) \subset L^4(\Omega)$, as well as Hölder's and Young's inequalities,

$$\int_0^t\!\!\int_\Omega |\bar\mu_t|\, |y|\, |z|\, dx\, ds \,\le\, \int_0^t \|\bar\mu_t(s)\|_H\, \|z(s)\|_{L^4(\Omega)}\, \|y(s)\|_{L^4(\Omega)}\, ds$$
$$\le\, \gamma \int_0^t \|z(s)\|_V^2\, ds \,+\, \frac{C_6}{\gamma}\int_0^t \|\bar\mu_t(s)\|_H^2\, \|y(s)\|_V^2\, ds\,. \quad (3.72)$$

Observe that by (2.6) the mapping $s \mapsto \|\bar\mu_t(s)\|_H^2$ belongs to $L^1(0,T)$.

At this point, we can conclude from (3.1) and (3.67), invoking Young's inequality, that

$$\int_0^t\!\!\int_\Omega 2\, \big|\mu_t^\lambda - \bar\mu_t\big|\, \big|\rho^\lambda - \bar\rho\big|\, |z|\, dx\, ds$$
$$\le\, 2\int_0^t \big\|(\mu_t^\lambda - \bar\mu_t)(s)\big\|_H\, \big\|(\rho^\lambda - \bar\rho)(s)\big\|_{L^\infty(Q)}\, \|z(s)\|_H\, ds$$
$$\le\, C_7\, \big\|(\rho^\lambda - \bar\rho)(s)\big\|_{L^\infty(Q)}^2 \int_0^t \big\|(\mu_t^\lambda - \bar\mu_t)(s)\big\|_H^2\, ds \,+\, \int_0^t \|z(s)\|_H^2\, ds$$
$$\le\, \int_0^t \|z(s)\|_H^2\, ds \,+\, C_8\, \lambda^4\,. \quad (3.73)$$

Finally, we invoke (3.1) and Hölder's and Young's inequalities, as well as the continuity of the embedding $H^1(\Omega) \subset L^4(\Omega)$, to obtain that

$$\int_0^t\!\!\int_\Omega \big|\rho_t^\lambda - \bar\rho_t\big|\, \big|\mu^\lambda - \bar\mu\big|\, |z|\, dx\, ds$$
$$\le\, \max_{0\le s\le t} \|z(s)\|_H \int_0^t \big\|(\rho_t^\lambda - \bar\rho_t)(s)\big\|_{L^4(\Omega)}\, \big\|(\mu^\lambda - \bar\mu)(s)\big\|_{L^4(\Omega)}\, ds$$
$$\le\, \gamma \max_{0\le s\le t} \|z(s)\|_H^2 \,+\, \frac{C_9}{\gamma}\int_0^t \big\|(\rho_t^\lambda - \bar\rho_t)(s)\big\|_V^2\, ds \int_0^t \big\|(\mu^\lambda - \bar\mu)(s)\big\|_V^2\, ds$$
$$\le\, \gamma \max_{0\le s\le t} \|z(s)\|_H^2 \,+\, C_{10}\, \lambda^4\,. \quad (3.74)$$

Combining the estimates (3.69)–(3.74), taking the maximum with respect to $t \in [0,T]$, adjusting $\gamma > 0$ appropriately small, and invoking Gronwall's lemma, we arrive at the conclusion that $(y^\lambda, z^\lambda) = (y,z)$ satisfies the inequality

$$\|y^\lambda\|^2_{H^1(0,T;H)\cap C^0([0,T];V)} \,+\, \|z^\lambda\|^2_{C^0([0,T];H)\cap L^2([0,T];V)} \,\le\, C_{11}\,\lambda^4\,. \tag{3.75}$$

