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OPTIMAL CONTROL OF THE BIDOMAIN SYSTEM (III): EXISTENCE OF MINIMIZERS AND FIRST-ORDER OPTIMALITY CONDITIONS

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Abstract. We consider optimal control problems for the bidomain equations of cardiac electrophysiology together with two-variable ionic models, *e.g.* the Rogers–McCulloch model. After ensuring the existence of global minimizers, we provide a rigorous proof for the system of first-order necessary optimality conditions. The proof is based on a stability estimate for the primal equations and an existence theorem for weak solutions of the adjoint system.

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1. Introduction

In this work, we continue our investigations of optimal control problems for the bidomain system. After the study of the monodomain approximation of the equations and a thorough stability and regularity analysis of weak solutions for the full bidomain equations, as contained in the previous papers [11, 12], we are now in position to analyze the related control problems with respect to the existence of minimizers as well as to provide a rigorous proof of the first-order necessary optimality conditions.

Let $\Omega \subset \mathbb{R}^3$ be a bounded domain and $T > 0$ a fixed time horizon. Then the bidomain system, representing a well-accepted description of the electrical activity of the heart, is given by[3]

$$\frac{\partial \Phi_{\mathrm{tr}}}{\partial t} + I_{\mathrm{ion}}(\Phi_{\mathrm{tr}}, W) - \mathrm{div}\,\big(M_i \,\nabla \Phi_i \big) = I_i \quad \text{for almost all } (x,t) \in \Omega \times [\,0,\,T\,]; \tag{1.1}$$

$$\frac{\partial \Phi_{\mathrm{tr}}}{\partial t} + I_{\mathrm{ion}}(\Phi_{\mathrm{tr}}, W) + \mathrm{div}\,\big(M_e \,\nabla \Phi_e \big) = -I_e \quad \text{for almost all } (x,t) \in \Omega \times [\,0,\,T\,]; \tag{1.2}$$

$$\frac{\partial W}{\partial t} + G(\Phi_{\mathrm{tr}}, W) = 0 \quad \text{for almost all } (x,t) \in \Omega \times [\,0,\,T\,]; \tag{1.3}$$

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3 The bidomain model has been considered first in [21]. A detailed introduction may be found *e.g.* in [20], pp. 21–56.

$$\mathfrak{n}^{\mathrm{T}} M_i \, \nabla \Phi_i \; = \; 0 \quad \text{for all} \;\; (x,t) \in \partial\Omega \times [\, 0, \, T \,] \, ; \tag{1.4}$$

$$\mathfrak{n}^{\mathrm{T}} M_e \, \nabla \Phi_e \; = \; 0 \quad \text{for all} \;\; (x,t) \in \partial\Omega \times [\, 0, \, T \,] \, ; \tag{1.5}$$

$$\Phi_{\mathrm{tr}}(x,0) \; = \; \Phi_i(x,0) - \Phi_e(x,0) \; = \; \Phi_0(x) \quad \text{and} \quad W(x,0) \; = \; W_0(x) \quad \text{for almost all} \;\; x \in \Omega. \tag{1.6}$$

In this model, Ω represents the spatial domain occupied by the cardiac muscle, the variables Φ_i and Φ_e denote the intracellular and extracellular electric potentials, and $\Phi_{\mathrm{tr}} = \Phi_i - \Phi_e$ is the transmembrane potential. The anisotropic electric properties of the intracellular and the extracellular tissue parts are modeled by conductivity tensors M_i and M_e. The specification of the model for the ionic current I_{ion} in (1.1) and (1.2) and the gating function G in (1.3) will be made below. We shall consider three so-called two-variable models wherein I_{ion} and G depend on Φ_{tr} as well as on a single gating variable W, which describes in a cumulative way the effects of the ion transport through the cell membranes (see Sect. 2.2.). Finally, the inhomogeneities I_i and I_e represent the intracellular and extracellular stimulation currents, respectively.

We shall investigate optimal control problems of the form

$$\text{(P)} \quad F(\Phi_{\mathrm{tr}}, \Phi_e, W, I_e) \; = \; \int_0^T \!\! \int_\Omega r\big(\, x, t, \Phi_{\mathrm{tr}}(x,t), \Phi_e(x,t), W(x,t) \, \big) \, \mathrm{d}x \, \mathrm{d}t \; + \; \frac{\mu}{2} \int_0^T \!\! \int_{\Omega_{\mathrm{con}}} I_e(x,t)^2 \, \mathrm{d}x \, \mathrm{d}t \; \longrightarrow \; \inf ! \tag{1.7}$$

subject to the bidomain equations (1.1)–(1.6) in its weak formulation (see (2.1)–(2.4) below)

and the control restriction $I_e \in \mathcal{C}$ (1.8)

where Ω_{con} is a Lipschitz subdomain of Ω and

$$\mathcal{C} \; = \; \big\{ \, Q \, I \; \big| \; I \in L^\infty \big[\, (\, 0, \, T \,) \, , \, L^2(\Omega) \, \big], \; \mathrm{supp} \, (I) \subseteq \Omega_{\mathrm{con}} \times [\, 0, \, T \,], \tag{1.9}$$
$$| \, I(x,t) \, | \; \leqslant \; R \;\; (\forall) \, (x,t) \in \Omega_T \, \big\} \; \subset \; L^\infty \big[\, (\, 0, \, T \,) \, , \, L^2(\Omega) \, \big].$$

For the description of the control domain, the linear operator $Q: \;\; L^2(\Omega_T) \to L^2(\Omega_T)$ defined by

$$Q \, I(x,t) \; = \; I(x,t) - \mathbb{1}_{\Omega_{\mathrm{con}}}(x) \cdot \frac{1}{|\, \Omega_{\mathrm{con}} \,|} \int_{\Omega_{\mathrm{con}}} I(\tilde{x},t) \, \mathrm{d}\tilde{x} \tag{1.10}$$

has been used. When applied to a function I with $\mathrm{supp}\,(I) \subseteq \Omega_{\mathrm{con}} \times [\, 0, T \,]$, Q extends by zero the orthogonal projection onto the complement of the subspace $\{ \, Z \, \big| \, \int_{\Omega_{\mathrm{con}}} Z(\tilde{x},t) \, \mathrm{d}\tilde{x} \; = \; 0 \text{ for a.a. } t \; \in \; (\, 0, \, T \,) \, \} \; \subset \; L^2 \big[\, (\, 0, \, T \,) \, , \, L^2(\Omega_{\mathrm{con}}) \, \big]$. Consequently, for $I_e \in \mathcal{C}$, we have

$$\int_\Omega I_e(x,t) \, \mathrm{d}x \; = \; \int_{\Omega_{\mathrm{con}}} I_e(x,t) \, \mathrm{d}x \; = \; 0 \quad \text{for almost all } t \in (\, 0, \, T \,), \tag{1.11}$$

what guarantees the solvability of the state equations (*cf.* Thm. 2.3 below). In problem (P), the extracellular excitation I_e acts as control, which is allowed to be applied on the subdomain Ω_{con} only.[4] The pointwise constraint within the description (1.9) of $\mathcal{C}$ is included due to the obvious fact that one cannot apply arbitrary large electrical stimulations to living tissue without damaging it. In mathematical terms, this restriction is necessary in order to establish a stability estimate for the bidomain system (Thm. 2.4).

Due to the complex dynamical behaviour of the state equations, an appropriate choice of the integrand r within the first term of the objective (1.7) for concrete applications is quite delicate. With arrhythmia or tachycardia in mind, it could be chosen as $r(x,t,\varphi,\eta,w) = \big(\varphi - \Phi_{\mathrm{des}}(t) \big)^2$ where Φ_{des} denotes some desired

[4]For physiological reasons, the intracellular excitation I_i must be set zero.

trajectory for the controlled state $\Phi_{\rm tr}$, which is part of a solution of (1.1)–(1.5) as well, *cf.* [16]. The second term expresses the requirement that – regardless of whether the pointwise restriction within (1.9) is active – the overall stimulus should be as small as possible. Consequently, solutions with little intervention to the cardiac system are favored.

Besides an existence theorem for global minimizers (Thm. 3.4), the main result of the present paper is the rigorous proof of the following *set of first-order necessary optimality conditions* for sufficiently regular local minimizers $(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)$ of (P), consisting of the variational inequality

$$\int_0^T \int_{\Omega_{\rm con}} \Big(\mu\, \hat{I}_e - Q\, P_2 \Big) \cdot \Big(I_e - \hat{I}_e \Big)\, {\rm d}x\, {\rm d}t \,\geqslant\, 0 \quad \text{for all admissible controls } I_e \tag{1.12}$$

and the adjoint system[5]

$$\int_0^T \int_\Omega \Big(-\frac{\partial P_1}{\partial t} + \frac{\partial I_{\rm ion}}{\partial \varphi}(\hat{\Phi}_{\rm tr}, \hat{W})\, P_1 + \frac{\partial G}{\partial \varphi}(\hat{\Phi}_{\rm tr}, \hat{W})\, P_3 \Big)\, \psi\, {\rm d}x\, {\rm d}t + \int_0^T \int_\Omega \nabla\psi^{\rm T} M_i\, (\, \nabla P_1 + \nabla P_2\,)\, {\rm d}x\, {\rm d}t \tag{1.13}$$
$$= -\int_0^T \int_\Omega \Big(\frac{\partial r}{\partial \varphi}(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W}) \Big)\, \psi\, {\rm d}x\, {\rm d}t \quad \forall\, \psi \in L^2\big[\,(\,0,\,T\,)\,,\ W^{1,2}(\Omega)\,\big],\ P_1(x,T) \equiv 0\,;$$

$$\int_0^T \int_\Omega \nabla\psi^{\rm T} M_i\, \nabla P_1\, {\rm d}x\, {\rm d}t + \int_0^T \int_\Omega \nabla\psi^{\rm T}\, (M_i + M_e)\, \nabla P_2\, {\rm d}x\, {\rm d}t \,=\, -\int_0^T \int_\Omega \frac{\partial r}{\partial \eta}(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W})\, \psi\, {\rm d}x\, {\rm d}t \tag{1.14}$$
$$\forall\, \psi \in L^2\big[\,(\,0,\,T\,)\,,\ W^{1,2}(\Omega)\,\big] \text{ with } \int_\Omega \psi(x,t)\, {\rm d}x = 0 \text{ for a.a. } t \in (\,0,\,T\,),\ \int_\Omega P_2(x,t)\, {\rm d}x = 0\ (\forall)\, t \in (\,0,\,T\,)\,;$$

$$\int_0^T \int_\Omega \Big(-\frac{\partial P_3}{\partial t} + \frac{\partial I_{\rm ion}}{\partial w}(\hat{\Phi}_{\rm tr}, \hat{W})\, P_1 + \frac{\partial G}{\partial w}(\hat{\Phi}_{\rm tr}, \hat{W})\, P_3 \Big)\, \psi\, {\rm d}x\, {\rm d}t \,=\, -\int_0^T \int_\Omega \Big(\frac{\partial r}{\partial w}(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W}) \Big)\, \psi\, {\rm d}x\, {\rm d}t \tag{1.15}$$
$$\forall\, \psi \in L^2\big[\,(\,0,\,T\,)\,,\ L^2(\Omega)\,\big],\ P_3(x,T) \equiv 0$$

for the multipliers P_1, P_2 and P_3 related to the weak state equations (2.1), (2.2) and (2.3) below, respectively (Thm. 5.2). The proof, which will be given by fitting the problem (P) into the framework of *weakly singular problems* in the sense of Ito/Kunisch (see [9], p. 17 f.), is based on two main ingredients. The first one is a stability estimate for the primal equations (Thm. 2.4), whose proof has been already provided in the previous publication [12]. Secondly, we need an existence proof for weak solutions of the adjoint system, which is contained in the present paper (Thm. 4.2). In difference to the monodomain approximation considered in [11], the proof of the optimality conditions requires additional regularity of the minimizer $(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e\,)$ in the case of the full bidomain system.

In the literature, only a few studies related to the optimal control of the bidomain system are available as yet, mostly restricted to the monodomain approximation. We mention [1, 5, 10, 13–16] and refer to [11], page 1527, for a closer discussion. Numerical work concerning open-loop control of the bidomain equations with the goal of dampening of excitation and reentry waves has been realized in [10, 14–16]. The problems were treated with gradient and Newton-type techniques applied to FEM discretizations of the state equations.

The paper is structured in the following way. In Section 2, the solution concepts for the bidomain equations are outlined. We present the ionic models to be used and summarize the existence and stability theorems for weak solutions of (1.1)–(1.6). Then, in Section 3, we restate the optimal control problem (1.7)–(1.8) within function spaces, subsequently analyzing the structure of the feasible domain and establishing the existence of global minimizers. Section 4 is concerned with the derivation of the adjoint system and the existence proof for a weak solution of it. Finally, in Section 5, we state and prove the first-order necessary optimality conditions for the control problem.

[5]Within the functions $r(x,t,\varphi,\eta,w)$, $I_{\rm ion}(\varphi,w)$ and $G(\varphi,w)$, the real variables φ, η and w are the placeholders for $\Phi_{\rm tr}$, Φ_e and W, respectively.

Notations.
We denote by $L^p(\Omega)$ the space of functions, which are in the pth power integrable ($1 \leqslant p < \infty$), or are measurable and essentially bounded ($p = \infty$), and by $W^{1,p}(\Omega)$ the Sobolev space of functions $\psi : \ \Omega \to \mathbb{R}$ which, together with their first-order weak partial derivatives, belong to the space $L^p(\Omega, \mathbb{R})$ ($1 \leqslant p < \infty$). For spaces of Bochner integrable mappings, *e.g.* $L^2\big[\,(0, T)\,,\ W^{1,2}(\Omega)\,\big]$, we refer to the summary in [11], page 1542. Ω_T is an abbreviation for $\Omega \times [\,0, T\,]$. The gradient ∇ is always taken only with respect to the spatial variables x. The characteristic function of the set $\mathrm{A} \subseteq \mathbb{R}^3$ is defined as $\mathbb{1}_\mathrm{A} : \ \mathbb{R}^3 \to \mathbb{R}$ with $\mathbb{1}_\mathrm{A}(x) = 1 \iff x \in \mathrm{A}$ and $\mathbb{1}_\mathrm{A}(x) = 0 \iff x \notin \mathrm{A}$. Finally, the nonstandard abbreviation "$(\forall)\, t \in \mathrm{A}$ "has to be read as "for almost all $t \in \mathrm{A}$" or "for all $t \in \mathrm{A}$ except for a Lebesgue null set", and the symbol $\mathfrak{o}$ denotes, depending on the context, the zero element or the zero function of the underlying space.

2. Weak solutions of the bidomain system

2.1. Parabolic-elliptic form of the bidomain system; strong and weak solutions

It is well-known that the bidomain system (1.1)–(1.6) can be equivalently stated in parabolic-elliptic form, *cf.* [4], page 459, and [12], page 4, (2.1)–(2.9). In its weak formulation, the system reads as follows:

$$\int_\Omega \Big(\frac{\partial \Phi_{\mathrm{tr}}}{\partial t} \cdot \psi + \nabla\psi^{\mathrm{T}} M_i(\,\nabla\Phi_{\mathrm{tr}} + \nabla\Phi_e\,) + I_{\mathrm{ion}}(\Phi_{\mathrm{tr}}, W)\,\psi \Big)\,\mathrm{d}x \;=\; \int_\Omega I_i\,\psi\,\mathrm{d}x \tag{2.1}$$

$$\forall\,\psi \in W^{1,2}(\Omega), \ \text{ for a.a. } t \in (\,0\,,\,T\,)\,;$$

$$\int_\Omega \Big(\nabla\psi^{\mathrm{T}} M_i \nabla\Phi_{\mathrm{tr}} + \nabla\psi^{\mathrm{T}}(M_i + M_e)\,\nabla\Phi_e \Big)\,\mathrm{d}x \;=\; \int_\Omega \Big(I_i + I_e \Big)\,\psi\,\mathrm{d}x \tag{2.2}$$

$$\forall\,\psi \in W^{1,2}(\Omega) \ \text{ with } \int_\Omega \psi(x)\,\mathrm{d}x = 0\,, \ \text{ for a.a. } t \in (\,0\,,\,T\,)\,;$$

$$\int_\Omega \Big(\frac{\partial W}{\partial t} + G(\Phi_{\mathrm{tr}}, W) \Big)\,\psi\,\mathrm{d}x \;=\; 0 \quad \forall\,\psi \in L^2(\Omega)\,, \ \text{ for a.a. } t \in (\,0\,,\,T\,)\,; \tag{2.3}$$

$$\Phi_{\mathrm{tr}}(x, 0) \;=\; \Phi_0(x) \quad \text{and} \quad W(x, 0) \;=\; W_0(x) \quad \text{for almost all } x \in \Omega. \tag{2.4}$$

Throughout the paper, the following assumptions about the data will be made:

Assumptions 2.1 (Basic assumptions on the data)**.**

1) $\Omega \subset \mathbb{R}^3$ is a bounded Lipschitz domain.
2) M_i, M_e : $\mathrm{cl}\,(\Omega) \to \mathbb{R}^{3\times 3}$ are symmetric, positive definite matrix functions with $L^\infty(\Omega)$-coefficients, obeying uniform ellipticity conditions:

$$0 \leqslant \mu_1 \,\|\,\xi\,\|^2 \leqslant \xi^{\mathrm{T}} M_i(x)\,\xi \leqslant \mu_2\,\|\,\xi\,\|^2 \ \text{ and } \ 0 \leqslant \mu_1\,\|\,\xi\,\|^2 \leqslant \xi^{\mathrm{T}} M_e(x)\,\xi \leqslant \mu_2\,\|\,\xi\,\|^2 \quad \forall\,\xi \in \mathbb{R}^3 \ \ \forall\,x \in \Omega \tag{2.5}$$

with μ_1, $\mu_2 > 0$.

The notions of strong and weak solutions are as follows:

Definition 2.2.

1) (Strong solution of the bidomain system)[6] A triple $(\Phi_{\mathrm{tr}}, \Phi_e, W)$ is called a strong solution of the bidomain system (2.1)–(2.4) on $[\,0\,,\,T\,]$ iff the functions Φ_{tr}, Φ_e and W satisfy (2.1)–(2.4) and belong to the spaces

$$\Phi_{\mathrm{tr}} \in L^2\big[\,(\,0\,,\,T\,)\,,\ W^{2,2}(\Omega)\,\big] \,\cap\, W^{1,2}\big[\,(\,0\,,\,T\,)\,,\ L^2(\Omega)\,\big]\,; \tag{2.6}$$

[6]Slightly modified from [4], p. 469, Definition 18.

$$\Phi_e \in L^2\big[\,(\,0\,,\,T\,)\,,\; W^{2,2}(\Omega)\,\big]\,; \tag{2.7}$$
$$W \in W^{1,2}\big[\,(\,0\,,\,T\,)\,,\; L^2(\Omega)\,\big] \tag{2.8}$$

where $\int_\Omega \Phi_e(x,t)\,\mathrm{d}x \;=\; 0$ holds for almost all $t \in (\,0\,,\,T\,)$.

2) (Weak solution of the bidomain system)[7] A triple $(\Phi_{\rm tr}, \Phi_e, W)$ is called a weak solution of the bidomain system (2.1)–(2.4) on $[\,0\,,\,T\,]$ iff the functions $\Phi_{\rm tr}$, Φ_e and W satisfy (2.1)–(2.4) and belong to the spaces

$$\Phi_{\rm tr} \in C^0\big[\,[\,0\,,\,T\,]\,,\, L^2(\Omega)\,\big] \,\cap\, L^2\big[\,(\,0\,,\,T\,)\,,\; W^{1,2}(\Omega)\,\big] \,\cap\, L^4(\Omega_T)\,; \tag{2.9}$$
$$\Phi_e \in L^2\big[\,(\,0\,,\,T\,)\,,\; W^{1,2}(\Omega)\,\big]\,; \tag{2.10}$$
$$W \in C^0\big[\,[\,0\,,\,T\,]\,,\, L^2(\Omega)\,\big] \tag{2.11}$$

where $\int_\Omega \Phi_e(x,t)\,\mathrm{d}x \;=\; 0$ holds for almost all $t \in (\,0\,,\,T\,)$.

2.2. Two-variable models for the ionic current

For the ionic current $I_{\rm ion}$ and the function G within the gating equation, the following three models will be considered:

a) The Rogers–McCulloch model[8].

$$I_{\rm ion}(\varphi, w) \;=\; b\cdot\varphi\,(\varphi-a)\,(\varphi-1)+\varphi\cdot w \;=\; b\,\varphi^3-(a+1)\,b\,\varphi^2+a\,b\,\varphi+\varphi\,w\,; \tag{2.12}$$
$$G(\varphi, w) \;=\; \varepsilon\,w-\varepsilon\,\kappa\,\varphi \tag{2.13}$$

with $0 < a < 1$, $b > 0$, $\kappa > 0$ and $\varepsilon > 0$. Consequently, the gating variable obeys the linear ODE

$$\partial W/\partial t+\varepsilon\,W \;=\; \varepsilon\,\kappa\,\Phi_{\rm tr}. \tag{2.14}$$

b) The FitzHugh–Nagumo model[9].

$$I_{\rm ion}(\varphi, w) \;=\; \varphi\,(\varphi-a)\,(\varphi-1)+w \;=\; \varphi^3-(a+1)\,\varphi^2+a\,\varphi+w\,; \tag{2.15}$$
$$G(\varphi, w) \;=\; \varepsilon\,w-\varepsilon\,\kappa\,\varphi \tag{2.16}$$

with $0 < a < 1$, $\kappa > 0$ and $\varepsilon > 0$. Consequently, the gating variable obeys the same linear ODE (2.14) as before.

c) The linearized Aliev–Panfilov model[10].

$$I_{\rm ion}(\varphi, w) \;=\; b\cdot\varphi\,(\varphi-a)\,(\varphi-1)+\varphi\cdot w \;=\; b\,\varphi^3-(a+1)\,b\,\varphi^2+a\,b\,\varphi+\varphi\,w\,; \tag{2.17}$$
$$G(\varphi, w) \;=\; \varepsilon\,w-\varepsilon\,\kappa\,\big(\,(a+1)\,\varphi-\varphi^2\,\big) \tag{2.18}$$

with $0 < a < 1$, $b > 0$, $\kappa > 0$ and $\varepsilon > 0$. The linear ODE for the gating variable is

$$\partial W/\partial t+\varepsilon\,W \;=\; \varepsilon\,\kappa\,\big(\,(a+1)\,\Phi_{\rm tr}-{\Phi_{\rm tr}}^2\,\big). \tag{2.19}$$

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[7] [4], p. 472, Definition 26.
[8] Introduced in [18].
[9] See [8] together with [17].
[10] The model, which appears to be a linearization of the original model derived in [2], is taken from [4], p. 480.

2.3. Existence and uniqueness of weak solutions; the stability estimate

In [12], the following results about weak solutions of the bidomain system (2.1)–(2.4) have been obtained:

Theorem 2.3 (Existence and uniqueness of weak solutions).[11] *Assume that the data within* (2.1)–(2.4) *obey Assumptions 2.1., and specify the Rogers–McCulloch or the FitzHugh–Nagumo model. Then the bidomain system* (2.1)–(2.4) *admits for arbitrary initial values* $\Phi_0 \in L^2(\Omega)$, $W_0 \in L^4(\Omega)$ *and inhomogeneities* I_i, $I_e \in L^\infty\big[\,(0\,,T\,)\,,\,\big(\,W^{1,2}(\Omega)\,\big)^*\,\big]$, *which satisfy the compatibility condition*

$$\int_\Omega \Big(\,I_i(x,t) + I_e(x,t)\,\Big)\,\mathrm{d}x \,=\, 0 \quad \textit{for almost all } t \in (\,0\,,\,T), \tag{2.20}$$

a uniquely determined weak solution $(\Phi_{\mathrm{tr}}, \Phi_e, W)$ *on* $[\,0\,,T\,]$ *according to Definition 2.2, 2). If the linearized Aliev–Panfilov model is specified, this assertion remains true provided that* W_0 *belongs to* $W^{1,3/2}(\Omega)$ *instead of* $L^4(\Omega)$.

In fact, a closer regularity analysis reveals that, under the assumptions of Theorem 2.3., the components (Φ_{tr}, W) of a given weak solution of the bidomain system belong to $\big(\,L^2\big[\,(\,0\,,T\,)\,,\,L^6(\Omega)\,\big] \,\cap\, L^q\big[\,(\,0\,,T\,),\,L^r(\Omega)\,\big]\,\big) \times C^0\big[\,[\,0\,,T\,]\,,\,L^4(\Omega)\,\big]$ in the case of the Rogers–McCulloch or the FitzHugh–Nagumo model and to $\big(\,L^2\big[\,(\,0\,,T\,)\,,\,L^6(\Omega)\,\big] \,\cap\, L^q\big[\,(\,0\,,T\,)\,,\,L^r(\Omega)\,\big]\,\big) \times C^0\big[\,[\,0\,,T\,]\,,\,L^{8/3}(\Omega)\,\big]$ in the case of the linearized Aliev–Panfilov model where $1 < q < \infty$ and $4 \leqslant r < 6$.

Theorem 2.4 (Stability estimate for weak solutions).[12] *Assume that the data within* (2.1)–(2.4) *obey Assumptions 2.1., and specify the Rogers–McCulloch or the FitzHugh–Nagumo model. Consider two weak solutions* $({\Phi_{\mathrm{tr}}}', {\Phi_e}', W')$, $({\Phi_{\mathrm{tr}}}'', {\Phi_e}'', W'')$ *of* (2.1)–(2.4), *which correspond to initial values* $\Phi_0' = \Phi_0'' = \Phi_0 \in L^2(\Omega)$, $W_0' = W_0'' = W_0 \in L^4(\Omega)$ *and inhomogeneities* ${I_i}'$, ${I_e}'$, ${I_i}''$ *and* ${I_e}'' \in L^\infty\big[\,(\,0\,,T\,)\,,\,\big(\,W^{1,2}(\Omega)\,\big)^*\,\big]$ *with*

$$\int_\Omega \Big(\,{I_i}'(x,t) + {I_e}'(x,t)\,\Big)\,\mathrm{d}x \,=\, \int_\Omega \Big(\,{I_i}''(x,t) + {I_e}''(x,t)\,\Big)\,\mathrm{d}x \,=\, 0 \quad \textit{for almost all } t \in (\,0\,,T\,)\,, \tag{2.21}$$

whose norms are bounded by $R > 0$. *Then the following estimate holds:*

$$\begin{aligned}
&\big\|\,{\Phi_{\mathrm{tr}}}' - {\Phi_{\mathrm{tr}}}''\,\big\|^2_{L^2\left[\,(\,0\,,T\,)\,,\,W^{1,2}(\Omega)\,\right]} + \big\|\,{\Phi_{\mathrm{tr}}}' - {\Phi_{\mathrm{tr}}}''\,\big\|^2_{C^0\left[\,[\,0\,,T\,]\,,\,L^2(\Omega)\,\right]} \\
&\quad + \big\|\,{\Phi_{\mathrm{tr}}}' - {\Phi_{\mathrm{tr}}}''\,\big\|_{W^{1,4/3}\left[\,(\,0\,,T\,)\,,\,\left(\,W^{1,2}(\Omega)\,\right)^*\,\right]} + \big\|\,{\Phi_e}' - {\Phi_e}''\,\big\|^2_{L^2\left[\,(\,0\,,T\,)\,,\,W^{1,2}(\Omega)\,\right]} \\
&\qquad + \|\,W' - W''\,\|^2_{L^2\left[\,(\,0\,,T\,)\,,\,L^2(\Omega)\,\right]} + \|\,W' - W''\,\|^2_{C^0\left[\,[\,0\,,T\,]\,,\,L^2(\Omega)\,\right]} + \|\,W' - W''\,\|^2_{W^{1,2}\left[\,(\,0\,,T\,)\,,\,L^2(\Omega)\,\right]} \\
&\qquad\qquad \leqslant C\,\Big(\,\big\|\,{I_i}' - {I_i}''\,\big\|^2_{L^\infty\left[\,(\,0\,,T\,)\,,\,\left(\,W^{1,2}(\Omega)\,\right)^*\,\right]} + \big\|\,{I_e}' - {I_e}''\,\big\|^2_{L^\infty\left[\,(\,0\,,T\,)\,,\,\left(\,W^{1,2}(\Omega)\,\right)^*\,\right]}\,\Big).
\end{aligned} \tag{2.22}$$

The constant $C > 0$ *does not depend on* ${I_i}'$, ${I_e}'$, ${I_i}''$ *and* ${I_e}''$ *but possibly on* Ω, R, Φ_0 *and* W_0. *If the linearized Aliev–Panfilov model is specified then the assertion remains true provided that* $W_0' = W_0'' = W_0$ *belong to* $W^{1,3/2}(\Omega)$ *instead of* $L^4(\Omega)$.

The assumptions in Theorems 2.3.–2.4. are in accordance to the analytical framework wherein the control problem (P) will be studied in the next sections.

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[11] [4], p. 473, Theorem 30, together with [12], p. 8, Theorem 2.8, slightly modified. An error within the proof of this and the next theorem will be fixed in a subsequent publication.

[12] [12], p. 7 f., Theorem 2.7, slightly modified.

3. The optimal control problem

3.1. Formulation of the problem within function spaces

In order to provide a precise statement of the optimal control problem (1.7)–(1.8) within an appropriate function space framework, we introduce the following spaces:

$$\mathrm{X}_1 = L^2\big[(0,T),\, W^{1,2}(\Omega)\big]; \quad \mathrm{X}_2 = \mathrm{X}_1 \cap \Big\{ Z \;\Big|\; \int_\Omega Z(x,t)\,\mathrm{d}x = 0 \;\; (\forall)\, t \in (0,T) \Big\}; \tag{3.1}$$

$$\mathrm{X}_3 = L^2\big[(0,T),\, L^2(\Omega)\big]; \quad \mathrm{X}_4 = L^\infty\big[(0,T),\, L^2(\Omega)\big]. \tag{3.2}$$

We will further specify the subspaces

$$\widetilde{\mathrm{X}}_1 = \mathrm{X}_1 \cap W^{1,4/3}\big[(0,T),\, \big(W^{1,2}(\Omega)\big)^*\big] \cap C^0\big[[0,T],\, L^2(\Omega)\big]; \quad \widetilde{\mathrm{X}}_2 = \mathrm{X}_2; \tag{3.3}$$

$$\widetilde{\mathrm{X}}_3 = \mathrm{X}_3 \cap W^{1,2}\big[(0,T),\, \big(L^2(\Omega)\big)^*\big] \cap C^0\big[[0,T],\, L^2(\Omega)\big], \tag{3.4}$$

which contain all polynomials and, consequently, lie dense in X_1, X_2 and X_3, as well as the target spaces

$$\mathrm{Z}_1 = L^{4/3}\big[(0,T),\, \big(W^{1,2}(\Omega)\big)^*\big]; \quad \mathrm{Z}_2 = L^2\big[(0,T),\, \big(W^{1,2}(\Omega)\big)^*\big]; \tag{3.5}$$

$$\mathrm{Z}_3 = L^2\big[(0,T),\, \big(L^2(\Omega)\big)^*\big]; \quad \mathrm{Z}_4 = \mathrm{Z}_5 = L^2(\Omega). \tag{3.6}$$

The quadruples $(\Phi_{\mathrm{tr}}, \Phi_e, W, I_e)$ of state and control variables will be chosen from the space $\widetilde{\mathrm{X}}_1 \times \widetilde{\mathrm{X}}_2 \times \widetilde{\mathrm{X}}_3 \times \mathrm{X}_4$. Recall the definition of $Q:\; L^2(\Omega_T) \to L^2(\Omega_T)$ as

$$Q\, I(x,t) = I(x,t) - \mathbb{1}_{\Omega_{\mathrm{con}}}(x) \cdot \frac{1}{|\,\Omega_{\mathrm{con}}\,|} \int_{\Omega_{\mathrm{con}}} I(\tilde{x},t)\,\mathrm{d}\tilde{x}. \tag{3.7}$$

With the aid of the operators

$$F:\; \mathrm{X}_1 \times \mathrm{X}_2 \times \mathrm{X}_3 \times \mathrm{X}_4 \to \mathbb{R}; \tag{3.8}$$

$$E_1:\; \widetilde{\mathrm{X}}_1 \times \widetilde{\mathrm{X}}_2 \times \widetilde{\mathrm{X}}_3 \to \mathrm{Z}_1; \quad E_2:\; \widetilde{\mathrm{X}}_1 \times \widetilde{\mathrm{X}}_2 \times \mathrm{X}_4 \to \mathrm{Z}_2; \quad E_3:\; \widetilde{\mathrm{X}}_1 \times \widetilde{\mathrm{X}}_3 \to \mathrm{Z}_3; \tag{3.9}$$

$$E_4:\; \widetilde{\mathrm{X}}_1 \to \mathrm{Z}_4; \quad E_5:\; \widetilde{\mathrm{X}}_3 \to \mathrm{Z}_5, \tag{3.10}$$

the problem (P) will be restated now in the following way:

$$(\mathrm{P}) \quad F(\Phi_{\mathrm{tr}}, \Phi_e, W, I_e) = \int_0^T \int_\Omega r\big(x,t,\Phi_{\mathrm{tr}}(x,t), \Phi_e(x,t), W(x,t)\big)\,\mathrm{d}x\,\mathrm{d}t + \frac{\mu}{2} \cdot \int_0^T \int_\Omega I_e(x,t)^2\,\mathrm{d}x\,\mathrm{d}t \longrightarrow \inf!; \tag{3.11}$$

$$E_1(\Phi_{\mathrm{tr}}, \Phi_e, W) = \mathfrak{o} \iff \int_\Omega \Big(\frac{\partial \Phi_{\mathrm{tr}}}{\partial t} + I_{\mathrm{ion}}(\Phi_{\mathrm{tr}}, W)\Big)\psi\,\mathrm{d}x + \int_\Omega \nabla\psi^{\mathrm{T}} M_i (\nabla\Phi_{\mathrm{tr}} + \nabla\Phi_e)\,\mathrm{d}x = 0 \quad \forall\,\psi \in W^{1,2}(\Omega) \;\; (\forall)\, t \in (0,T); \tag{3.12}$$

$$E_2(\Phi_{\mathrm{tr}}, \Phi_e, I_e) = \mathfrak{o} \iff \int_\Omega \Big(\nabla\psi^{\mathrm{T}} M_i \nabla\Phi_{\mathrm{tr}} + \nabla\psi^{\mathrm{T}} (M_i + M_e) \nabla\Phi_e\Big)\,\mathrm{d}x - \int_\Omega I_e\,\psi\,\mathrm{d}x = 0 \quad \forall\,\psi \in W^{1,2}(\Omega) \text{ with } \int_\Omega \psi(x)\,\mathrm{d}x = 0 \;\; (\forall)\, t \in (0,T); \tag{3.13}$$

$$E_3(\Phi_{\mathrm{tr}}, W) = \mathfrak{o} \iff \int_\Omega \Big(\frac{\partial W(t)}{\partial t} + G(\Phi_{\mathrm{tr}}(t), W(t))\Big)\psi\,\mathrm{d}x = 0 \quad \forall\,\psi \in L^2(\Omega) \;\; (\forall)\, t \in (0,T); \tag{3.14}$$

$$E_4(\Phi_{\rm tr}) = \mathfrak{o} \iff \Phi_{\rm tr}(x,0) - \Phi_0(x) = 0 \quad (\forall)\, x \in \Omega\,; \tag{3.15}$$

$$E_5(W) = \mathfrak{o} \iff W(x,0) - W_0(x) = 0 \quad (\forall)\, x \in \Omega\,; \tag{3.16}$$

$$I_e \in \mathcal{C} = \Big\{ Q\, I \;\Big|\; I \in L^\infty\big[\,(\,0\,,\,T\,)\,,\, L^2(\Omega)\big]\,,\ \operatorname{supp}(I) \subseteq \Omega_{\rm con} \times [\,0\,,\,T\,]\,, \\ |\, I(x,t)\,| \leqslant R \;\; (\forall)\,(x,t) \in \Omega_T \Big\} \subset L^\infty\big[\,(\,0\,,\,T\,)\,,\, L^2(\Omega)\big]. \tag{3.17}$$

Assumptions 2.1 are imposed on the data of problem (P). The numbers $T > 0$, $\mu > 0$ and $R > 0$ as well as the Lipschitz subdomain $\Omega_{\rm con} \subseteq \Omega$ are fixed. The functions $I_{\rm ion}$ and G will be specified according to any of the models from Section 2.2. In the case of the Rogers–McCulloch or the FitzHugh–Nagumo model, we fix initial values $\Phi_0 \in L^2(\Omega)$ and $W_0 \in L^4(\Omega)$ while in the case of the linearized Aliev–Panfilov model, $\Phi_0 \in L^2(\Omega)$ and $W_0 \in W^{1,3/2}(\Omega)$ will be used. Concerning the objective functional F, we assume the integrand

$$r(x,t,\varphi,\eta,w):\ \Omega \times [\,0\,,\,T\,] \times \mathbb{R}^3 \to \mathbb{R} \tag{3.18}$$

to be measurable with respect to x and t and continuous with respect to φ, η and w. With regard to (3.7) and (3.17), in the second term of F the original integration domain $\Omega_{\rm con}$ from (1.7) can be replaced by Ω.