Finally, testing (3.63) by $-\Delta y^\lambda$, and using (3.68), we find that also

$$\|y^\lambda\|^2_{L^2(0,T;W)} \,\le\, C_{12}\,\lambda^4\,. \tag{3.76}$$

This concludes the proof of the assertion. ∎

Corollary 3.4 *Let the assumptions* (A1)–(A3) *be fulfilled, and let $\bar u \in U_{ad}$ be an optimal control for the problem* **(CP)** *with associated state $(\bar\rho,\bar\mu) = S(\bar u)$. Then, for every $v \in U_{ad}$,*

$$\int_0^T\!\!\int_\Omega \beta_2\,\bar u(v-\bar u)\,dx\,dt + \int_\Omega (\bar\rho(T)-\rho_T)\,\xi(T)\,dx + \int_0^T\!\!\int_\Omega \beta_1\,(\bar\mu-\mu_T)\,\eta\,dx\,dt \,\ge\, 0, \tag{3.77}$$

where (ξ,η) is the unique solution to the linearized system (3.21)–(3.24) *associated with $h = v - \bar u$.*

Proof. Let $v \in U_{ad}$ be arbitrary. Then $h = v - \bar u$ is an admissible direction, since $\bar u + \lambda h \in U_{ad}$ for $0 < \lambda \le 1$. For any such λ, we have

$$\begin{aligned} 0 \,&\le\, \frac{J(\bar u + \lambda h, S(\bar u + \lambda h)) - J(\bar u, S(\bar u))}{\lambda} \\ &\le\, \frac{J(\bar u + \lambda h, S(\bar u + \lambda h)) - J(\bar u, S(\bar u + \lambda h))}{\lambda} \,+\, \frac{J(\bar u, S(\bar u + \lambda h)) - J(\bar u, S(\bar u))}{\lambda}\,. \end{aligned}$$

It follows immediately from the definition of the cost functional J that the first summand on the right-hand side of this inequality converges to $\int_0^T\!\int_\Omega \beta_2\,\bar u\,h\,dx\,dt$ as $\lambda \searrow 0$. For the second summand, we obtain from Proposition 3.3 that

$$\lim_{\lambda\searrow 0} \frac{J(\bar u, S(\bar u + \lambda h)) - J(\bar u, S(\bar u))}{\lambda} = \int_\Omega (\bar\rho(T)-\rho_T)\,\xi(T)\,dx + \int_0^T\!\!\int_\Omega \beta_1\,(\bar\mu-\mu_T)\,\eta\,dx\,dt\,,$$

whence the assertion follows. ∎

3.3 The optimality system

Let $\bar u \in U_{ad}$ be an optimal control for **(CP)** with associated state $(\bar\rho,\bar\mu) = S(\bar u)$. Then, for every $v \in U_{ad}$, (3.77) holds. We now aim to eliminate (ξ,η) by introducing the adjoint state variables. To this end, we consider the *adjoint system*:

$$-(\varepsilon + 2\bar{\rho})\, q_t - \bar{\rho}_t\, q - \Delta q = p + \beta_1\, (\bar{\mu} - \mu_T) \quad \text{a.e. in } Q, \tag{3.78}$$

$$\frac{\partial q}{\partial \mathbf{n}} = 0 \quad \text{a.e. in } \Sigma, \qquad q(x,T) = 0 \quad \text{a.e. in } \Omega, \tag{3.79}$$

$$-\delta p_t - \Delta p + f''(\bar{\rho})\, p = \bar{\mu}\, q_t - \bar{\mu}_t\, q \quad \text{in } Q, \tag{3.80}$$

$$\frac{\partial p}{\partial \mathbf{n}} = 0 \quad \text{on } \Sigma, \qquad \delta\, p(T) = \bar{\rho}(T) - \rho_T \quad \text{in } \Omega\,, \tag{3.81}$$

which is a linear backward-in-time parabolic system for the adjoint state variables p and q.