3.2. Structure of the feasible domain

Proposition 3.1. *For the problem* (3.11)–(3.17)*, the control-to-state-mapping* $\mathcal{C} \ni I_e \longmapsto (\Phi_{\rm tr}, \Phi_e, W) \in {\rm X}_1 \times {\rm X}_2 \times {\rm X}_3$ *is well-defined.*

Proof.
Recall that $\int_\Omega I_e(x,t)\,{\rm d}x = 0$ for almost all $t \in (\,0,\,T)$. Consequently, the data within the problem (3.11)–(3.17) satisfy the assumptions of Theorem 2.3. with $I_i = \mathfrak{o}$, and the existence of a uniquely determined weak solution $(\Phi_{\rm tr}, \Phi_e, W)$ of the bidomain system is guaranteed for any feasible control $I_e \in \mathcal{C} \subset L^\infty\big[\,(\,0\,,\,T\,)\,,\, L^2(\Omega)\big]$. $\square$

Proposition 3.2. *The control domain* $\mathcal{C} \subset L^\infty(\Omega_T)$ *forms a closed, convex, weak*-sequentially compact subset of the space* ${\rm X}_4$*.*

Proof.
Obviously, $\mathcal{C}$ is a convex subset of ${\rm X}_4$. In order to confirm closedness, consider a norm-convergent sequence $\{\, Q\, I^N \,\}$ with members in $\mathcal{C} \cap {\rm X}_4$ and limit element $\hat{I}$. Since the sequence $\{\, I^N \,\}$ of the generating functions is uniformly bounded in $L^\infty\big[\,(\,0\,,\,T\,)\,,\, L^2(\Omega_{\rm con})\big]$, it admits a weak*-convergent subsequence $I^{N'}$ with a limit element $\tilde{I}$ still satisfying the conditions $\operatorname{supp}(\tilde{I}) \subseteq \Omega_{\rm con} \times [\,0\,,\,T\,]$ and $|\,\tilde{I}(x,t)\,| \leqslant R\ (\forall)\,(x,t) \in \Omega_T$. The weak*-continuity of the operator Q implies then $Q\, I^{N'} \xrightarrow{\;*\;}{}^{{\rm X}_4}\, Q\,\tilde{I}$ and $\hat{I} = Q\,\tilde{I} \in \mathcal{C}$. Now the weak*-sequential compactness of $\mathcal{C}$ is obtained from [19], (p. 301), Theorem VI.6.6. (together with p. 152), Theorem IV.4.11. Finally, $\|\, I \,\|_{L^\infty(\Omega_T)} \leqslant R$ implies $\|\, Q\, I \,\|_{L^\infty(\Omega_T)} \leqslant 2\,R$, and $\mathcal{C}$ belongs even to $L^\infty(\Omega_T)$. $\square$

Proposition 3.3. *The feasible domain* $\mathcal{B}$ *of the problem* (3.11)–(3.17) *is nonempty and closed with respect to the following topology in* ${\rm X}_1 \times {\rm X}_2 \times {\rm X}_3 \times {\rm X}_4$*: weak convergence with respect to the first three components, and weak*-convergence with respect to the fourth component.*

Proof.
The existence of feasible solutions follows *via* Theorem 2.3 from Proposition 3.1. Consider now a sequence of feasible solutions $\{\, ({\Phi_{\rm tr}}^N, {\Phi_e}^N, W^N, {I_e}^N) \,\}$ with ${\Phi_{\rm tr}}^N \rightharpoonup^{{\rm X}_1} \hat{\Phi}_{\rm tr}$, ${\Phi_e}^N \rightharpoonup^{{\rm X}_2} \hat{\Phi}_e$, $W^N \rightharpoonup^{{\rm X}_3} \hat{W}$ and ${I_e}^N \xrightarrow{\;*\;}{}^{{\rm X}_4} \hat{I}_e$. From Proposition 3.2, we already know that $\hat{I}_e$ belongs to $\mathcal{C}$. Further, from [12], page 7, Theorem 2.6, we obtain uniform bounds with respect to N for the norms of ${\Phi_{\rm tr}}^N$, ${\Phi_e}^N$, W^N, $\partial{\Phi_{\rm tr}}^N/\partial t$ and $\partial W^N/\partial t$, implying weak convergence of $\partial{\Phi_{\rm tr}}^{N'}/\partial t$, $\nabla{\Phi_{\rm tr}}^{N'}$ and $\partial W^{N'}/\partial t$ as well as a.e. pointwise convergence of ${\Phi_{\rm tr}}^{N'}$ on Ω_T along a suitable subsequence. Consequently, passing to the limit $N' \to \infty$ in (2.1)–(2.4), we may confirm that $(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W})$ solves the bidomain system with right-hand sides $I_i = \mathfrak{o}$ and $\hat{I}_e$. $\square$

3.3. Existence of global minimizers

Theorem 3.4 (Existence of global minimizers in (P))**.** *We impose the assumptions from Section 3.1. on the data of the problem* (3.11)–(3.17)*. Assume further that the integrand* $r(x,t,\varphi,\eta,w): \ \Omega \times [\,0\,,T\,] \times \mathbb{R}^3 \to \mathbb{R}$ *is bounded from below and convex with respect to* φ*,* η *and* w*. Then the problem* (3.11)–(3.17) *admits a global minimizer.*

Proof. Since r is bounded from below, the problem (3.11)–(3.17) admits a minimizing sequence $\{\,({\Phi_{\rm tr}}^N, {\Phi_e}^N, W^N, {I_e}^N)\,\}$ of feasible solutions. Due to the uniform boundedness of $\|\, {I_e}^N \,\|_{X_4}$ with respect to N, the norms $\|\, {\Phi_{\rm tr}}^N \,\|_{X_1}$, $\|\, {\Phi_e}^N \,\|_{X_2}$ and $\|\, W^N \,\|_{X_3}$ are uniformly bounded as well (*cf.* again [12], p. 7, Thm. 2.6), and we may pass to a subsequence $\{\,({\Phi_{\rm tr}}^{N'}, {\Phi_e}^{N'}, W^{N'}, {I_e}^{N'})\,\}$, which converges to a feasible quadruple $(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)$ in the sense of Proposition 3.3. The lower semicontinuity of the objective follows as in [6] (p. 96), Theorem 3.23, and page 97, Remark 3.25(ii). Consequently, denoting the minimal value of (P) by m, we get

$$\begin{aligned} m \,=\, \lim{}_{N'\to\infty} F({\Phi_{\rm tr}}^{N'}, {\Phi_e}^{N'}, W^{N'}, {I_e}^{N'}) \qquad (3.19) \\ \geqslant \liminf{}_{N'\to\infty} F({\Phi_{\rm tr}}^{N'}, {\Phi_e}^{N}p, W^{N'}, {I_e}^{N'}) \,\geqslant\, F(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e) \,\geqslant\, m\,, \end{aligned}$$

and the quadruple $(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)$ is a global minimizer of (P). □

4. The adjoint equations

4.1. Derivation of the adjoint system

Throughout the following sections, we will further assume that the integrand $r(x,t,\varphi,\eta,w)$ within the objective (3.11) is continuously differentiable with respect to the variables φ, η and w. For the optimal control problem (P), let us introduce now the formal Lagrange function

$$\begin{aligned} \mathcal{L}(\Phi_{\rm tr}, \Phi_e, W, I_e, P_1, P_2, P_3, P_4, P_5) \,=\, F(\Phi_{\rm tr}, \Phi_e, W, I_e) + \langle\, P_1\,,\, E_1(\Phi_{\rm tr}, \Phi_e, W)\,\rangle \qquad (4.1) \\ + \langle\, P_2\,,\, E_2(\Phi_{\rm tr}, \Phi_e, I_e)\,\rangle + \langle\, P_3\,,\, E_3(\Phi_{\rm tr}, W)\,\rangle + \langle\, P_4\,,\, E_4(\Phi_{\rm tr})\,\rangle + \langle\, P_5\,,\, E_5(W)\,\rangle \end{aligned}$$

with multipliers

$$P_1 \,\in\, L^4\big[\,(\,0\,,T\,)\,,\ W^{1,2}(\Omega)\,\big]\,; \qquad (4.2)$$

$$P_2 \,\in\, L^2\big[\,(\,0\,,T\,)\,,\ W^{1,2}(\Omega)\,\big] \,\cap\, \Big\{\, Z \;\Big|\; \int_\Omega Z(x,t)\,{\rm d}x \,=\, 0\ \ (\forall)\, t \in (\,0\,,T\,)\,\Big\}\,; \qquad (4.3)$$

$$P_3 \,\in\, L^2\big[\,(\,0\,,T\,)\,,\, L^2(\Omega)\,\big]\,; \quad P_4,\, P_5 \,\in\, \big(\,L^2(\Omega)\,\big)^*. \qquad (4.4)$$

Differentiating $\mathcal{L}$ at the point $(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)$ in a formal way with respect to the variables $\Phi_{\rm tr}$, Φ_e and W, we find the adjoint equations

$$\begin{aligned} D_{\Phi_{\rm tr}} F\,(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e) + \langle\, P_1\,,\, D_{\Phi_{\rm tr}}\, E_1(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W})\,\rangle \qquad (4.5) \\ + \langle\, P_2\,,\, D_{\Phi_{\rm tr}}\, E_2(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{I}_e)\,\rangle + \langle\, P_3\,,\, D_{\Phi_{\rm tr}}\, E_3(\hat{\Phi}_{\rm tr}, \hat{W})\,\rangle + \langle\, P_4\,,\, D_{\Phi_{\rm tr}}\, E_4(\hat{\Phi}_{\rm tr})\,\rangle \,=\, 0\,; \end{aligned}$$

$$D_{\Phi_e} F\,(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e) + \langle\, P_1\,,\, D_{\Phi_e}\, E_1(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W})\,\rangle + \langle\, P_2\,,\, D_{\Phi_e}\, E_2(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{I}_e)\,\rangle \,=\, 0\,; \qquad (4.6)$$

$$D_W\, F(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e) + \langle\, P_1\,,\, D_W\, E_1(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W})\,\rangle + \langle\, P_3\,,\, D_W\, E_3(\hat{\Phi}_{\rm tr}, \hat{W})\,\rangle + \langle\, P_5\,,\, D_W\, E_5(\hat{W})\,\rangle \,=\, 0. \qquad (4.7)$$

After choosing $P_4 = -P_1(\,\cdot\,,0)$ and $P_5 = -P_3(\,\cdot\,,0)$ (this choice is possible by Theorem 4.2. below), the adjoint system takes the following form:

$$\int_0^T \int_\Omega \left(-\frac{\partial P_1}{\partial t} + \frac{\partial I_{\mathrm{ion}}}{\partial \varphi}(\hat{\Phi}_{\mathrm{tr}}, \hat{W})\, P_1 + \frac{\partial G}{\partial \varphi}(\hat{\Phi}_{\mathrm{tr}}, \hat{W})\, P_3 \right) \psi \,\mathrm{d}x\,\mathrm{d}t + \int_0^T \int_\Omega \nabla\psi^{\mathrm{T}} M_i \,(\, \nabla P_1 + \nabla P_2 \,)\,\mathrm{d}x\,\mathrm{d}t \tag{4.8}$$
$$= -\int_0^T \int_\Omega \left(\frac{\partial r}{\partial \varphi}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \right) \psi \,\mathrm{d}x\,\mathrm{d}t \quad \forall\, \psi \in L^2\big[\,(\,0\,,T\,)\,,\; W^{1,2}(\Omega)\,\big]\,,\; P_1(x,T) \equiv 0\,;$$

$$\int_0^T \int_\Omega \nabla\psi^{\mathrm{T}} M_i \nabla P_1 \,\mathrm{d}x\,\mathrm{d}t + \int_0^T \int_\Omega \nabla\psi^{\mathrm{T}} (M_i + M_e) \nabla P_2 \,\mathrm{d}x\,\mathrm{d}t = -\int_0^T \int_\Omega \frac{\partial r}{\partial \eta}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W})\, \psi \,\mathrm{d}x\,\mathrm{d}t \tag{4.9}$$
$$\forall\, \psi \in L^2\big[\,(\,0\,,T\,)\,,\; W^{1,2}(\Omega)\,\big] \text{ with } \int_\Omega \psi(x,t)\,\mathrm{d}x = 0 \quad (\forall)\, t \in (\,0\,,T\,)\,,\; \int_\Omega P_2(x,t)\,\mathrm{d}x = 0 \quad (\forall)\, t \in (\,0\,,T\,)\,;$$

$$\int_0^T \int_\Omega \left(-\frac{\partial P_3}{\partial t} + \frac{\partial I_{\mathrm{ion}}}{\partial w}(\hat{\Phi}_{\mathrm{tr}}, \hat{W})\, P_1 + \frac{\partial G}{\partial w}(\hat{\Phi}_{\mathrm{tr}}, \hat{W})\, P_3 \right) \psi \,\mathrm{d}x\,\mathrm{d}t = -\int_0^T \int_\Omega \left(\frac{\partial r}{\partial w}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \right) \psi \,\mathrm{d}x\,\mathrm{d}t \tag{4.10}$$
$$\forall\, \psi \in L^2\big[\,(\,0\,,T\,)\,,\, L^2(\Omega)\,\big]\,,\; P_3(x,T) \equiv 0.$$

4.2. The reduced form of the adjoint system

First, we apply to the system (4.8)–(4.10) the transformation $s = T - t$, thus defining $\widetilde{P}_i(x,s) = P_i(x, T-s)$, $1 \leqslant i \leqslant 3$, $\widetilde{\Phi_{\mathrm{tr}}}(x,s) = \hat{\Phi}_{\mathrm{tr}}(x, T-s)$, $\widetilde{\Phi_e}(x,s) = \hat{\Phi}_e(x,T-s)$, $\widetilde{W}(x,s) = \hat{W}(x,T-s)$ and $\widetilde{I}_e(x,s) = \hat{I}_e(x,T-s)$ etc. By abuse of notation, we suppress all tildes, thus simply replacing t by s and $-\partial P_1/\partial t$, $-\partial P_3/\partial t$ by $\partial P_1/\partial s$ and $\partial P_3/\partial s$, respectively. Then the adjoint system, in analogy to the primal bidomain equations, can be rewritten in terms of the bidomain bilinear form as a reduced system:

$$\frac{\mathrm{d}}{\mathrm{d}s} \langle\, P_1(s)\,,\, \psi \,\rangle + A\,(\, P_1(s)\,,\, \psi\,) + \int_\Omega \left(\frac{\partial I_{\mathrm{ion}}}{\partial \varphi}(\hat{\Phi}_{\mathrm{tr}}, \hat{W})\, P_1 + \frac{\partial G}{\partial \varphi}(\hat{\Phi}_{\mathrm{tr}}, \hat{W})\, P_3 \right) \psi \,\mathrm{d}x = \langle\, \widetilde{S}(s)\,,\, \psi \,\rangle \tag{4.11}$$
$$\forall\, \psi \in\, W^{1,2}(\Omega)\,;$$

$$\frac{\mathrm{d}}{\mathrm{d}s} \langle\, P_3(s)\,,\, \psi \,\rangle + \int_\Omega \left(\frac{\partial I_{\mathrm{ion}}}{\partial w}(\hat{\Phi}_{\mathrm{tr}}, \hat{W})\, P_1 + \frac{\partial G}{\partial w}(\hat{\Phi}_{\mathrm{tr}}, \hat{W})\, P_3 \right) \psi \,\mathrm{d}x = -\langle\, \frac{\partial r}{\partial w}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W})\,,\, \psi \,\rangle \tag{4.12}$$
$$\forall\, \psi \in L^2(\Omega)\,;$$

$$P_1(x,0) = 0 \quad (\forall)\, x \in \Omega\,; \quad P_3(x,0) = 0 \quad (\forall)\, x \in \Omega \tag{4.13}$$

on $[\,0\,,T\,]$ in distributional sense (*cf.* [12], p. 5f.), Theorem 2.4. Here the bidomain bilinear form $A : \; W^{1,2}(\Omega) \times W^{1,2}(\Omega) \to \mathbb{R}$ is defined as *ibid.*, page 5, (2.22), through

$$A(\psi_1\,,\, \psi_2) = \int_\Omega \nabla\psi_1^{\mathrm{T}} M_i \nabla\psi_2 \,\mathrm{d}x + \int_\Omega \nabla\widetilde{\psi}_e^{\mathrm{T}} M_i \nabla\psi_2 \,\mathrm{d}x \tag{4.14}$$

where $\widetilde{\psi}_e \in W^{1,2}(\Omega)$ is the uniquely determined solution of the variational equation

$$\int_\Omega \nabla\widetilde{\psi}_e^{\mathrm{T}} (M_i + M_e) \nabla\psi \,\mathrm{d}x = -\int_\Omega \nabla\psi_1^{\mathrm{T}} M_i \nabla\psi \,\mathrm{d}x \quad \forall\, \psi \in\, W^{1,2}(\Omega) \text{ with } \int_\Omega \psi \,\mathrm{d}x = 0 \tag{4.15}$$
$$\text{satisfying } \int_\Omega \widetilde{\psi}_e \,\mathrm{d}x = 0\,,$$

and the linear functionals $\widetilde{S}(s) \in \big(\, W^{1,2}(\Omega)\,\big)^*$ are defined through

$$\Big\langle\, \widetilde{S}(s)\,,\, \psi \,\Big\rangle = -\Big\langle\, \frac{\partial r}{\partial \varphi}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W})\,,\, \psi \,\Big\rangle - \int_\Omega \nabla\overline{\psi}_e^{\mathrm{T}} M_i \nabla\psi \,\mathrm{d}x \tag{4.16}$$

where $\overline{\psi}_e \in W^{1,2}(\Omega)$ is the uniquely determined solution of the variational equation

$$\int_\Omega \nabla\overline{\psi}_e^{\mathrm{T}}(M_i + M_e)\,\nabla\psi\,\mathrm{d}x \,=\, \left\langle \frac{\partial r}{\partial\eta}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W})\,,\,\psi \right\rangle \quad \forall\,\psi \in W^{1,2}(\Omega) \;\text{ with }\; \int_\Omega \psi\,\mathrm{d}x = 0 \qquad (4.17)$$

$$\text{satisfying } \int_\Omega \overline{\psi}_e\,\mathrm{d}x = 0.$$

The component P_2 of the solution of (4.8)–(4.10) is uniquely determined as the sum $P_2 = \widetilde{\psi}_e + \overline{\psi}_e$. Note that this reformulation is even possible without imposing the additional compatibility condition

$$\int_\Omega \frac{\partial r}{\partial\eta}\big(\,\hat{\Phi}_{\mathrm{tr}}(x,s), \hat{\Phi}_e(x,s), \hat{W}(x,s)\,\big)\,\mathrm{d}x \,=\, 0 \quad (\forall)\,s \in (\,0\,,\,T\,). \qquad (4.18)$$

4.3. Existence and regularity of weak solutions

Theorem 4.1 (*A priori* estimates for weak solutions of the adjoint system)**.** *The optimal control problem* (3.11)–(3.17) *is studied under the assumptions from Section 3.1. Within the problem, we specify the Rogers–McCulloch model. Assume further that the integrand $r(x,t,\varphi,\eta,w)$ is continuously differentiable with respect to φ, η and w.*

1) If $(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)$ is a feasible solution of (P) *with*

$$\frac{\partial r}{\partial\varphi}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W})\,,\; \frac{\partial r}{\partial\eta}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W})\,,\; \frac{\partial r}{\partial w}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \in L^2(\Omega_T) \qquad (4.19)$$

then every weak solution $(P_1, P_2, P_3) \in L^2\big[\,(\,0\,,\,T\,)\,,\,W^{1,2}(\Omega)\,\big] \times L^2\big[\,(\,0\,,\,T\,)\,,\,W^{1,2}(\Omega)\,\big] \times L^2(\Omega_T)$ of the adjoint system (4.8)–(4.10) *obeys the estimate*

$$\begin{aligned} &\|\,P_1\,\|^2_{L^\infty[\,(0,T),\,L^2(\Omega)\,]} + \|\,P_1\,\|^2_{L^2[\,(0,T),\,W^{1,2}(\Omega)\,]} + \|\,P_2\,\|^2_{L^2[\,(0,T),\,W^{1,2}(\Omega)\,]} + \|\,P_3\,\|^2_{L^\infty[\,(0,T),\,L^2(\Omega)\,]} \\ &\quad\leqslant C\,\left(\left\| \frac{\partial r}{\partial\varphi}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \right\|^2_{L^2(\Omega_T)} + \left\| \frac{\partial r}{\partial\eta}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \right\|^2_{L^2(\Omega_T)} + \left\| \frac{\partial r}{\partial w}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \right\|^2_{L^2(\Omega_T)} \right) \end{aligned} \qquad (4.20)$$

where the constant $C > 0$ does not depend on P_1, P_2, P_3 but on $(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)$ and the data of (P)*.*

2) Let $q = 10/9$. If $(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)$ is a feasible solution of (P) *with*

$$\frac{\partial r}{\partial\varphi}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W})\,,\; \frac{\partial r}{\partial\eta}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W})\,,\; \frac{\partial r}{\partial w}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \in L^{2q}\big[\,(\,0\,,\,T\,)\,,\,L^2(\Omega)\,\big] \qquad (4.21)$$

then every weak solution $(P_1, P_2, P_3) \in L^2\big[\,(\,0\,,\,T\,)\,,\,W^{1,2}(\Omega)\,\big] \times L^2\big[\,(\,0\,,\,T\,)\,,\,W^{1,2}(\Omega)\,\big] \times L^2(\Omega_T)$ of the adjoint system (4.8)–(4.10) obeys (4.20) *as well as the further estimate*

$$\begin{aligned} &\|\,P_1\,\|^2_{C^0[\,[0,T],\,L^2(\Omega)\,]} + \|\,\partial P_1/\partial s\,\|^q_{L^q[\,(0,T),\,(W^{1,2}(\Omega))^*\,]} + \|\,P_3\,\|^2_{C^0[\,[0,T],\,L^2(\Omega)\,]} \\ &\quad + \|\,\partial P_3/\partial s\,\|^q_{L^q[\,(0,T),\,L^2(\Omega)\,]} \leqslant \left(1 + \left\| \frac{\partial r}{\partial\varphi}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \right\|^{2q}_{L^{2q}[\,(0,T),\,L^2(\Omega)\,]} \right. \\ &\qquad \left. + \left\| \frac{\partial r}{\partial\eta}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \right\|^{2q}_{L^{2q}[\,(0,T),\,L^2(\Omega)\,]} + \left\| \frac{\partial r}{\partial w}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \right\|^2_{L^2(\Omega_T)} \right) \end{aligned} \qquad (4.22)$$

where the constant $C > 0$ does not depend on P_1, P_2, P_3 but on $(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)$ and the data of (P)*.*

The *a priori* estimates yield the following existence and uniqueness theorem for the adjoint system:

Theorem 4.2 (Existence and uniqueness of weak solutions for the adjoint system)**.**
Under the assumptions of Theorem 4.1, 2), the adjoint system (4.8)–(4.10) *admits a uniquely determined weak solution* (P_1, P_2, P_3) *with*

$$P_1 \in C^0\big[\,[\,0\,,T\,]\,,\,L^2(\Omega)\,\big] \cap L^2\big[\,(\,0\,,T\,)\,,\,W^{1,2}(\Omega)\,\big] \cap W^{1,q}\big[\,(\,0\,,T\,)\,,\,\big(\,W^{1,2}(\Omega)\,\big)^*\,\big]; \tag{4.23}$$

$$P_2 \in L^2\big[\,(\,0\,,T\,)\,,\,W^{1,2}(\Omega)\,\big]; \quad \int_\Omega P_2(x,t)\,\mathrm{d}x = 0 \ \ (\forall)\,t \in (\,0\,,T\,); \tag{4.24}$$

$$P_3 \in C^0\big[\,[\,0\,,T\,]\,,\,L^2(\Omega)\,\big] \cap W^{1,q}\big[\,(\,0\,,T\,)\,,\,L^2(\Omega)\,\big]. \tag{4.25}$$

Note that, even under the assumptions of Theorems 4.1, 2) and 4.2, the regularity of $P_1 \in L^4\big[\,(\,0\,,T\,)\,,\,W^{1,2}(\Omega)\,\big]$ as required in (4.1) and (4.2) cannot be guaranteed.

4.4. Proofs

Proof of Theorem 4.1. Throughout the proof, C denotes a generical positive constant, which may appropriately change from line to line. Further, we will specify in (3.12)–(3.14) the Rogers–McCulloch model. The necessary alterations in the case of the other models will be discussed at the end of the subsection.

- **Step 1.** *An estimate for the right-hand side of* (4.11). We start with

Lemma 4.3. *Under the assumptions of Theorem 4.1., for arbitrary* $\varepsilon_0' > 0$ *the following estimate holds:*

$$\Big|\Big\langle\,\widetilde{S}(s),\,\psi\,\Big\rangle\Big| \leqslant \frac{C}{\varepsilon_0'}\left(\Big\|\,\frac{\partial r}{\partial\varphi}(\hat{\Phi}_{\mathrm{tr}},\hat{\Phi}_e,\hat{W})\,\Big\|^2_{L^2(\Omega)} + \Big\|\,\frac{\partial r}{\partial\eta}(\hat{\Phi}_{\mathrm{tr}},\hat{\Phi}_e,\hat{W})\,\Big\|^2_{L^2(\Omega)}\right) + C\,\varepsilon_0'\,\|\,\psi\,\|^2_{W^{1,2}(\Omega)}. \tag{4.26}$$

The constant $C > 0$ *does not depend on* ε_0' *and* ψ*.*

Proof. Inserting $\overline{\psi}_e \in W^{1,2}(\Omega)$ as a feasible test function into (4.17), we get from the uniform ellipticity of M_i and M_e and the Poincaré inequality:

$$\begin{aligned} C\,\|\,\overline{\psi}_e\,\|^2_{W^{1,2}(\Omega)} &\leqslant \int_\Omega \nabla\overline{\psi}_e^{\mathrm{T}}(M_i+M_e)\,\nabla\overline{\psi}_e^{\mathrm{T}}\,\mathrm{d}x \leqslant \big|\,\langle\,\frac{\partial r}{\partial\eta}(\hat{\Phi}_{\mathrm{tr}},\hat{\Phi}_e,\hat{W}),\,\overline{\psi}_e^{\mathrm{T}}\,\rangle\big| \\ &\leqslant \frac{1}{2\,\delta_1}\Big\|\,\frac{\partial r}{\partial\eta}(\hat{\Phi}_{\mathrm{tr}},\hat{\Phi}_e,\hat{W})\,\Big\|^2_{(\,W^{1,2}(\Omega)\,)^*} + \frac{\delta_1}{2}\,\|\,\overline{\psi}_e\,\|^2_{W^{1,2}(\Omega)} \quad (\forall)\,s \in (\,0,\,T\,), \end{aligned} \tag{4.27}$$

for arbitrary $\delta_1 > 0$. Inserting $\delta_1 = C$, we arrive at

$$\frac{C}{2}\,\|\,\overline{\psi}_e\,\|^2_{W^{1,2}(\Omega)} \leqslant \frac{1}{2\,C}\Big\|\,\frac{\partial r}{\partial\eta}(\hat{\Phi}_{\mathrm{tr}},\hat{\Phi}_e,\hat{W})\,\Big\|^2_{(\,W^{1,2}(\Omega)\,)^*} \leqslant \frac{1}{2\,C}\Big\|\,\frac{\partial r}{\partial\eta}(\hat{\Phi}_{\mathrm{tr}},\hat{\Phi}_e,\hat{W})\,\Big\|^2_{L^2(\Omega)}. \tag{4.28}$$

From (4.16), we obtain

$$\Big|\Big\langle\,\widetilde{S}(s)\,,\,\psi\,\Big\rangle\Big| \leqslant \Big|\Big\langle\,\frac{\partial r}{\partial\varphi}(\hat{\Phi}_{\mathrm{tr}},\hat{\Phi}_e,\hat{W})\,,\,\psi\,\Big\rangle\Big| + \big|\,\langle\,\nabla\overline{\psi}_e^{\mathrm{T}}M_i\,,\,\nabla\psi\,\rangle\,\big| \tag{4.29}$$

$$\leqslant \frac{1}{2\,\delta_2}\Big\|\,\frac{\partial r}{\partial\varphi}(\hat{\Phi}_{\mathrm{tr}},\hat{\Phi}_e,\hat{W})\,\Big\|^2_{(\,W^{1,2}(\Omega)\,)^*} + \frac{\delta_2}{2}\,\|\,\psi\,\|^2_{W^{1,2}(\Omega)} + \frac{1}{2\,\delta_3}\,\|\,\overline{\psi}_e\,\|^2_{L^2(\Omega)} + \frac{\delta_3}{2}\,\|\,M_i\,\|^2\cdot\|\,\psi\,\|^2_{L^2(\Omega)} \tag{4.30}$$

$$\leqslant \frac{1}{2\,\delta_2}\Big\|\,\frac{\partial r}{\partial\varphi}(\hat{\Phi}_{\mathrm{tr}},\hat{\Phi}_e,\hat{W})\,\Big\|^2_{L^2(\Omega)} + \frac{1}{2\,\delta_3}\,\|\,\overline{\psi}_e\,\|^2_{W^{1,2}(\Omega)} + \left(\frac{\delta_2}{2} + \frac{(\mu_2)^2\,\delta_3}{2}\right)\|\,\psi\,\|^2_{W^{1,2}(\Omega)} \tag{4.31}$$

$$\leqslant \frac{C}{\delta_2}\Big\|\,\frac{\partial r}{\partial\varphi}(\hat{\Phi}_{\mathrm{tr}},\hat{\Phi}_e,\hat{W})\,\Big\|^2_{L^2(\Omega)} + \frac{C}{\delta_3}\Big\|\,\frac{\partial r}{\partial\eta}(\hat{\Phi}_{\mathrm{tr}},\hat{\Phi}_e,\hat{W})\,\Big\|^2_{L^2(\Omega)} + C\left(\frac{\delta_2}{2} + \frac{(\mu_2)^2\delta_3}{2}\right)\|\,\psi\,\|^2_{W^{1,2}(\Omega)} \tag{4.32}$$

by (2.5) and (4.28). Taking $\delta_3 = \delta_2/(\mu_2)^2$, we get (4.26). □

• **Step 2.** *The estimates for* $\| P_1 \|_{L^\infty\left[\,[0,T\,],\,L^2(\Omega)\right]}$ *and* $\| P_3 \|_{L^\infty\left[\,[0,T\,],\,L^2(\Omega)\right]}$. Specifying the derivatives of $I_{\rm ion}$ and G according to the Rogers–McCulloch model, we have

$$\frac{\partial I_{\rm ion}}{\partial \varphi}(\hat{\Phi}_{\rm tr}, \hat{W}) \;=\; 3\,b\,(\hat{\Phi}_{\rm tr})^2 - 2\,(a+1)\,b\,\hat{\Phi}_{\rm tr} + ab + \hat{W}\,; \quad \frac{\partial G}{\partial \varphi}(\hat{\Phi}_{\rm tr}, \hat{W}) \;\equiv\; -\varepsilon\,\kappa\,; \tag{4.33}$$

$$\frac{\partial I_{\rm ion}}{\partial w}(\hat{\Phi}_{\rm tr}, \hat{W}) \;=\; \hat{\Phi}_{\rm tr}\,; \quad \frac{\partial G}{\partial w}(\hat{\Phi}_{\rm tr}, \hat{W}) \;\equiv\; \varepsilon. \tag{4.34}$$

Inserting $P_1(s)$ as a feasible test function into (4.11), we get for arbitrary ε_0', $\varepsilon_1(s) > 0$ with [12], page 6, Theorem 2.4, 2), and Lemma 4.3 above[13]

$$\frac{1}{2}\,\frac{\mathrm{d}}{\mathrm{d}s}\,\|\,P_1(s)\,\|^2_{L^2(\Omega)} + \Big(\,A(P_1,P_1) + \beta\,\|\,P_1\,\|^2_{L^2(\Omega)}\Big) + \int_\Omega \frac{\partial I_{\rm ion}}{\partial \varphi}(\hat{\Phi}_{\rm tr}, \hat{W})\,P_1(s)^2\,\mathrm{d}x \tag{4.35}$$
$$\leqslant \int_\Omega \Big|\,\frac{\partial G}{\partial \varphi}(\hat{\Phi}_{\rm tr}, \hat{W})\Big|\,|\,P_1\,P_3\,| + |\,\langle\,\widetilde{S}(s),\,P_1\,\rangle\,| + \beta\,\|\,P_1\,\|^2_{L^2(\Omega)} \quad \Longrightarrow$$

$$\frac{1}{2}\,\frac{\mathrm{d}}{\mathrm{d}s}\,\|\,P_1(s)\,\|^2_{L^2(\Omega)} + \beta\,\|\,P_1\,\|^2_{W^{1,2}(\Omega)} + \int_\Omega \big(\,ab + 3\,b\,(\hat{\Phi}_{\rm tr})^2\,\big)\,P_1(s)^2\,\mathrm{d}x \tag{4.36}$$
$$\leqslant C\int_\Omega \Big(\,|\,\hat{\Phi}_{\rm tr}\,| + |\,\hat{W}\,|\,\Big)\,|\,P_1\,|^2\,\mathrm{d}x + \varepsilon\,\kappa\int_\Omega |\,P_1\,P_3\,|\,\mathrm{d}x$$
$$+\;\frac{C}{\varepsilon_0'}\,\left(\Big\|\,\frac{\partial r}{\partial \varphi}(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W})\Big\|^2_{L^2(\Omega)} + \Big\|\,\frac{\partial r}{\partial \eta}(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W})\Big\|^2_{L^2(\Omega)}\right) + C\,\varepsilon_0'\,\|\,P_1\,\|^2_{W^{1,2}(\Omega)} + \beta\,\|\,P_1\,\|^2_{L^2(\Omega)} \quad \Longrightarrow$$

$$\frac{1}{2}\,\frac{\mathrm{d}}{\mathrm{d}s}\,\|\,P_1(s)\,\|^2_{L^2(\Omega)} + \beta\,\|\,P_1\,\|^2_{W^{1,2}(\Omega)} \tag{4.37}$$
$$\leqslant C\,\varepsilon_1(s)\int_\Omega \Big(\,|\,\hat{\Phi}_{\rm tr}\,|^2 + |\,\hat{W}\,|^2\,\Big)\,|\,P_1\,|^2\,\mathrm{d}x + \frac{C}{\varepsilon_1(s)}\,\|\,P_1\,\|^2_{L^2(\Omega)} + C\,\Big(\,\|\,P_1\,\|^2_{L^2(\Omega)} + \|\,P_3\,\|^2_{L^2(\Omega)}\Big)$$
$$+\;\frac{C}{\varepsilon_0'}\,\left(\Big\|\,\frac{\partial r}{\partial \varphi}(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W})\Big\|^2_{L^2(\Omega)} + \Big\|\,\frac{\partial r}{\partial \eta}(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W})\Big\|^2_{L^2(\Omega)}\right) + C\,\varepsilon_0'\,\|\,P_1\,\|^2_{W^{1,2}(\Omega)} + \beta\,\|\,P_1\,\|^2_{L^2(\Omega)}$$

$$\leqslant C\,\varepsilon_1(s)\,\left(\Big\|\,\hat{\Phi}_{\rm tr}\,\Big\|^2_{L^4(\Omega)} + \Big\|\,\hat{W}\,\Big\|^2_{L^4(\Omega)}\right)\cdot\|\,P_1\,\|^2_{W^{1,2}(\Omega)} + C\,\left(1 + \frac{1}{\varepsilon_1(s)}\right)\,\|\,P_1\,\|^2_{L^2(\Omega)} \tag{4.38}$$
$$+\;\frac{C}{\varepsilon_0'}\,\left(\Big\|\,\frac{\partial r}{\partial \varphi}(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W})\Big\|^2_{L^2(\Omega)} + \Big\|\,\frac{\partial r}{\partial \eta}(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W})\Big\|^2_{L^2(\Omega)}\right) + C\,\varepsilon_0'\,\|\,P_1\,\|^2_{W^{1,2}(\Omega)} + C\,\|\,P_3\,\|^2_{L^2(\Omega)}.$$

We choose $\varepsilon_1(s) = \varepsilon_1'/\,\big(\,1 + \Big\|\,\hat{\Phi}_{\rm tr}(s)\,\Big\|^2_{L^4(\Omega)} + \Big\|\,\hat{W}(s)\,\Big\|^2_{L^4(\Omega)}\big)$ with $\varepsilon_1' > 0$ and continue (4.38) with

$$\ldots \leqslant C\,\varepsilon_1'\,\cdot\|\,P_1\,\|^2_{W^{1,2}(\Omega)} + C\,\left(1 + \frac{1}{\varepsilon_1'}\,\left(1 + \Big\|\,\hat{\Phi}_{\rm tr}(s)\,\Big\|^2_{L^4(\Omega)} + \Big\|\,\hat{W}(s)\,\Big\|^2_{L^4(\Omega)}\right)\right)\cdot\|\,P_1\,\|^2_{L^2(\Omega)} \tag{4.39}$$
$$+\;\frac{C}{\varepsilon_0'}\,\left(\Big\|\,\frac{\partial r}{\partial \varphi}(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W})\Big\|^2_{L^2(\Omega)} + \Big\|\,\frac{\partial r}{\partial \eta}(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W})\Big\|^2_{L^2(\Omega)}\right) + C\,\varepsilon_0'\,\|\,P_1\,\|^2_{W^{1,2}(\Omega)} + C\,\|\,P_3\,\|^2_{L^2(\Omega)}.$$

Further, inserting $P_3(s)$ as a feasible test function into (4.12), we find with $\varepsilon_2(s) > 0$

$$\frac{1}{2}\,\frac{\mathrm{d}}{\mathrm{d}s}\,\|\,P_3(s)\,\|^2_{L^2(\Omega)}$$
$$\leqslant \int_\Omega \Big|\,\frac{\partial I_{\rm ion}}{\partial w}(\hat{\Phi}_{\rm tr}, \hat{W})\Big|\,|\,P_1\,P_3\,|\,\mathrm{d}x + \int_\Omega \Big|\,\frac{\partial G}{\partial w}(\hat{\Phi}_{\rm tr}, \hat{W})\Big|\;|\,P_3\,|^2\,\mathrm{d}x + \int_\Omega \Big|\,\frac{\partial r}{\partial w}(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W})\Big|\;|P_3\,|\,\mathrm{d}x \tag{4.40}$$