It must be expected that the adjoint state variables (p,q) be less regular than the state variables $(\bar{\rho}, \bar{\mu})$. Indeed, we only have $p(T) \in L^2(\Omega)$, and thus (3.80) and (3.81) should be interpreted in the ususal weak sense. That is, we look for a vector-valued function $p \in H^1(0,T;V^*) \cap C^0([0,T];H) \cap L^2(0,T;V)$ that, in addition to the final time condition (3.81), satisfies

$$\begin{aligned} &\langle -\delta\, p_t(t), v\rangle_{V^*,V} \;+\; \int_\Omega \nabla p(t) \cdot \nabla v\, dx \;+\; \int_\Omega f''(\bar{\rho}(t))\, p(t)\, v\, dx \\ &= \int_\Omega \left(\bar{\mu}(t)\, q_t(t) - \bar{\mu}_t(t)\, q(t)\right)\, v\, dx\,, \end{aligned} \tag{3.82}$$

for every $v \in V$ and almost every $t \in (0,T)$. Notice that if $q \in H^1(0,T;H) \cap C^0([0,T];V)$, then it is easily seen that $\bar{\mu}\, q_t - \bar{\mu}_t\, q \in L^{3/2}(Q)$, so that the integral on the right-hand side of (3.82) makes sense. On the other hand, if p has the expected regularity then the solution to (3.78), (3.79) should belong to $H^1(0,T;H) \cap C^0([0,T];V) \cap L^2(0,T;W)$.

Lemma 3.5 *Suppose that the system* (3.78)–(3.81) *has a unique solution* (p,q) *where* $p \in H^1(0,T;V^*) \cap C^0([0,T];H) \cap L^2(0,T;V)$ *and* $q \in H^1(0,T;H) \cap C^0([0,T];V) \cap L^2(0,T;W)$*. Then we have*

$$\int_\Omega (\bar{\rho}(x,T) - \rho_T(x))\, \xi(x,T)\, dx \;+\; \int_0^T \!\! \int_\Omega \beta_1\, (\bar{\mu} - \mu_T)\, \eta\, dx\, dt = \int_0^T \!\! \int_\Omega q\, h\, dx\, dt\,. \tag{3.83}$$

Proof. The assertion follows from repeated integration by parts, using the well-known integration by parts formula

$$\int_0^T \big(\langle v_t(t), w(t)\rangle_{V^*,V} \;+\; \langle w_t(t), v(t)\rangle_{V^*,V}\big)\, dt = \int_\Omega \big(v(T)w(T) - v(0)w(0)\big)\, dx,$$

which holds for all functions $v, w \in H^1(0,T;V^*) \cap L^2(0,T;V)$. Since this calculation is standard in optimal control theory, we may leave it to the reader to work out the details. ∎

Proposition 3.6 *The adjoint system* (3.78)–(3.81) *has a unique solution* (p,q) *with* $p \in H^1(0,T;V^*) \cap C^0([0,T];H) \cap L^2(0,T;V)$ *and* $q \in H^1(0,T;H) \cap C^0([0,T];V) \cap L^2(0,T;W)$*, where* (3.80) and $(3.81)_1$ *are understood in the sense of* (3.82).

Proof. We proceed in a series of steps.

Step 1: Approximation. As in the proof of Proposition 3.2, we employ a delay technique. However, this time we have to use a *negative* delay, since the system (3.78)–(3.81) runs backwards in time.

For $0 < \tau < T$, we define the translation operator $\tilde{\mathcal{T}}_\tau : L^1(0,T;H) \to L^1(0,T;H)$ by putting, for every $v \in L^1(0,T;H)$ and almost all $t \in (0,T)$,

$$\big(\tilde{\mathcal{T}}_\tau v\big)(t) = v(t+\tau) \quad \text{if } t \le T-\tau, \quad \text{and} \quad \big(\tilde{\mathcal{T}}_\tau v\big)(t) = 0 \quad \text{if } t > T-\tau; \tag{3.84}$$

clearly, we have that $\|\tilde{\mathcal{T}}_\tau v\|_{L^2(Q)} \le \|v\|_{L^2(Q)}$, for every $v \in L^2(Q)$ and any $\tau \in (0,T)$.