[13]Note that $\varepsilon > 0$ is fixed from the Rogers–McCulloch model.

$$\leqslant \int_\Omega \big|\, \hat{\varPhi}_{\rm tr}\, P_1\, P_3 \,\big|\, {\rm d}x + \varepsilon \, \|\, P_3 \,\|^2_{L^2(\Omega)} + C \left\| \frac{\partial r}{\partial w}(\hat{\varPhi}_{\rm tr}, \hat{\varPhi}_e, \hat{W}) \right\|^2_{L^2(\Omega)} + C \, \|\, P_3 \,\|^2_{L^2(\Omega)} \tag{4.41}$$

$$\leqslant C\,\varepsilon_2(s) \int_\Omega \big|\, \hat{\varPhi}_{\rm tr}\, P_1 \,\big|^2 \, {\rm d}x + C\left(1 + \frac{1}{\varepsilon_2(s)}\right) \|\, P_3 \,\|^2_{L^2(\Omega)} + C \left\| \frac{\partial r}{\partial w}(\hat{\varPhi}_{\rm tr}, \hat{\varPhi}_e, \hat{W}) \right\|^2_{L^2(\Omega)} \tag{4.42}$$

$$\leqslant C\,\varepsilon_2(s) \left\| \hat{\varPhi}_{\rm tr} \right\|^2_{L^4(\Omega)} \cdot \|\, P_1 \,\|^2_{W^{1,2}(\Omega)} + C\left(1 + \frac{1}{\varepsilon_2(s)}\right) \|\, P_3 \,\|^2_{L^2(\Omega)} + C \left\| \frac{\partial r}{\partial w}(\hat{\varPhi}_{\rm tr}, \hat{\varPhi}_e, \hat{W}) \right\|^2_{L^2(\Omega)}. \tag{4.43}$$

Choosing now $\varepsilon_2(s) = \varepsilon_2' / \big(1 + \big\| \hat{\varPhi}_{\rm tr}(s) \big\|^2_{L^4(\Omega)}\big)$ with $\varepsilon_2' > 0$, (4.43) may be continued as

$$\ldots \leqslant C\,\varepsilon_2' \,\|\, P_1 \,\|^2_{W^{1,2}(\Omega)} + C\left(1 + \frac{1}{\varepsilon_2'}\left(1 + \left\| \hat{\varPhi}_{\rm tr}(s) \right\|^2_{L^4(\Omega)}\right)\right) \|\, P_3 \,\|^2_{L^2(\Omega)} + C \left\| \frac{\partial r}{\partial w}(\hat{\varPhi}_{\rm tr}, \hat{\varPhi}_e, \hat{W}) \right\|^2_{L^2(\Omega)}. \tag{4.44}$$

Combining (4.39) and (4.44), we obtain

$$\begin{aligned} &\frac{\rm d}{{\rm d}s}\left(\|\, P_1(s) \,\|^2_{L^2(\Omega)} + \|\, P_3(s) \,\|^2_{L^2(\Omega)} \right) + 2\,\beta \,\|\, P_1 \,\|^2_{W^{1,2}(\Omega)} \qquad (4.45)\\ &\quad \leqslant C\,(\,\varepsilon_0' + \varepsilon_1' + \varepsilon_2'\,) \,\|\, P_1 \,\|^2_{W^{1,2}(\Omega)} + C\left(1 + \frac{1}{\varepsilon_1'}\left(1 + \left\| \hat{\varPhi}_{\rm tr}(s) \right\|^2_{L^4(\Omega)} + \left\| \hat{W}(s) \right\|^2_{L^4(\Omega)}\right)\right) \|\, P_1 \,\|^2_{L^2(\Omega)}\\ &\qquad + C\left(1 + \frac{1}{\varepsilon_2'}\left(1 + \left\| \hat{\varPhi}_{\rm tr}(s) \right\|^2_{L^4(\Omega)}\right)\right) \|\, P_3 \,\|^2_{L^2(\Omega)}\\ &\qquad + \frac{C}{\varepsilon_0'}\left(\left\| \frac{\partial r}{\partial \varphi}(\hat{\varPhi}_{\rm tr}, \hat{\varPhi}_e, \hat{W}) \right\|^2_{L^2(\Omega)} + \left\| \frac{\partial r}{\partial \eta}(\hat{\varPhi}_{\rm tr}, \hat{\varPhi}_e, \hat{W}) \right\|^2_{L^2(\Omega)} \right) + C \left\| \frac{\partial r}{\partial w}(\hat{\varPhi}_{\rm tr}, \hat{\varPhi}_e, \hat{W}) \right\|^2_{L^2(\Omega)}. \end{aligned}$$

Now we fix the parameters ε_0', ε_1', $\varepsilon_2' > 0$ in such a way that the terms with $\|\, P_1 \,\|_{W^{1,2}(\Omega)}$ on both sides of (4.45) will be annihilated, thus arriving at

$$\frac{\rm d}{{\rm d}s}\left(\|\, P_1(s) \,\|^2_{L^2(\Omega)} + \|\, P_3(s) \,\|^2_{L^2(\Omega)} \right) \leqslant A(s)\left(\|\, P_1(s) \,\|^2_{L^2(\Omega)} + \|\, P_3(s) \,\|^2_{L^2(\Omega)} \right) + B(s) \quad \text{where} \tag{4.46}$$

$$A(s) \;=\; C\left(1 + \left\| \hat{\varPhi}_{\rm tr}(s) \right\|^2_{L^4(\Omega)} + \left\| \hat{W}(s) \right\|^2_{L^4(\Omega)}\right); \tag{4.47}$$

$$B(s) \;=\; C\Big(\left\| \frac{\partial r}{\partial \varphi}(\hat{\varPhi}_{\rm tr}, \hat{\varPhi}_e, \hat{W}) \right\|^2_{L^2(\Omega)} + \left\| \frac{\partial r}{\partial \eta}(\hat{\varPhi}_{\rm tr}, \hat{\varPhi}_e, \hat{W}) \right\|^2_{L^2(\Omega)} + \left\| \frac{\partial r}{\partial w}(\hat{\varPhi}_{\rm tr}, \hat{\varPhi}_e, \hat{W}) \right\|^2_{L^2(\Omega)} \Big). \tag{4.48}$$

Then Gronwall's inequality yields for all $s \in [\,0,\, T\,]$:

$$\|\, P_1(s) \,\|^2_{L^2(\Omega)} + \|\, P_3(s) \,\|^2_{L^2(\Omega)} \leqslant {\rm e}^{\int_0^s A(\sigma)\,{\rm d}\sigma} \left(\|\, P_1(0) \,\|^2_{L^2(\Omega)} + \|\, P_3(0) \,\|^2_{L^2(\Omega)} + \int_0^s B(\sigma)\,{\rm d}\sigma \right) \tag{4.49}$$

$$\leqslant {\rm e}^{CT} \left(\left\| \frac{\partial r}{\partial \varphi}(\hat{\varPhi}_{\rm tr}, \hat{\varPhi}_e, \hat{W}) \right\|^2_{L^2(\Omega_T)} + \left\| \frac{\partial r}{\partial \eta}(\hat{\varPhi}_{\rm tr}, \hat{\varPhi}_e, \hat{W}) \right\|^2_{L^2(\Omega_T)} + \left\| \frac{\partial r}{\partial w}(\hat{\varPhi}_{\rm tr}, \hat{\varPhi}_e, \hat{W}) \right\|^2_{L^2(\Omega_T)} \right) \tag{4.50}$$

since $\hat{\varPhi}_{\rm tr} \in L^4(\Omega_T)$ and $\hat{W} \in C^0\big[\,[\,0,\, T\,],\, L^4(\Omega)\,\big]$. Consequently, we get the estimate

$$\begin{aligned} \|\, P_1 \,\|^2_{L^\infty[\,(\,0,\,T\,)\,,\,L^2(\Omega)\,]} + \|\, P_3 \,\|^2_{L^\infty[\,(\,0,\,T\,)\,,\,L^2(\Omega)\,]} \leqslant C\Bigg(&\left\| \frac{\partial r}{\partial \varphi}(\hat{\varPhi}_{\rm tr}, \hat{\varPhi}_e, \hat{W}) \right\|^2_{L^2(\Omega_T)} \qquad (4.51)\\ &+ \left\| \frac{\partial r}{\partial \eta}(\hat{\varPhi}_{\rm tr}, \hat{\varPhi}_e, \hat{W}) \right\|^2_{L^2(\Omega_T)} + \left\| \frac{\partial r}{\partial w}(\hat{\varPhi}_{\rm tr}, \hat{\varPhi}_e, \hat{W}) \right\|^2_{L^2(\Omega_T)} \Bigg). \end{aligned}$$

• **Step 3.** *The estimate for* $\| P_1 \|^2_{L^2[(0,T),\,W^{1,2}(\Omega)]}$. We return to (4.45). Then $\varepsilon_0',\ \varepsilon_1',\ \varepsilon_2' > 0$ may be alternatively chosen in such a way that $C\,(\varepsilon_0' + \varepsilon_1' + \varepsilon_2') = \beta$ and, consequently,

$$\frac{\mathrm{d}}{\mathrm{d}s}\Big(\| P_1(s) \|^2_{L^2(\Omega)} + \| P_3(s) \|^2_{L^2(\Omega)} \Big) + \beta \, \| P_1(s) \|^2_{W^{1,2}(\Omega)} \leqslant A(s) \Big(\| P_1(s) \|^2_{L^2(\Omega)} + \| P_3(s) \|^2_{L^2(\Omega)} \Big) + B(s) \tag{4.52}$$

where $A(s)$ and $B(s)$ are calculated as above. Together with (4.51), we obtain

$$\frac{\mathrm{d}}{\mathrm{d}s}\Big(\| P_1(s) \|^2_{L^2(\Omega)} + \| P_3(s) \|^2_{L^2(\Omega)} \Big) + \beta \, \| P_1(s) \|^2_{W^{1,2}(\Omega)} \tag{4.53}$$
$$\leqslant C\,A(s) \Big(\Big\| \frac{\partial r}{\partial \varphi}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \Big\|^2_{L^2(\Omega_T)} + \Big\| \frac{\partial r}{\partial \eta}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \Big\|^2_{L^2(\Omega_T)} + \Big\| \frac{\partial r}{\partial w}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \Big\|^2_{L^2(\Omega_T)} \Big) + B(s).$$

We integrate (4.53) over $[\,0,\,T\,]$ and get, inserting the initial values $P_1(0) = \mathfrak{o}$, $P_3(0) = \mathfrak{o}$

$$\| P_1(T) \|^2_{L^2(\Omega)} + \| P_3(T) \|^2_{L^2(\Omega)} + \beta \, \| P_1 \|^2_{L^2[(0,T),\,W^{1,2}(\Omega)]} \tag{4.54}$$
$$\leqslant C \Big(\Big\| \frac{\partial r}{\partial \varphi}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \Big\|^2_{L^2(\Omega_T)} + \Big\| \frac{\partial r}{\partial \eta}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \Big\|^2_{L^2(\Omega_T)} + \Big\| \frac{\partial r}{\partial w}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \Big\|^2_{L^2(\Omega_T)} \Big) \quad \Longrightarrow$$

$$\| P_1 \|^2_{L^2[(0,T),\,W^{1,2}(\Omega)]} \tag{4.55}$$
$$\leqslant C \Big(\Big\| \frac{\partial r}{\partial \varphi}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \Big\|^2_{L^2(\Omega_T)} + \Big\| \frac{\partial r}{\partial \eta}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \Big\|^2_{L^2(\Omega_T)} + \Big\| \frac{\partial r}{\partial w}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \Big\|^2_{L^2(\Omega_T)} \Big).$$

• **Step 4.** *The estimate for* $\| \partial P_1/\partial s \|^2_{L^q[(0,T),\,(W^{1,2}(\Omega))^*]}$ *with* $q = 10/9 < 2$. Exploiting the definition of the dual norm, we start with

$$\| \partial P_1/\partial s \|^q_{L^q[(0,T),\,(W^{1,2}(\Omega))^*]} = \int_0^T \sup_{\|\psi\|_{W^{1,2}(\Omega)} = 1} \big| \langle \partial P_1(s)/\partial s\,,\, \psi \rangle \big|^q \,\mathrm{d}s \tag{4.56}$$

$$= \int_0^T \sup_{\cdots} \Big| -A(P_1, \psi) - \int_\Omega \Big(\frac{\partial I_{\mathrm{ion}}}{\partial \varphi}(\hat{\Phi}_{\mathrm{tr}}, \hat{W})\, P_1 + \frac{\partial G}{\partial \varphi}(\hat{\Phi}_{\mathrm{tr}}, \hat{W})\, P_3 \Big) \psi \,\mathrm{d}x + \langle \widetilde{S}(s)\,,\,\psi \rangle \Big|^q \,\mathrm{d}s \tag{4.57}$$

$$\leqslant C \int_0^T \Big(\sup_{\cdots} |\, A(P_1, \psi) \,|^q + \sup_{\cdots} \Big(\int_\Omega \Big(|\,\hat{\Phi}_{\mathrm{tr}}\,|^2 + |\,\hat{\Phi}_{\mathrm{tr}}\,| + |\,\hat{W}\,| + 1 \Big) |\,P_1\,|\,|\,\psi\,| \,\mathrm{d}x \Big)^q \tag{4.58}$$
$$+ \sup_{\cdots} \varepsilon^q \kappa^q \Big(\int_\Omega |\,P_3\,|\,|\,\psi\,| \,\mathrm{d}x \Big)^q + \sup_{\cdots} |\,\langle \widetilde{S}(s)\,,\,\psi \rangle\,|^q \Big) \,\mathrm{d}s.$$

The four terms on the right-hand side of (4.58) will be estimated separately. For the first term, we get with [12], page 6, Theorem 2.4, 2), and (4.55)

$$\int_0^T \sup_{\cdots} |\, A(P_1, \psi) \,|^q \,\mathrm{d}s \leqslant \int_0^T \sup_{\cdots} \gamma^q \, \| P_1(s) \|^q_{W^{1,2}(\Omega)} \, \| \psi \|^q_{W^{1,2}(\Omega)} \,\mathrm{d}s \tag{4.59}$$

$$\leqslant \gamma^q \, \| P_1 \|^q_{L^q[(0,T),\,W^{1,2}(\Omega)]} \leqslant C \, \| P_1 \|^q_{L^2[(0,T),\,W^{1,2}(\Omega)]} \tag{4.60}$$

$$\leqslant C \Big(\Big\| \frac{\partial r}{\partial \varphi}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \Big\|^2_{L^2(\Omega_T)} + \Big\| \frac{\partial r}{\partial \eta}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \Big\|^2_{L^2(\Omega_T)} + \Big\| \frac{\partial r}{\partial w}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \Big\|^2_{L^2(\Omega_T)} \Big)^{q/2}. \tag{4.61}$$

For the second term, we obtain

$$\int_0^T \sup_{\cdots} \Big(\int_\Omega \Big(|\,\hat{\Phi}_{\mathrm{tr}}\,|^2 + |\,\hat{\Phi}_{\mathrm{tr}}\,| + |\,\hat{W}\,| + 1 \Big) |\,P_1\,|\,|\,\psi\,| \,\mathrm{d}x \Big)^q \,\mathrm{d}s \tag{4.62}$$

$$\leqslant C\left(\sup_{\dots}\int_0^T\int_\Omega\left|\hat{\Phi}_{\mathrm{tr}}\right|^{2q}\left|P_1\right|^q\left|\psi\right|^q\,\mathrm{d}x\,\mathrm{d}s+\sup_{\dots}\int_0^T\int_\Omega\left|\hat{\Phi}_{\mathrm{tr}}\right|^{q}\left|P_1\right|^q\left|\psi\right|^q\,\mathrm{d}x\,\mathrm{d}s\right. \tag{4.63}$$
$$\left.+\sup_{\dots}\int_0^T\int_\Omega\left|\hat{W}\right|^{q}\left|P_1\right|^q\left|\psi\right|^q\,\mathrm{d}x\,\mathrm{d}s+\sup_{\dots}\int_0^T\int_\Omega\left|P_1\right|^q\left|\psi\right|^q\,\mathrm{d}x\,\mathrm{d}s\right) = J_1+J_2+J_3+J_4.$$

We start with the estimation of J_1, thus getting

$$J_1 = \sup_{\dots}\int_0^T\int_\Omega\left|\hat{\Phi}_{\mathrm{tr}}\right|^{20/9}\left|P_1\right|^{10/9}\left|\psi\right|^{10/9}\,\mathrm{d}x\,\mathrm{d}s \tag{4.64}$$
$$= \sup_{\dots}\int_0^T\left(\int_\Omega\left|\hat{\Phi}_{\mathrm{tr}}\right|^{40/11}\mathrm{d}x\right)^{33/54}\left(\int_\Omega\left|P_1\right|^{60/11}\mathrm{d}x\right)^{11/54}\left(\int_\Omega\left|\psi\right|^{6}\mathrm{d}x\right)^{10/54}\mathrm{d}s \tag{4.65}$$
$$= \sup_{\dots}\int_0^T\left\|\hat{\Phi}_{\mathrm{tr}}\right\|^{20/9}_{L^{40/11}(\Omega)}\cdot\left\|P_1\right\|^{10/9}_{L^{60/11}(\Omega)}\cdot\left\|\psi\right\|^{10/9}_{L^{6}(\Omega)}\,\mathrm{d}s \tag{4.66}$$
$$\leqslant \sup_{\dots}C\int_0^T\left\|\hat{\Phi}_{\mathrm{tr}}\right\|^{20/9}_{L^{40/11}(\Omega)}\cdot\left\|P_1\right\|^{10/9}_{W^{1,2}(\Omega)}\cdot\left\|\psi\right\|^{10/9}_{W^{1,2}(\Omega)}\,\mathrm{d}s = C\int_0^T\left\|\hat{\Phi}_{\mathrm{tr}}\right\|^{20/9}_{L^{40/11}(\Omega)}\cdot\left\|P_1\right\|^{10/9}_{W^{1,2}(\Omega)}\,\mathrm{d}s \tag{4.67}$$
$$\leqslant C\left(\int_0^T\left\|\hat{\Phi}_{\mathrm{tr}}(s)\right\|^{5}_{L^{40/11}(\Omega)}\mathrm{d}s\right)^{8/18}\left(\int_0^T\left\|P_1(s)\right\|^{2}_{W^{1,2}(\Omega)}\mathrm{d}s\right)^{10/18} \tag{4.68}$$
$$\leqslant C\cdot\left\|\hat{\Phi}_{\mathrm{tr}}\right\|^{20/9}_{L^5\left[(0,T),\,L^{40/11}(\Omega)\right]}\cdot\left\|P_1\right\|^{10/9}_{L^2\left[(0,T),\,W^{1,2}(\Omega)\right]}. \tag{4.69}$$