We then consider for $\tau \in (0,T)$ the following approximating problem: find functions

$$\begin{aligned} &p^\tau \in H^1(0,T;V^*) \cap C^0([0,T];H) \cap L^2(0,T;V), \\ &q^\tau \in H^1(0,T;H) \cap C^0([0,T];V) \cap L^2(0,T;W) \end{aligned} \tag{3.85}$$

that solve the system

$$-(\varepsilon + 2\bar\rho)\, q^\tau_t - \Delta q^\tau + q^\tau = (1+\bar\rho_t)\, \tilde{\mathcal{T}}_\tau q^\tau + \tilde{\mathcal{T}}_\tau p^\tau + \beta_1(\bar\mu - \mu_T) \quad \text{a.e. in } Q, \tag{3.86}$$

$$\frac{\partial q^\tau}{\partial \mathbf{n}} = 0 \quad \text{a.e. on } \Sigma, \quad q^\tau(x,T) = 0 \quad \text{a.e. in } \Omega, \tag{3.87}$$

$$\begin{aligned} &\langle -\delta\, p^\tau_t(t), v\rangle_{V^*,V} + \int_\Omega \nabla p^\tau(t)\cdot\nabla v\,dx + \int_\Omega f''(\bar\rho(t))\, p^\tau(t)\, v\,dx \\ &\quad = \int_\Omega \Big(\bar\mu(t)\, q^\tau_t(t) - \bar\mu_t(t) q^\tau(t)\Big) v\,dx \quad \forall\, v \in V, \quad \text{for a.e. } t \in (0,T), \end{aligned} \tag{3.88}$$

$$\delta\, p^\tau(T) = \bar\rho(T) - \rho_T \quad \text{a.e. in } \Omega. \tag{3.89}$$

We choose for $\tau \in (0,T)$ the discrete values $\tau = T/N$, where $N \in \mathbb{N}$ is arbitrary, and we put $t_n = n\,\tau$, $0 \le n \le N$, and $I_n = (t_n, T)$. For $n = N-1, \ldots, 1, 0$, we solve the problem:

$$-(\varepsilon + 2\bar\rho)\, q_{n,t} - \Delta q_n + q_n = (1+\bar\rho_t)\, \tilde{\mathcal{T}}_\tau q_n + \tilde{\mathcal{T}}_\tau p_n + \beta_1(\bar\mu - \mu_T) \quad \text{a.e. in } \Omega \times I_n, \tag{3.90}$$

$$\frac{\partial q_n}{\partial \mathbf{n}} = 0 \quad \text{a.e. on } \Sigma, \quad q_n(x,T) = 0 \quad \text{a.e. in } \Omega, \tag{3.91}$$

$$\begin{aligned} &\langle -\delta\, p_{n,t}(t), v\rangle_{V^*,V} + \int_\Omega \nabla p_n(t)\cdot\nabla v\,dx + \int_\Omega f''(\bar\rho(t))\, p_n(t)\, v\,dx \\ &\quad = \int_\Omega \Big(\bar\mu(t)\, q_{n,t}(t) - \bar\mu_t(t)\, q_n(t)\Big)\, v\,dx \quad \text{for all } v \in V, \quad \text{for a.e. } t \in (t_n,T), \end{aligned} \tag{3.92}$$

$$\delta\, p_n(T) = \bar\rho(T) - \rho_T \quad \text{a.e. in } \Omega. \tag{3.93}$$

Here, $\tilde{\mathcal{T}}_\tau$ acts on functions that are not defined on the entire interval $(0,T)$; however, for $n < N-1$ it is still defined by (3.84), while for $n = N-1$ we simply put $\tilde{\mathcal{T}}_\tau p_n = \tilde{\mathcal{T}}_\tau q_n = 0$.