Since $\hat{\Phi}_{\mathrm{tr}} \in L^{p'}\left[(0,T),\,L^{p''}(\Omega)\right]$ for all $1 < p' < \infty$, $4 \leqslant p'' < 6$, we get a bound analogous to (4.61). Continuing with J_2, we find in completely analogous manner

$$J_2 = \sup_{\dots}\int_0^T\int_\Omega\left|\hat{\Phi}_{\mathrm{tr}}\right|^{10/9}\left|P_1\right|^{10/9}\left|\psi\right|^{10/9}\,\mathrm{d}x\,\mathrm{d}s \tag{4.70}$$
$$\leqslant \sup_{\dots}C\int_0^T\left\|\hat{\Phi}_{\mathrm{tr}}\right\|^{10/9}_{L^{20/11}(\Omega)}\cdot\left\|P_1\right\|^{10/9}_{W^{1,2}(\Omega)}\cdot\left\|\psi\right\|^{10/9}_{W^{1,2}(\Omega)}\,\mathrm{d}s = C\int_0^T\left\|\hat{\Phi}_{\mathrm{tr}}\right\|^{10/9}_{L^{20/11}(\Omega)}\cdot\left\|P_1\right\|^{10/9}_{W^{1,2}(\Omega)}\,\mathrm{d}s \tag{4.71}$$
$$\leqslant C\left(\int_0^T\left\|\hat{\Phi}_{\mathrm{tr}}(s)\right\|^{10/4}_{L^{20/11}(\Omega)}\mathrm{d}s\right)^{8/18}\left(\int_0^T\left\|P_1(s)\right\|^{2}_{W^{1,2}(\Omega)}\mathrm{d}s\right)^{10/18} \tag{4.72}$$
$$\leqslant C\cdot\left\|\hat{\Phi}_{\mathrm{tr}}\right\|^{10/9}_{L^{10/4}\left[(0,T),\,L^{20/11}(\Omega)\right]}\cdot\left\|P_1\right\|^{10/9}_{L^2\left[(0,T),\,W^{1,2}(\Omega)\right]}. \tag{4.73}$$

Noticing that, in the case of the Rogers–McCulloch model, $\hat{W}$ belongs even to $C^0\left[[0,T],\,L^4(\Omega)\right]$, we may estimate J_3 in the same way:

$$J_3 = \sup_{\dots}\int_0^T\int_\Omega\left|\hat{W}\right|^{10/9}\left|P_1\right|^{10/9}\left|\psi\right|^{10/9}\,\mathrm{d}x\,\mathrm{d}s \tag{4.74}$$
$$\leqslant \sup_{\dots}C\int_0^T\left\|\hat{W}\right\|^{10/9}_{L^{20/11}(\Omega)}\cdot\left\|P_1\right\|^{10/9}_{W^{1,2}(\Omega)}\cdot\left\|\psi\right\|^{10/9}_{W^{1,2}(\Omega)}\,\mathrm{d}s = C\int_0^T\left\|\hat{W}\right\|^{10/9}_{L^{20/11}(\Omega)}\cdot\left\|P_1\right\|^{10/9}_{W^{1,2}(\Omega)}\,\mathrm{d}s \tag{4.75}$$
$$\leqslant C\left(\int_0^T\left\|\hat{W}(s)\right\|^{10/4}_{L^{20/11}(\Omega)}\mathrm{d}s\right)^{8/18}\left(\int_0^T\left\|P_1(s)\right\|^{2}_{W^{1,2}(\Omega)}\mathrm{d}s\right)^{10/18} \tag{4.76}$$

$$\leqslant C\cdot\left\|\hat{W}\right\|^{10/9}_{L^{10/4}\left[(0,T),\,L^{20/11}(\Omega)\right]}\cdot\left\|P_1\right\|^{10/9}_{L^2\left[(0,T),\,W^{1,2}(\Omega)\right]} \tag{4.77}$$

$$\leqslant C \cdot \big\| \hat{W} \big\|^{10/9}_{L^\infty\left[(0,T),\,L^4(\Omega)\right]} \cdot \| P_1 \|^{10/9}_{L^2\left[(0,T),\,W^{1,2}(\Omega)\right]}. \tag{4.78}$$

Defining the function $S(x,s) \equiv 1$, the estimation of J_4 yields

$$J_4 = \sup_{\cdots} \int_0^T \int_\Omega |\, S \,|^{10/9} \,|\, P_1 \,|^{10/9} \,|\, \psi \,|^{10/9} \,\mathrm{d}x\,\mathrm{d}s \tag{4.79}$$
$$\leqslant C \cdot \| S \|^{10/9}_{L^{10/4}\left[(0,T),\,L^{20/11}(\Omega)\right]} \cdot \| P_1 \|^{10/9}_{L^2\left[(0,T),\,W^{1,2}(\Omega)\right]}.$$

Summing up, we get from (4.63), (4.69), (4.73), (4.78) and (4.79):

$$\int_0^T \sup_{\cdots} \left(\int_\Omega \Big(|\,\hat{\Phi}_{\mathrm{tr}}\,|^2 + |\,\hat{\Phi}_{\mathrm{tr}}\,| + |\,\hat{W}\,| + 1 \Big) \,|\, P_1 \,|\,|\, \psi \,|\,\mathrm{d}x \right)^q \mathrm{d}s \tag{4.80}$$
$$\leqslant C \left(\Big\| \frac{\partial r}{\partial \varphi}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \Big\|^2_{L^2(\Omega_T)} + \Big\| \frac{\partial r}{\partial \eta}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \Big\|^2_{L^2(\Omega_T)} + \Big\| \frac{\partial r}{\partial w}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \Big\|^2_{L^2(\Omega_T)} \right)^{q/2}.$$

The third term at the right-hand side of (4.58) will be estimated through

$$\int_0^T \sup_{\cdots} \varepsilon^q \kappa^q \left(\int_\Omega |\, P_3 \,|\,|\, \psi \,|\,\mathrm{d}x \right)^q \mathrm{d}s \leqslant \sup_{\cdots} C \int_0^T \int_\Omega |\, P_3 \,|^{10/9} \,|\, \psi \,|^{10/9} \,\mathrm{d}x\,\mathrm{d}s \tag{4.81}$$

$$\leqslant \sup_{\cdots} C \int_0^T \left(\int_\Omega |\, P_3 \,|^2 \,\mathrm{d}x \right)^{10/18} \left(\int_\Omega |\, \psi \,|^{10/4} \,\mathrm{d}x \right)^{8/18} \mathrm{d}s = \sup_{\cdots} C \int_0^T \| P_3 \|^{10/9}_{L^2(\Omega)} \cdot \| \psi \|^{10/9}_{L^{10/4}(\Omega)} \tag{4.82}$$

$$\leqslant \sup_{\cdots} C \int_0^T \| P_3 \|^{10/9}_{L^2(\Omega)} \cdot \| \psi \|^{10/9}_{W^{1,2}(\Omega)} = C \| P_3 \|^q_{L^q\left[(0,T),\,L^2(\Omega)\right]} \leqslant C \| P_3 \|^q_{L^\infty\left[(0,T),\,L^2(\Omega)\right]} \tag{4.83}$$

$$\leqslant C \left(\Big\| \frac{\partial r}{\partial \varphi}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \Big\|^2_{L^2(\Omega_T)} + \Big\| \frac{\partial r}{\partial \eta}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \Big\|^2_{L^2(\Omega_T)} + \Big\| \frac{\partial r}{\partial w}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \Big\|^2_{L^2(\Omega_T)} \right)^{q/2}. \tag{4.84}$$

Finally, Lemma 4.3 implies for the fourth term at the right-hand side of (4.58):

$$\int_0^T \sup_{\cdots} |\,\langle\, \widetilde{S}(s)\,,\, \psi \,\rangle\,|^q \,\mathrm{d}s \leqslant C \left(1 + \int_0^T \left(\Big\| \frac{\partial r}{\partial \varphi}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \Big\|^2_{L^2(\Omega)} + \Big\| \frac{\partial r}{\partial \eta}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \Big\|^2_{L^2(\Omega)} \right)^q \mathrm{d}s \right) \tag{4.85}$$

$$\leqslant C \left(1 + \int_0^T \left(\Big\| \frac{\partial r}{\partial \varphi}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \Big\|^{2q}_{L^2(\Omega)} + \Big\| \frac{\partial r}{\partial \eta}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \Big\|^{2q}_{L^2(\Omega)} \right) \mathrm{d}s \right) \tag{4.86}$$

$$\leqslant C \left(1 + \Big\| \frac{\partial r}{\partial \varphi}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \Big\|^{20/9}_{L^{20/9}\left[(0,T),\,L^2(\Omega)\right]} + \Big\| \frac{\partial r}{\partial \eta}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \Big\|^{20/9}_{L^{20/9}\left[(0,T),\,L^2(\Omega)\right]} \right). \tag{4.87}$$

Together with (4.61), (4.80), (4.84) and (4.87), (4.58) yields the claimed estimate

$$\| \partial P_1 / \partial s \|^q_{L^q\left[(0,T),\,(W^{1,2}(\Omega))^*\right]} \tag{4.88}$$
$$\leqslant C \left(\Big\| \frac{\partial r}{\partial \varphi}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \Big\|^2_{L^2(\Omega_T)} + \Big\| \frac{\partial r}{\partial \eta}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \Big\|^2_{L^2(\Omega_T)} + \Big\| \frac{\partial r}{\partial w}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \Big\|^2_{L^2(\Omega_T)} \right)^{q/2}$$
$$+ C \left(1 + \Big\| \frac{\partial r}{\partial \varphi}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \Big\|^{20/9}_{L^{20/9}\left[(0,T),\,L^2(\Omega)\right]} + \Big\| \frac{\partial r}{\partial \eta}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \Big\|^{20/9}_{L^{20/9}\left[(0,T),\,L^2(\Omega)\right]} \right).$$

• **Step 5.** *The estimate for* $\| \partial P_3/\partial s \|^q_{L^q\left[(0,T),\left(L^2(\Omega)\right)^*\right]}$. We start again by using the dual norm

$$\| \partial P_3/\partial s \|^q_{L^q\left[(0,T),\left(L^2(\Omega)\right)^*\right]} = \int_0^T \sup_{\|\psi\|_{L^2(\Omega)}=1} \big| \langle \partial P_3(s)/\partial s\,,\,\psi \rangle \big|^q \,\mathrm{d}s \tag{4.89}$$

$$= \int_0^T \sup_{\cdots} \Big| \int_\Omega \Big(-\hat{\Phi}_{\mathrm{tr}}\, P_1 - \varepsilon\, P_3 - \frac{\partial r}{\partial w}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \Big)\, \psi \,\mathrm{d}x \Big|^q \,\mathrm{d}s \tag{4.90}$$

$$\leqslant C \int_0^T \sup_{\cdots} \Big(\Big(\int_\Omega |\hat{\Phi}_{\mathrm{tr}}|\,|P_1|\,|\psi|\,\mathrm{d}x \Big)^q + \Big(\varepsilon \int_\Omega |P_3|\,|\psi|\,\mathrm{d}x \Big)^q + \Big(\int_\Omega \Big| \frac{\partial r}{\partial w}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \Big|\,|\psi|\,\mathrm{d}x \Big)^q \Big) \,\mathrm{d}s$$

$$\leqslant C \Big(\sup_{\cdots} \int_0^T \int_\Omega |\hat{\Phi}_{\mathrm{tr}}|^q\,|P_1|^q\,|\psi|^q \,\mathrm{d}x\,\mathrm{d}s + \sup_{\cdots} \int_0^T \Big(\int_\Omega |P_3|\,|\psi|\,\mathrm{d}x \Big)^q \mathrm{d}s \tag{4.91}$$

$$+ \sup_{\cdots} \int_0^T \Big(\int_\Omega \Big| \frac{\partial r}{\partial w}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \Big|\,|\psi|\,\mathrm{d}x \Big)^q \mathrm{d}s \Big) = J_5 + J_6 + J_7.$$

The three terms on the right-hand side of (4.91) will be estimated separately. For the first term, we get

$$J_5 = \sup_{\cdots} C \int_0^T \int_\Omega |\hat{\Phi}_{\mathrm{tr}}|^{10/9}\,|P_1|^{10/9}\,|\psi|^{10/9} \,\mathrm{d}x\,\mathrm{d}s \tag{4.92}$$

$$\leqslant \sup_{\cdots} C \Big(\int_0^T \int_\Omega |\hat{\Phi}_{\mathrm{tr}}|^5 \,\mathrm{d}x\,\mathrm{d}s \Big)^{2/9} \Big(\int_0^T \int_\Omega |P_1|^5 \,\mathrm{d}x\,\mathrm{d}s \Big)^{2/9} \Big(\int_0^T \int_\Omega |\psi|^2 \,\mathrm{d}x\,\mathrm{d}s \Big)^{5/9} \tag{4.93}$$

$$= \sup_{\|\psi(s)\|_{L^2(\Omega)}=1} C \cdot \Big\| \hat{\Phi}_{\mathrm{tr}} \Big\|^{10/9}_{L^5(\Omega_T)} \cdot \| P_1 \|^{10/9}_{L^5(\Omega_T)} \cdot \Big(\int_0^T \| \psi(s) \|^2_{L^2(\Omega)} \,\mathrm{d}x\,\mathrm{d}s \Big)^{5/9} \tag{4.94}$$

$$\leqslant C \cdot \Big\| \hat{\Phi}_{\mathrm{tr}} \Big\|^{10/9}_{L^5(\Omega_T)} \cdot \Big(\| P_1 \|^{10/9}_{L^2\left[(0,T),\,W^{1,2}(\Omega)\right]} + \| \partial P_1/\partial s \|^{10/9}_{L^{10/9}\left[(0,T),\left(W^{1,2}(\Omega)\right)^*\right]} \Big) \cdot T^{5/9} \tag{4.95}$$

by application of the Aubin–Dubinskij lemma to P_1. Since $\hat{\Phi}_{\mathrm{tr}} \in L^5(\Omega_T)$, we may use (4.55) and (4.88) in order to conclude that

$$J_5 \leqslant C \Big(\Big\| \frac{\partial r}{\partial \varphi}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \Big\|^2_{L^2(\Omega_T)} + \Big\| \frac{\partial r}{\partial \eta}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \Big\|^2_{L^2(\Omega_T)} + \Big\| \frac{\partial r}{\partial w}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \Big\|^2_{L^2(\Omega_T)} \Big)^{q/2} \tag{4.96}$$

$$+ C \Big(1 + \Big\| \frac{\partial r}{\partial \varphi}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \Big\|^{20/9}_{L^{20/9}\left[(0,T),\,L^2(\Omega)\right]} + \Big\| \frac{\partial r}{\partial \eta}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \Big\|^{20/9}_{L^{20/9}\left[(0,T),\,L^2(\Omega)\right]} \Big).$$

For the second term, we find

$$J_6 = \sup_{\cdots} C \int_0^T \Big(\int_\Omega |P_3|\,|\psi|\,\mathrm{d}x \Big)^q \mathrm{d}s \leqslant \sup_{\cdots} C \int_0^T \Big(\| P_3(s) \|^2_{L^2(\Omega)} + \| \psi(s) \|^2_{L^2(\Omega)} \Big)^{10/9} \mathrm{d}s \tag{4.97}$$

$$\leqslant C \Big(1 + \| P_3 \|^{20/9}_{L^\infty\left[(0,T),\,L^2(\Omega)\right]} \Big) \tag{4.98}$$

$$\leqslant C \Big(1 + \Big\| \frac{\partial r}{\partial \varphi}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \Big\|^2_{L^2(\Omega_T)} + \Big\| \frac{\partial r}{\partial \eta}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \Big\|^2_{L^2(\Omega_T)} + \Big\| \frac{\partial r}{\partial w}(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}) \Big\|^2_{L^2(\Omega_T)} \Big)^q \tag{4.99}$$

by (4.51). For the third term, we get

$$J_7 = \sup_{\cdots} \int_0^T \Big(\int_\Omega \Big| \frac{\partial r}{\partial w}(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W}) \Big| \, |\, \psi \,|\, {\rm d}x \Big)^q \, {\rm d}s \leqslant \sup_{\cdots} \int_0^T \Big(\Big\| \frac{\partial r}{\partial w}(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W}) \Big\|^2_{L^2(\Omega)} \tag{4.100}$$

$$+ \, \| \, \psi(s) \, \|^2_{L^2(\Omega)} \Big)^q {\rm d}s \leqslant C \, \Big(1 + \Big\| \frac{\partial r}{\partial w}(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W}) \Big\|^{20/9}_{L^{2q}\big[\,(\,0\,,\,T\,)\,,\,L^2(\Omega)\big]} \Big) \, . \tag{4.101}$$

Combining now (4.91) with (4.96), (4.99) and (4.101), we arrive at the claimed estimate

$$\begin{aligned} & \| \, \partial P_3/\partial s \, \|^q_{L^q\big[\,(\,0\,,\,T\,)\,,\,\big(\,L^2(\Omega)\,\big)^*\,\big]} \\ & \leqslant C \Big(\Big\| \frac{\partial r}{\partial \varphi}(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W}) \Big\|^2_{L^2(\Omega_T)} + \Big\| \frac{\partial r}{\partial \eta}(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W}) \Big\|^2_{L^2(\Omega_T)} + \Big\| \frac{\partial r}{\partial w}(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W}) \Big\|^2_{L^2(\Omega_T)} \Big)^{q/2} \\ & \quad + C \Big(1 + \Big\| \frac{\partial r}{\partial \varphi}(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W}) \Big\|^{20/9}_{L^{20/9}\big[\,(\,0\,,\,T\,)\,,\,L^2(\Omega)\big]} + \Big\| \frac{\partial r}{\partial \eta}(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W}) \Big\|^{20/9}_{L^{20/9}\big[\,(\,0\,,\,T\,)\,,\,L^2(\Omega)\big]} \Big). \end{aligned} \tag{4.102}$$

• **Step 6.** *The estimate for* $\| \, P_2 \, \|^2_{L^2\big[\,(\,0\,,\,T\,)\,,\,W^{1,2}(\Omega)\big]}$. Inserting $P_2(s) \in W^{1,2}(\Omega)$ with $\int_\Omega P_2(x,s)\,{\rm d}x = 0$ as a feasible test function into (4.9), the uniform ellipticity of M_i, M_e and the Poincaré inequality imply

$$\| \, P_2(s) \, \|^2_{W^{1,2}(\Omega)} \leqslant C \int_\Omega \nabla P_2^{\rm T} (M_i + M_e) \, \nabla P_2 \, {\rm d}x \tag{4.103}$$

$$\leqslant C \Big| \int_\Omega \nabla P_2^{\rm T} \, M_i \, \nabla P_1 \, {\rm d}x + \int_\Omega \frac{\partial r}{\partial \eta}(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W}) \, P_2 \, {\rm d}x \Big| \tag{4.104}$$

$$\leqslant C \, \Big(\| \, P_1 \, \|_{W^{1,2}(\Omega)} \cdot \| \, P_2 \, \|_{W^{1,2}(\Omega)} + \int_\Omega \Big| \frac{\partial r}{\partial \eta}(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W}) \Big| \, |\, P_2 \,|\, {\rm d}x \Big) \tag{4.105}$$

since, by Assumption 2.1, 2), the entries of M_i are essentially bounded. Consequently, applying the generalized Cauchy inequality twice, we get

$$\begin{aligned} \| \, P_2(s) \, \|^2_{W^{1,2}(\Omega)} \leqslant C \, \Big(& \frac{1}{\varepsilon_3'} \, \| \, P_1 \, \|^2_{W^{1,2}(\Omega)} + \varepsilon_3' \, \| \, P_2 \, \|^2_{W^{1,2}(\Omega)} \\ & + \frac{1}{\varepsilon_4'} \, \Big\| \frac{\partial r}{\partial \eta}(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W}) \Big\|^2_{L^2(\Omega)} + \varepsilon_4' \, \| \, P_2 \, \|^2_{W^{1,2}(\Omega)} \Big) \end{aligned} \tag{4.106}$$

for arbitrary ε_3', $\varepsilon_4' > 0$. Choosing $(\varepsilon_3' + \varepsilon_4') = 1/(2\,C)$, we arrive at

$$\frac{1}{2} \, \| \, P_2(s) \, \|^2_{W^{1,2}(\Omega)} \leqslant C \, \Big(\| \, P_1 \, \|^2_{W^{1,2}(\Omega)} + \Big\| \frac{\partial r}{\partial \eta}(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W}) \Big\|^2_{L^2(\Omega)} \Big) \quad \Longrightarrow \tag{4.107}$$

$$\| \, P_2 \, \|^2_{L^2\big[\,(\,0\,,\,T\,)\,,\,W^{1,2}(\Omega)\big]} \leqslant C \, \Big(\| \, P_1 \, \|^2_{L^2\big[\,(\,0\,,\,T\,)\,,\,W^{1,2}(\Omega)\big]} + \Big\| \frac{\partial r}{\partial \eta}(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W}) \Big\|^2_{L^2(\Omega_T)} \Big) \tag{4.108}$$

where the right-hand side is bounded by (4.55).

• **Step 7.** *Conclusion of the proof.* The fact that P_1 belongs even to $C^0\big[\,[\,0\,,\,T\,]\,,\,L^2(\Omega)\,\big]$ can be confirmed analogously to [4], page 478, Section 5.3. As a consequence of the imbedding theorem [7], page 286, Theorem 2, $P_3 \in C^0\big[\,[\,0\,,\,T\,]\,,\,L^2(\Omega)\,\big]$ holds true as well. Consequently, the norms on the left-hand side of (4.51) can be replaced by $C^0\big[\,[\,0\,,\,T\,]\,,\,L^2(\Omega)\,\big]$-norms, and the proof is complete. □

Proof of Theorem 4.2.

• **Step 1.** *Approximate solutions for the reduced adjoint system.* By [4], page 464, Theorem 6, the bidomain bilinear form $A(\,\cdot\,,\,\cdot\,)$ gives rise to an orthonormal basis of eigenfunctions $\{\,\psi_i\,\}$ within the space $W^{1,2}(\Omega)$, which are related to eigenvalues $0 = \lambda_0 < \lambda_1 \leqslant \lambda_2 \leqslant \ldots$. For $N \in \mathbb{N}_0$, let us define the subspaces

$$\mathrm{X}^N(\Omega) \,=\, \Big\{\, \psi = \sum_{i=0}^{N} c_i\,\psi_i \;\Big|\; c_0\,,\ldots,\,c_N \in \mathbb{R}\,\Big\} \subset W^{1,2}(\Omega)\,, \tag{4.109}$$

and the functions $P_1^N,\, P_3^N:\ \Omega \times [\,0\,,\,T\,] \to \mathrm{X}^N$ according to

$$P_1^N(x,s) \,=\, \sum_{i=0}^{N} p_{i,N}(s)\,\psi_i(x)\,; \quad P_3^N(x,s) \,=\, \sum_{i=0}^{N} q_{i,N}(s)\,\psi_i(x) \tag{4.110}$$

where $p_{i,N},\, q_{i,N}:\ [\,0\,,\,T\,] \to \mathbb{R}$ are solutions of the initial value problem

$$\frac{\mathrm{d}p_{j,N}(s)}{\mathrm{d}s} \,+\, \lambda_j\,p_{j,N}(s) + \sum_{i=0}^{N} p_{i,N}(s)\cdot\int_\Omega \frac{\partial I_{\mathrm{ion}}}{\partial\varphi}(\hat{\Phi}_{\mathrm{tr}},\hat{W})\,\psi_i(x)\,\psi_j(x)\,\mathrm{d}x \tag{4.111}$$

$$+\sum_{i=0}^{N} q_{i,N}(s)\cdot\int_\Omega \frac{\partial G}{\partial\varphi}(\hat{\Phi}_{\mathrm{tr}},\hat{W})\,\psi_i(x)\,\psi_j(x)\,\mathrm{d}x \,=\, \langle\, \widetilde{S}(s)\,,\,\psi_j\,\rangle\,, \quad 0 \leqslant j \leqslant N\,;$$

$$\frac{\mathrm{d}q_{j,N}(s)}{\mathrm{d}s} \,+\, \sum_{i=0}^{N} p_{i,N}(s)\cdot\int_\Omega \frac{\partial I_{\mathrm{ion}}}{\partial w}(\hat{\Phi}_{\mathrm{tr}},\hat{W})\,\psi_i(x)\,\psi_j(x)\,\mathrm{d}x \tag{4.112}$$

$$+\sum_{i=0}^{N} q_{i,N}(s)\cdot\int_\Omega \frac{\partial G}{\partial w}(\hat{\Phi}_{\mathrm{tr}},\hat{W})\,\psi_i(x)\,\psi_j(x)\,\mathrm{d}x \,=\, -\left\langle\, \frac{\partial r}{\partial w}(\hat{\Phi}_{\mathrm{tr}},\hat{\Phi}_e,\hat{W})\,,\,\psi_j\,\right\rangle\,, \quad 0 \leqslant j \leqslant N\,;$$

$$p_{j,N}(0) \,=\, 0\,;\; q_{j,N}(0) \,=\, 0 \quad 0 \leqslant j \leqslant N. \tag{4.113}$$

Specifying the data for (4.111)–(4.113) according to the Rogers–McCulloch model, the problem reads as

$$\frac{\mathrm{d}p_{j,N}(s)}{\mathrm{d}s} \,+\, \lambda_j\,p_{j,N}(s) + \sum_{i=0}^{N} p_{i,N}(s)\cdot\int_\Omega \Big(\,3\,b\,(\hat{\Phi}_{\mathrm{tr}})^2 + 2\,(a+1)\,b\,\hat{\Phi}_{\mathrm{tr}} + \hat{W} + a\,b\,\Big)\,\psi_i\,\psi_j\,\mathrm{d}x \tag{4.114}$$

$$-\,\varepsilon\,\kappa\,q_{j,N}(s) \,=\, \langle\, \widetilde{S}(s)\,,\,\psi_j\,\rangle\,, \quad 0 \leqslant j \leqslant N\,;$$

$$\frac{\mathrm{d}q_{j,N}(s)}{\mathrm{d}s} \,+\, \sum_{i=0}^{N} p_{i,N}(s)\cdot\int_\Omega \hat{\Phi}_{\mathrm{tr}}\,\psi_i\,\psi_j\,\mathrm{d}x \,+\, \varepsilon\,q_{j,N}(s) \,=\, -\left\langle\, \frac{\partial r}{\partial w}(\hat{\Phi}_{\mathrm{tr}},\hat{\Phi}_e,\hat{W})\,,\,\psi_j\,\right\rangle\,, \quad 0 \leqslant j \leqslant N; \tag{4.115}$$

$$p_{j,N}(0) \,=\, 0\,;\; q_{j,N}(0) \,=\, 0 \quad 0 \leqslant j \leqslant N. \tag{4.116}$$

Obviously, all integrals with respect to x are well-defined and the coefficients as well as the right-hand sides are integrable with respect to s at least. Then, by [23], page 92, Theorem II.4.6, the initial-value problem (4.114)–(4.116) admits a unique solution $\big(\,p_{0,N},\,\ldots,\,p_{N,N}\,,\,q_{0,N}\,,\,\ldots,\,q_{N,N}\,\big) \in \big(\,W^{1,1}(\,0\,,\,T\,)\,\big)^{2\,(N+1)}$. As a consequence of the orthogonality relations, P_1^N and P_3^N obey the equations

$$\frac{\mathrm{d}}{\mathrm{d}s}\langle\, P_1^N(s)\,,\,\psi\,\rangle + A\big(\,P_1^N(s)\,,\,\psi\,\big) + \int_\Omega \left(\,\frac{\partial I_{\mathrm{ion}}}{\partial\varphi}(\hat{\Phi}_{\mathrm{tr}},\hat{W})\,P_1^N + \frac{\partial G}{\partial\varphi}(\hat{\Phi}_{\mathrm{tr}},\hat{W})\,P_3^N\,\right)\,\psi\,\mathrm{d}x \tag{4.117}$$

$$=\,\left\langle\, \widetilde{S}(s)\,,\,\psi\,\right\rangle \quad \forall\,\psi \in \mathrm{X}^N(\Omega)\,;$$

$$\frac{\mathrm{d}}{\mathrm{d}s}\langle\, P_3^N(s)\,,\,\psi\,\rangle + \int_\Omega \left(\,\frac{\partial I_{\mathrm{ion}}}{\partial w}(\hat{\Phi}_{\mathrm{tr}},\hat{W})\,P_1^N + \frac{\partial G}{\partial w}(\hat{\Phi}_{\mathrm{tr}},\hat{W})\,P_3^N\,\right)\,\psi\,\mathrm{d}x \tag{4.118}$$

$$=\,-\left\langle\, \frac{\partial r}{\partial w}(\hat{\Phi}_{\mathrm{tr}},\hat{\Phi}_e,\hat{W})\,,\,\psi\,\right\rangle \quad \forall\,\psi \in \mathrm{X}^N(\Omega).$$

In this sense, the functions P_1^N, P_3^N can be interpreted as approximate solutions of the reduced adjoint system.

• **Step 2.** A priori *estimates for the approximate solutions* P_1^N, P_3^N. The functions P_1^N, P_3^N obey the *a priori* estimates from Theorem 4.1, 2). More precisely, the following holds:

Lemma 4.4. *Let the assumptions of Theorem 4.1, 2), hold for the data of* (P) *and a feasible solution* $(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)$ *where* $q = 10/9$. *Then for all* $N \in \mathbb{N}_0$, *the functions* P_1^N, P_3^N *satisfy the estimate*

$$\| P_1^N \|^2_{C^0[\,[0,T], L^2(\Omega)]} + \| P_1^N \|^2_{L^2[\,(0,T), W^{1,2}(\Omega)]} + \| \partial P_1^N/\partial s \|^q_{L^q[\,(0,T), (W^{1,2}(\Omega))^*]} \tag{4.119}$$
$$+ \| P_3^N \|^2_{C^0[\,[0,T], L^2(\Omega)]} + \| \partial P_3^N/\partial s \|^q_{L^q[\,(0,T), L^2(\Omega)]} \leqslant C$$

for a constant $C > 0$ *independent of* N.

Proof. We rely on the Proof of Theorem 4.1. First, we observe that Lemma 4.3, (4.51) and (4.55) remain true if P_1 and P_3 are replaced by P_1^N and P_3^N since, in Steps 2 and 3 of the proof above, the reduced equations must be studied only for the special test functions $P_1^N(s)$, $P_3^N(s) \in \mathrm{X}^N(\Omega)$. Further, we observe that

$$\| \partial P_1^N/\partial s \|^q_{L^q[\,(0,T), (W^{1,2}(\Omega))^*]} = \int_0^T \sup_{\|\psi\|_{W^{1,2}(\Omega)}=1} \big| \langle \partial P_1^N(s)/\partial s, \psi \rangle \big|^q \, \mathrm{d}s \tag{4.120}$$

$$= \int_0^T \sup_{\left\| \sum_{j=0}^{\infty} c_j \psi_j \right\|_{W^{1,2}(\Omega)}=1} \left| \left\langle \sum_{i=0}^{N} \frac{\mathrm{d}p_{i,N}(s)}{\mathrm{d}s} \psi_i , \sum_{j=0}^{\infty} c_j \psi_j \right\rangle \right|^q \mathrm{d}s \tag{4.121}$$

$$= \int_0^T \sup_{\left\| \sum_{j=0}^{\infty} c_j \psi_j \right\|_{W^{1,2}(\Omega)}=1} \left| \left\langle \sum_{i=0}^{N} \frac{\mathrm{d}p_{i,N}(s)}{\mathrm{d}s} \psi_i , \sum_{j=0}^{N} c_j \psi_j \right\rangle \right|^q \mathrm{d}s \tag{4.122}$$

$$= \int_0^T \sup_{\psi \in \mathrm{X}^N,\ \|\psi\|_{W^{1,2}(\Omega)}=1} \big| \langle \partial P_1^N(s)/\partial s, \psi \rangle \big|^q \, \mathrm{d}s. \tag{4.123}$$

By (4.117), the calculations from the Proof of Theorem 4.1, Step 4, can be repeated now, resulting in a uniform bound for $\| \partial P_1^N/\partial s \|^q_{L^q[\,(0,T), (W^{1,2}(\Omega))^*]}$. In the same manner, we may repeat the derivation from Step 5 since

$$\| \partial P_3^N/\partial s \|^q_{L^q[\,(0,T), (L^2(\Omega))^*]} = \int_0^T \sup_{\|\psi\|_{L^2(\Omega)}=1} \big| \langle \partial P_3^N(s)/\partial s, \psi \rangle \big|^q \, \mathrm{d}s \tag{4.124}$$

$$= \int_0^T \sup_{\psi \in \mathrm{X}^N,\ \|\psi\|_{L^2(\Omega)}=1} \big| \langle \partial P_3^N(s)/\partial s, \psi \rangle \big|^q \, \mathrm{d}s, \tag{4.125}$$

and we obtain a uniform bound for $\| \partial P_3^N/\partial s \|^q_{L^q[\,(0,T), L^2(\Omega)]}$ as well. The arguments from Step 7 hold without alterations. □

• **Step 3.** *The solution for the reduced adjoint system.* Lemma 4.4 implies that we may select a subsequence $\{ (P_1^{N'}, P_3^{N'}) \}$ of $\{ (P_1^N, P_3^N) \}$ with convergence to limit elements in the following sense:

$$P_1^{N'} \rightharpoonup^{L^2[\,(0,T), W^{1,2}(\Omega)]} P_1; \tag{4.126}$$

$$dP_1^{N'}/\mathrm{d}s \rightharpoonup^{L^q\left[\,(0\,,T\,)\,,\,\left(\,W^{1,2}(\Omega)\right)^*\,\right]}\ \widetilde{P}\,; \tag{4.127}$$

$$P_3^{N'} \rightharpoonup^{L^2\left[\,(0\,,T\,)\,,\,L^2(\Omega)\,\right]}\ P_3\,; \tag{4.128}$$

$$dP_3^{N'}/\mathrm{d}s \rightharpoonup^{L^q\left[\,(0\,,T\,)\,,\,\left(\,L^2(\Omega)\right)^*\,\right]}\ \widetilde{Q}. \tag{4.129}$$

Consequently, taking an arbitrary element $\psi_j \in W^{1,2}(\Omega)$ from the orthonormal base, we find

$$\begin{aligned}
&\langle\, \widetilde{P}(s)\,,\,\psi_j\,\rangle + A\big(\,P_1(s)\,,\,\psi_j\,\big) + \int_\Omega \left(\frac{\partial I_{\mathrm{ion}}}{\partial\varphi}(\hat{\Phi}_{\mathrm{tr}},\hat{W})\,P_1 + \frac{\partial G}{\partial\varphi}(\hat{\Phi}_{\mathrm{tr}},\hat{W})\,P_3\right)\psi_j\,\mathrm{d}x \,-\, \langle\,\widetilde{S}(s)\,,\,\psi_j\,\rangle \\
&= \lim_{N'\to\infty}\left(\frac{\mathrm{d}}{\mathrm{d}s}\langle\,P_1^{N'}(s)\,,\psi_j\,\rangle + A\big(\,P_1^{N'}(s)\,,\,\psi_j\big) + \int_\Omega\left(\frac{\partial I_{\mathrm{ion}}}{\partial\varphi}(\hat{\Phi}_{\mathrm{tr}},\hat{W})\,P_1^{N'}\right.\right. \\
&\qquad\left.\left. + \frac{\partial G}{\partial\varphi}(\hat{\Phi}_{\mathrm{tr}},\hat{W})\,P_3^{N'}\right)\psi_j\,\mathrm{d}x \,-\, \langle\,\widetilde{S}(s)\,,\,\psi_j\,\rangle\right) \,=\, 0
\end{aligned} \tag{4.130}$$

since $\psi_j \in \mathrm{X}^{N'}$ for all sufficiently large $N' \in \mathbb{N}$. For the same reason, it holds that

$$\begin{aligned}
&\langle\,\widetilde{Q}(s)\,,\,\psi_j\,\rangle + \int_\Omega\left(\frac{\partial I_{\mathrm{ion}}}{\partial w}(\hat{\Phi}_{\mathrm{tr}},\hat{W})\,P_1 + \frac{\partial G}{\partial w}(\hat{\Phi}_{\mathrm{tr}},\hat{W})\,P_3\right)\psi_j\,\mathrm{d}x + \langle\,\frac{\partial r}{\partial w}(\hat{\Phi}_{\mathrm{tr}},\hat{\Phi}_e,\hat{W})\,,\,\psi_j\,\rangle \\
&= \lim_{N'\to\infty}\left(\frac{\mathrm{d}}{\mathrm{d}s}\langle\,P_3^{N'}(s)\,,\,\psi_j\,\rangle + \int_\Omega\left(\frac{\partial I_{\mathrm{ion}}}{\partial w}(\hat{\Phi}_{\mathrm{tr}},\hat{W})\,P_1^{N'} + \frac{\partial G}{\partial w}(\hat{\Phi}_{\mathrm{tr}},\hat{W})\,P_3^{N'}\right)\psi_j\,\mathrm{d}x\right. \\
&\qquad\left. + \left\langle\,\frac{\partial r}{\partial w}(\hat{\Phi}_{\mathrm{tr}},\hat{\Phi}_e,\hat{W})\,,\,\psi_j\,\right\rangle\right) \,=\, 0.
\end{aligned} \tag{4.131}$$

Weak continuity of the distributional differential operator implies that $\widetilde{P} = dP_1/\mathrm{d}s$ and $\widetilde{Q} = dP_3/\mathrm{d}s$ in the sense of distributions. Further, it obviously holds that $P_1(x,0) = \lim_{N'\to\infty} P_1^N(x,0) = 0$ and $P_3(x,0) = \lim_{N'\to\infty} P_3^N(x,0) = 0$. Since $\{\,\psi_i\,\}$ lies dense in $W^{1,2}(\Omega)$ as well as in $L^2(\Omega)$, the functions P_1 and P_3 form a weak solution of the reduced adjoint system.