Whenever the pairs (p_k, q_k) with

$$p_k \in H^1(I_k; V^*) \cap C^0(\bar{I}_k; H) \cap L^2(I_k; V), \tag{3.94}$$
$$q_k \in H^1(I_k; H) \cap C^0(\bar{I}_k; V) \cap L^2(I_k; W), \tag{3.95}$$

have been constructed for $0 < n \leq k \leq N-1$, we look for the pair (ξ_{n-1}, η_{n-1}) that coincides with (ξ_n, η_n) in I_n. Note that the linear parabolic problem (3.90), (3.91) has a unique solution q_{n-1} on $\Omega \times I_{n-1}$ that satisfies (3.95) for $k = n-1$ (see, e. g., [12]) . On inserting q_{n-1} in (3.92) (with n replaced by $n-1$), we then find (e. g., by using an appropriate Galerkin approximation) that the linear parabolic problem (3.92), (3.93) admits a unique solution p_{n-1} that fulfills (3.94) for $k = n-1$. Hence, we conclude that $(p^\tau, q^\tau) = (p_0, q_0)$ satisfies (3.86)–(3.89) and (3.85).

Step 2: A priori estimates. We now prove a series of a priori estimates for the functions (p^τ, q^τ). In the following, we denote by C_i $(i \in \mathbb{N})$ some generic positive constants, which may depend on $\varepsilon, \delta, \rho_*, \rho^*, \mu^*, T, K_1^*, K_2^*$, but not on τ (i. e., not on N). For the sake of simplicity, we omit the superscript τ and simply write (p, q).

We multiply (3.86) by $-q_t$ and integrate over $\Omega \times [t, T]$ to obtain, using Young's inequality,

$$\begin{aligned}
&\frac{\varepsilon}{2} \int_t^T \|q_t(s)\|_H^2\, ds + \frac{1}{2}\left(\|\nabla q(t)\|_H^2 + \|q(t)\|_H^2\right) \\
&\leq C_1 + C_2 \int_t^T \left(\|p(s)\|_H^2 + \|q(s)\|_H^2\right) ds + \int_t^T \int_\Omega |\bar{\rho}_t|\, |\tilde{\mathcal{T}}_\tau q|\, |q_t|\, dx\, ds\,.
\end{aligned} \tag{3.96}$$

Moreover, by virtue of Hölder's and Young's inequalities, and invoking the continuity of the embedding $H^1(\Omega) \subset L^4(\Omega)$, we have, for any $\gamma > 0$, that

$$\begin{aligned}
&\int_t^T \int_\Omega |\bar{\rho}_t|\, |\tilde{\mathcal{T}}_\tau q|\, |q_t|\, dx\, ds \leq \int_t^T \|\bar{\rho}_t(s)\|_{L^4(\Omega)}\, \|\tilde{\mathcal{T}}_\tau q(s)\|_{L^4(\Omega)}\, \|q_t(s)\|_H\, ds \\
&\leq \gamma \int_t^T \|q_t(s)\|_H^2\, ds + \frac{C_3}{\gamma} \int_t^{T-\tau} \|\bar{\rho}_t(s)\|_V^2\, \|q(s+\tau)\|_V^2\, ds\,.
\end{aligned} \tag{3.97}$$

Observe that by (2.6) the mapping $s \mapsto \|\bar{\rho}_t(s)\|_V^2$ belongs to $L^1(0,T)$.

Next, we insert $v = p(t)$ in (3.88) and integrate over $[t, T]$, where $t \in [0, T]$. We find, using (3.93), that

$$\begin{aligned}
&\frac{\delta}{2} \|p(t)\|_H^2 + \frac{1}{2} \int_t^T \|\nabla p(s)\|_H^2\, ds \leq C_4 + C_5 \int_t^T \|p(s)\|_H^2\, ds \\
&+ \int_t^T \int_\Omega |\bar{\mu}|\, |q_t|\, |p|\, dx\, ds + \int_t^T \int_\Omega |\bar{\mu}_t|\, |q|\, |p|\, dx\, ds\,.
\end{aligned} \tag{3.98}$$

Let us denote for short the last two integrals on the right-hand side of (3.98) by I_1 and I_2, respectively. Since $\bar{\mu} \in L^\infty(Q)$, we have that

$$I_1 \leq \gamma \int_t^T \|q_t(s)\|_H^2\, ds + \frac{C_6}{\gamma} \int_t^T \|p(s)\|_H^2\, ds\,. \tag{3.99}$$

Moreover, we conclude from (2.6), invoking Hölder's and Young's inequalities, that

$$
\begin{aligned}
I_2 \;&\le\; \int_t^T \|\bar\mu_t(s)\|_H\,\|q(s)\|_{L^4(\Omega)}\,\|p(s)\|_{L^4(\Omega)}\,ds \\
&\le\; \gamma \int_t^T \|p(s)\|_V^2\,ds \;+\; \frac{C_7}{\gamma}\int_t^T \|\bar\mu_t(s)\|_H^2\,\|q(s)\|_V^2\,ds\,,
\end{aligned}
\tag{3.100}
$$

where the mapping $s \mapsto \|\bar\mu_t(s)\|_H^2$ belongs to $L^1(0,T)$.

Now, we combine the estimates (3.96)–(3.100). On choosing $\gamma > 0$ sufficiently small, and on applying Gronwall's lemma, we find that

$$
\|p\|_{C^0([0,T];H)\cap L^2(0,T;V)} \;+\; \|q\|_{H^1(0,T;H)\cap C^0([0,T];V)} \;\le\; C_8\,. \tag{3.101}
$$

It is now a standard matter to verify, by comparison in (3.86) and (3.88), respectively, that also

$$
\|p\|_{H^1(0,T;V^*)} \;+\; \|q\|_{L^2(0,T;W)} \;\le\; C_9\,. \tag{3.102}
$$

Step 3: Passage to the limit. Let (p_N,q_N) denote the solution to the system (3.86)–(3.87) associated with $\tau_N = T/N$, for $N \in \mathbb{N}$. In Step 2, we have shown that there is some $C>0$, which does not depend on N, such that

$$
\|p_N\|_{H^1(0,T;V^*)\cap C^0([0,T];H)\cap L^2(0,T;V)} \;+\; \|q_N\|_{H^1(0,T;H)\cap C^0([0,T];V)\cap L^2(0,T;W)} \;\le\; C.
$$

Hence, there is a subsequence, which is again indexed by N, such that

$$
\begin{aligned}
&p_N \to p, \quad \text{weakly star in } H^1(0,T;V^*)\cap L^\infty(0,T;H)\cap L^2(0,T;V),\\
&q_N \to q, \quad \text{weakly star in } H^1(0,T;H)\cap L^\infty(0,T;V)\cap L^2(0,T;W).
\end{aligned}
$$

By compact embedding, we also have the strong convergences (see, e. g., [16])

$$
p_N \to p, \quad \text{strongly in } L^2(Q), \qquad q_N \to q, \quad \text{strongly in } C^0([0,T];H)\cap L^2(0,T;V).
$$

From this, we can conclude the following convergences:

$$
\begin{aligned}
&\bar\rho\, q_{N,t} \to \bar\rho\, q_t \quad \text{weakly in } L^2(Q), \quad \Delta q_N \to \Delta q \quad \text{weakly in } L^2(Q),\\
&\tilde{\mathcal{T}}_{T/N} q_N \to q \quad \text{strongly in } L^2(Q), \quad \tilde{\mathcal{T}}_{T/N} p_N \to p \quad \text{strongly in } L^2(Q),\\
&\bar\rho_t\, \tilde{\mathcal{T}}_{T/N} q_N \to \bar\rho_t\, q \quad \text{strongly in } L^1(Q).
\end{aligned}
$$

Hence, passing to the limit as $N \to \infty$ in (3.86)–(3.87) for $\tau = T/N$, we find that the pair (p,q) gives a strong solution to the parabolic problem (3.78)–(3.79). Next, we notice that the weak convergence of $\{p_N\}$ to p in $H^1(0,T;V^*)\cap L^2(0,T;V)$ implies that $p_N \to p$ weakly in $C^0([0,T];H)$. We may thus conclude, in particular, that $\delta\, p(T) = \bar\rho(T) - \rho_T$. Since $f''(\bar\rho)$ and $\bar\mu$ are bounded, we also have the following convergences:

$$
f''(\bar\rho)\, p_N \to f''(\bar\rho)\, p \quad \text{strongly in } L^2(Q), \quad \bar\mu\, q_{N,t} \to \bar\mu\, q_t \quad \text{weakly in } L^2(Q).
$$

Therefore, (3.82) is fulfilled for any v in $C^1(\overline{\Omega})$, which is a dense subset of $H^1(\Omega)$, because Ω is a Lipschitz domain. From this, it easily follows that (3.82) is satisfied for every $v \in H^1(\Omega)$. In conclusion, the pair (p, q) is a solution to the adjoint system (3.78)–(3.81) that enjoys the asserted smoothness properties.

Uniqueness remains to be shown. But if (p_1, q_1), (p_2, q_2) are two solutions having the above properties, then the pair (p, q), where $p = p_1 - p_2$ and $q = q_1 - q_2$, satisfies (3.78)–(3.81), where the inhomogeneities $\beta_1(\bar{\mu} - \mu_T)$ and $\bar{\rho} - \rho_T$ on the right-hand sides of (3.78) and (3.81), respectively, cancel out by subtraction. We may then repeat the a priori estimates of Step 2 to see that in the present situation the constants C_1 and C_4 appearing, respectively, in (3.96) and (3.98), simply do not occur. Consequently, the application of Gronwall's lemma yields $p = q = 0$. This concludes the proof. ∎

In summary, we have proved the following result concerning first-order necessary optimality conditions.

Theorem 3.7 *Suppose that $\bar{u} \in U_{ad}$ is an optimal control for* **(CP)** *with associated state $(\bar{\rho}, \bar{\mu}) = S(\bar{u})$. Then the adjoint system* (3.78)–(3.81) *has a unique weak solution (p, q) with $p \in H^1(0,T;V^*) \cap C^0([0,T];H) \cap L^2(0,T;V)$, $\quad q \in H^1(0,T;H) \cap C^0([0,T];V) \cap L^2(0,T;W)$; moreover, for any $v \in U_{ad}$, we have the inequality:*

$$\int_0^T \int_\Omega \beta_2 \, \bar{u} \, (v - \bar{u}) \, dx \, dt \; + \int_0^T \int_\Omega q \, (v - \bar{u}) \, dx \, dt \; \geq \; 0 \, . \tag{3.103}$$

Remark: 5. Since U_{ad} is a nonempty, closed and convex subset of $L^2(Q)$, (3.103) has the following implications:

- For $\beta_2 > 0$, the optimal control $\bar{u}$ is nothing but the $L^2(Q)$ orthogonal projection of $-\beta_2^{-1} q$ onto U_{ad}. In other words,

  $$\bar{u}(x,t) = \mathcal{P}_{[0,U(x,t)]} \left(-\beta_2^{-1} \, q(x,t) \right) \quad \text{a. e. in } Q \, ,$$

  where, for any $a, b \in \mathrm{I\!R}$ such that $a \leq b$, $\mathcal{P}_{[a,b]}(u) := \min \{b, \, \max \{a, u\}\}$.

- For $\beta_2 = 0$, we have that almost everywhere

  $$\bar{u}(x,t) = \begin{cases} 0 & \text{if } q(x,t) > 0 \\ U(x,t) & \text{if } q(x,t) < 0 \end{cases} \, ,$$

  a *bang-bang* situation where no information can be recovered for points at which $q(x,t) = 0$.

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