• **Step 4.** *Completion of the adjoint solution.* As indicated in Section 4.2., the solution (P_1, P_3) of the reduced adjoint system may be completed to a weak solution (P_1, P_2, P_3) of the adjoint system where $P_2 \in L^2\big[\,(0\,,T\,)\,,\,W^{1,2}(\Omega)\,\big]$ with $\int_\Omega P_2(x,s)\,\mathrm{d}x = 0\ (\forall)\,s \in (\,0\,,T\,)$ is uniquely determined by P_1, P_3. The claimed regularity of the solution is guaranteed by Theorem 4.1, 2).

• **Step 5.** *Uniqueness.* Since the reduced adjoint system is linear with respect to P_1 and P_3, estimate (4.20) yields the uniqueness of its weak solution (P_1, P_3) within the space $\big(\,L^\infty\big[\,(\,0\,,T\,)\,,\,L^2(\Omega)\,\big] \cap L^2\big[\,(\,0\,,T\,)\,,\,W^{1,2}(\Omega)\,\big]\,\big) \times L^\infty\big[\,(\,0\,,T\,)\,,\,L^2(\Omega)\,\big]$. The completion of (P_1, P_3) to a weak solution (P_1, P_2, P_3) of the adjoint system is uniquely determined as well. This finishes the Proof of Theorem 4.2. □

Remark 4.5. 1) If the Rogers–McCulloch model in (3.12)–(3.14) is replaced by the FitzHugh–Nagumo model then the Proofs of Theorems 4.1. and 4.2. can be repeated with only minor alterations.

2) Theorems 4.1. and 4.2. remain even true if (3.12)–(3.14) is considered with the linearized Aliev–Panfilov model. In the proofs, we must work with

$$\frac{\partial G}{\partial\varphi}(\hat{\Phi}_{\mathrm{tr}},\hat{W}) \,=\, -\varepsilon\,\kappa\,(a+1) + 2\,\varepsilon\,\kappa\,\hat{\Phi}_{\mathrm{tr}} \tag{4.132}$$

instead of $\partial G(\hat{\Phi}_{\rm tr}, \hat{W})/\partial\varphi \equiv -\varepsilon\,\kappa$. Thus the estimations (4.36)–(4.55) have to be modified in the following way: On the right-hand side of (4.36), the term $\varepsilon\,\kappa \int_\Omega |\,P_1\,P_3\,|\,{\rm d}x$ must be replaced by

$$\varepsilon\,\kappa\,(a+1)\int_\Omega \big|\,P_1\,P_3\,\big|\,{\rm d}x \,+\, \varepsilon\,\kappa \int_\Omega \big|\,\hat{\Phi}_{\rm tr}\,P_1\,P_3\,\big|\,{\rm d}x. \tag{4.133}$$

The estimation of the first member of (4.133) runs as above, for the second one we get with arbitrary $\varepsilon_3(s) > 0$:

$$\int_\Omega \big|\,\hat{\Phi}_{\rm tr}\,P_1\,P_3\,\big|\,{\rm d}x \,\leqslant\, C\,\varepsilon_3(s) \int_\Omega \big|\,\hat{\Phi}_{\rm tr}\,P_1\,\big|^2\,{\rm d}x + \frac{C}{\varepsilon_3(s)}\,\|\,P_3\,\|^2_{L^2(\Omega)} \tag{4.134}$$

$$\leqslant\, C\,\varepsilon_3(s)\,\Big\|\,\hat{\Phi}_{\rm tr}\,\Big\|^2_{L^4(\Omega)} \cdot \|\,P_1\,\|^2_{L^4(\Omega)} + \frac{C}{\varepsilon_3(s)}\,\|\,P_3\,\|^2_{L^2(\Omega)}. \tag{4.135}$$

We choose $\varepsilon_3(s) = \varepsilon_3'/\big(1 + \Big\|\,\hat{\Phi}_{\rm tr}\,\Big\|^2_{L^4(\Omega)}\big)$ with $\varepsilon_3' > 0$, thus getting

$$\int_\Omega \big|\,\hat{\Phi}_{\rm tr}\,P_1\,P_3\,\big|\,{\rm d}x \,\leqslant\, C\,\varepsilon'\,\|\,P_1\,\|^2_{W^{1,2}(\Omega)} + \frac{C}{\varepsilon_3'}\,\big(1 + \Big\|\,\hat{\Phi}_{\rm tr}\,\Big\|^2_{L^4(\Omega)}\big)\,\|\,P_3\,\|^2_{L^2(\Omega)}\,, \tag{4.136}$$

and with appropriate choices of $\varepsilon_3' > 0$, we may proceed as above. Further alterations concern the estimations (4.58)–(4.88). In (4.58), the term $\sup_{\dots}\,\varepsilon^q\,\kappa^q\,\big(\int_\Omega |\,P_3\,|\,|\psi\,|\,{\rm d}x\big)^q$ must be replaced by

$$\sup_{\dots}\,\varepsilon^q\,\kappa^q\,(a+1)^q\left(\int_\Omega |\,P_3\,|\,|\psi\,|\,{\rm d}x\right)^q + \sup_{\dots}\,\varepsilon^q\,\kappa^q\left(\int_\Omega |\,\hat{\Phi}_{\rm tr}\,P_3\,\psi\,|\,{\rm d}x\right)^q. \tag{4.137}$$

Despite of the lesser regularity of $\hat{W}$ for the linearized Aliev–Panfilov model, the estimations (4.70)–(4.80) can be maintained since the solution satisfies $\hat{W} \in C^0\big[\,[\,0\,,\,T\,]\,,\,L^{8/3}(\Omega)\,\big] \hookrightarrow L^{10/4}\big[\,(\,0\,,\,T\,)\,,\,L^{20/11}(\Omega)\,\big]$. In (4.81)–(4.84), we must add an estimate for the second term from (4.137). Consider therefore

$$\sup_{\dots}\int_0^T \int_\Omega \big|\,\hat{\Phi}_{\rm tr}\,\big|^{10/9}\,\big|\,P_3\,\big|^{10/9}\,\big|\,\psi\,\big|^{10/9}\,{\rm d}x\,{\rm d}s$$

$$\leqslant\, C\,\sup_{\dots}\int_0^T \left(\int_\Omega \big|\,\hat{\Phi}_{\rm tr}\,\big|^5\,{\rm d}x\right)^{4/18} \left(\int_\Omega \big|\,\psi\,\big|^5\,{\rm d}x\right)^{4/18} \left(\int_\Omega \big|\,P_3\,\big|^2\,{\rm d}x\right)^{10/18} {\rm d}s \tag{4.138}$$

$$\leqslant\, C\,\sup_{\dots}\int_0^T \left(\Big\|\,\hat{\Phi}_{\rm tr}\,\Big\|^{10/9}_{L^5(\Omega)} \cdot \|\,\psi\,\|^{10/9}_{W^{1,2}(\Omega)} \cdot \|\,P_3\,\|^{10/9}_{L^2(\Omega)}\right) {\rm d}s \,=\, C\int_0^T \left(\Big\|\,\hat{\Phi}_{\rm tr}\,\Big\|^{10/9}_{L^5(\Omega)} \cdot \|\,P_3\,\|^{10/9}_{L^2(\Omega)}\right) {\rm d}s \tag{4.139}$$

$$\leqslant\, C\,\Big\|\,\hat{\Phi}_{\rm tr}\,\Big\|^{10/9}_{L^{10/9}\left[\,(\,0\,,T\,)\,,\,L^5(\Omega)\,\right]} \cdot \|\,P_3\,\|^{10/9}_{L^\infty\left[\,(\,0\,,T\,)\,,\,L^2(\Omega)\,\right]}\,, \tag{4.140}$$

and we may proceed as above. The other parts of the Proof of Theorem 4.1. as well as the Proof of Theorem 4.2. remain unchanged.

5. Necessary optimality conditions

5.1. Statement of the theorems

Definition 5.1 (Weak local minimizer)**.** A quadruple $(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)$, which is feasible in (P), is called a weak local minimizer of (P) iff there exists a number $\varepsilon > 0$ such that for all admissible $(\Phi_{\rm tr}, \Phi_e, W, I_e)$ the conditions

$$\Big\|\,\Phi_{\rm tr} - \hat{\Phi}_{\rm tr}\,\Big\|_{{\rm X}_1} \,\leqslant\, \varepsilon\,,\;\; \Big\|\,\Phi_e - \hat{\Phi}_e\,\Big\|_{{\rm X}_2} \,\leqslant\, \varepsilon\,,\;\; \Big\|\,W - \hat{W}\,\Big\|_{{\rm X}_3} \,\leqslant\, \varepsilon\,,\;\; \Big\|\,I_e - \hat{I}_e\,\Big\|_{{\rm X}_4} \,\leqslant\, \varepsilon \tag{5.1}$$

imply the relation $F(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e) \leqslant F(\Phi_{\rm tr}, \Phi_e, W, I_e)$.

The necessary optimality conditions for weak local minimizers of (P) can be formulated as follows:

Theorem 5.2 (First-order necessary optimality conditions for the control problem (P)). *We consider problem* (P)*,* (3.11)–(3.17)*, under the assumptions of Section 3.1. with the Rogers–McCulloch or the FitzHugh–Nagumo model. Assume further that 1)* $\Omega \subset \mathbb{R}^3$ *admits a* $C^{1,1}$*-boundary, 2)* M_i, $M_e :\ \mathrm{cl}\,(\Omega) \to \mathbb{R}^{3\times 3}$ *are symmetric, positive definite matrix functions obeying* (2.5) *with* $W^{1,\infty}(\Omega)$*-coefficients, and 3) the integrand* $r(x,t,\varphi,\eta,w)$ *is continuously differentiable with respect to* φ*,* η *and* w*. Let* $(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)$ *be a weak local minimizer of* (P) *such that* $(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W})$ *is a strong solution of the bidomain system on* $[\,0\,,\,T\,]$, $\hat{I}_e \in W^{1,2}\big[\,(\,0\,,\,T\,)\,,\,L^2(\Omega)\,\big]$ *and*

$$\frac{\partial r}{\partial \varphi}(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W})\,,\ \frac{\partial r}{\partial \eta}(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W})\,,\ \frac{\partial r}{\partial w}(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W}) \in L^{2q}\big[\,(\,0\,,\,T\,)\,,\,L^2(\Omega)\,\big] \tag{5.2}$$

where $q \geqslant 10/9$*. Then there exist multipliers* $P_1 \in L^4\big[\,(\,0\,,\,T\,)\,,\,W^{1,2}(\Omega)\,\big]$, $P_2 \in L^2\big[\,(\,0\,,\,T\,)\,,\,W^{1,2}(\Omega)\,\big] \cap \big\{\,Z \;\big|\; \int_\Omega Z(x,t)\,\mathrm{d}x = 0\ (\forall)\,t \in (\,0\,,\,T\,)\,\big\}$ *and* $P_3 \in L^2(\Omega_T)$*, satisfying together with* $(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)$ *the adjoint equations* (4.8)–(4.10)*, which are solved in weak sense, as well as the optimality condition*

$$\int_0^T \int_{\Omega_{\rm con}} \Big(\,\mu\,\hat{I}_e - Q\,P_2\,\Big)\cdot\big(\,I_e - \hat{I}_e\,\big)\,\mathrm{d}x\,\mathrm{d}t\ \geqslant\ 0 \quad \forall\,I_e \in \mathcal{C}. \tag{5.3}$$

If the linearized Aliev–Panfilov model is specified then all assertions remain true provided that $\partial r(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W})/\partial w$ *belongs to* $L^3(\Omega_T)$ *instead of* $L^2(\Omega_T)$*.*

The assumptions of Theorem 5.2. reflect the fact that there is a regularity gap between the weak solutions of the primal and adjoint equations. The duality pairing between $\partial\Phi_{\rm tr}/\partial t \in L^{4/3}\big[\,(\,0\,,\,T\,)\,,\,\big(\,W^{1,2}(\Omega)\,\big)^*\,\big]$ and $P_1 \in L^2\big[\,(\,0\,,\,T\,)\,,\,W^{1,2}(\Omega)\,\big]$ is not well-defined, and hence further regularity is required. In order to gain this regularity, we have to impose that $(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W})$ is a *strong* solution of the bidomain system rather than a weak one. Sufficient conditions for strong local solvability of (3.12)–(3.14) may be found in [22].

Corollary 5.3 (Pointwise formulation of the optimality condition). *Under the assumptions of Theorem 5.2., let the optimal control* $\hat{I}_e$ *be represented as* $\hat{I}_e = Q\,\hat{I}$ *with* $\hat{I} \in L^\infty\big[\,(\,0\,,\,T\,)\,,\,L^2(\Omega)\,\big]$, $\mathrm{supp}\,(\hat{I}) \subseteq \Omega_{\rm con} \times [\,0\,,\,T\,]$ *and* $|\,\hat{I}(x,t)\,| \leqslant R$ *for almost all* $(x,t) \in \Omega_T$*. The optimality condition* (5.3) *from Theorem 5.2. then implies the following Pontryagin minimum condition, which holds a.e. pointwise:*

$$\hat{I}(x_0,t_0)\cdot\Big(\,\mu\cdot Q\,\hat{I}(x_0,t_0) - Q\,P_2(x_0,t_0)\,\Big) = \underset{-R\leqslant\eta\leqslant R}{\mathrm{Min}}\ \eta\,\Big(\,\mu\cdot Q\,\hat{I}(x_0,t_0) - Q\,P_2(x_0,t_0)\,\Big) \tag{5.4}$$

$$(\forall)\,(x_0,t_0) \in\ \Omega_{\rm con} \times\ [\,0\,,\,T\,].$$

Consequently, for a.e. $(x,t) \in \Omega_{\rm con} \times\ [\,0\,,\,T\,]$ *the following implications hold:*

$$\begin{aligned} &Q\,\hat{I}(x,t) - \frac{1}{\mu}\,Q\,P_2(x,t)\ >\ 0\ \implies\ \hat{I}(x,t)\ = -R\,;\\ &Q\,\hat{I}(x,t) - \frac{1}{\mu}\,Q\,P_2(x,t)\ <\ 0\ \implies\ \hat{I}(x,t)\ =\ \ \ R\ \text{ and}\\ &\hat{I}(x,t)\ \in (\,-R\,,\,R\,)\ \implies\ Q\,\hat{I}(x,t) - \frac{1}{\mu}\,Q\,P_2(x,t)\ =\ 0. \end{aligned} \tag{5.5}$$

Corollary 5.4 (Regularity of weak local minimizers). *Under the assumptions of Theorem 5.2., consider a weak local minimizer* $(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)$ *of* (P)*, whose control part* $\hat{I}_e = Q\,\hat{I}$ *is generated by a function* $\hat{I}$ *with* $|\,\hat{I}(x,t)\,| < R$ *a.e. Then* $\hat{I}_e\,\big|\,\Omega_{\rm con}$ *belongs to the space* $L^\infty\big(\,\Omega_{\rm con}\,\times\,[\,0\,,\,T\,]\,\big) \cap L^2\big[\,(\,0\,,\,T\,),\ W^{1,2}(\Omega_{\rm con})\,\big]$

Fur numerical purposes, it is useful to specify the Gâteaux derivative of the reduced cost functional $\widetilde{F}: \mathcal{C} \to \mathbb{R}$. It is defined through

$$\widetilde{F}(I_e) = F\big(\Phi_{\mathrm{tr}}(I_e), \Phi_e(I_e), W(I_e), I_e\big) \tag{5.6}$$

with the aid of the control-to-state mapping $I_e \longmapsto \big(\Phi_{\mathrm{tr}}(I_e), \Phi_e(I_e), W(I_e)\big)$, which is well-defined by Proposition 3.1.

Corollary 5.5 (First variation of the reduced cost functional)**.** *Under the assumptions of Theorem 5.2., the Gâteaux derivative of the reduced cost functional $\widetilde{F}$ at $\hat{I}_e \in \mathcal{C}$ is given through*

$$D_{I_e}\widetilde{F}(\hat{I}_e) = \mu\, \hat{I}_e - Q\, P_2(\hat{I}_e) \tag{5.7}$$

where $\big(P_1(\hat{I}_e), P_2(\hat{I}_e), P_3(\hat{I}_e)\big)$ denotes the solution of the adjoint system (4.8)–(4.10) *corresponding to $\big(\Phi_{\mathrm{tr}}(\hat{I}_e), \Phi_e(\hat{I}_e), W(\hat{I}_e), \hat{I}_e\big)$.*

5.2. Proof of the necessary optimality conditions

Proof of Theorem 5.2. As mentioned in the introduction, the proof of the necessary optimality conditions for (P) is based on the stability estimate for the bidomain system (Thm. 2.4) and the existence theorem for the adjoint system (Thm. 4.2), which will be invoked in Steps 2 and 3 of the proof, respectively.

• **Step 1.** *Variation of the weak local minimizer in a feasible direction.* Assume that $(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)$ is a weak local minimizer of (P). If $I_e \in \mathcal{C}$ is an arbitrary feasible control with $\big\| I_e - \hat{I}_e \big\|_{L^\infty[(0,T), L^2(\Omega)]} \leqslant \varepsilon$ then, by Proposition 3.2., all controls

$$I_e(s) = \hat{I}_e + s\,(I_e - \hat{I}_e), \; 0 \leqslant s \leqslant 1, \tag{5.8}$$

belong to $\mathcal{C}$ as well. By Proposition 3.1., for every $I_e(s) \in L^\infty[(0,T), L^2(\Omega)]$, there exists a corresponding weak solution $(\Phi_{\mathrm{tr}}(s), \Phi_e(s), W(s)) \in \mathrm{X}_1 \times \mathrm{X}_2 \times \mathrm{X}_3$ for the bidomain system on $[0,T]$. Thus the quadruples $(\Phi_{\mathrm{tr}}(s), \Phi_e(s), W(s), I_e(s))$ are feasible in (P) for all $0 \leqslant s \leqslant 1$. On the other hand, from [12], page 7, Theorem 2.7, it follows that every feasible solution of (P) within a closed ball

$$\mathrm{U}_\varepsilon(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}, \hat{I}_e) = \mathrm{K}(\hat{\Phi}_{\mathrm{tr}}, C\varepsilon) \times \mathrm{K}(\hat{\Phi}_e, C\varepsilon) \times \mathrm{K}(\hat{W}, C\varepsilon) \times \mathrm{K}(\hat{I}_e, \varepsilon) \subset \mathrm{X}_1 \times \mathrm{X}_2 \times \mathrm{X}_3 \times \mathrm{X}_4 \tag{5.9}$$

can be generated in this way.

• **Step 2.**

Lemma 5.6. *For all $I_e \in \mathcal{C}$, $\big\| I_e - \hat{I}_e \big\|_{L^\infty[(0,T), L^2(\Omega)]} \leqslant \varepsilon$ implies that*

$$\lim_{s\to 0+0} \frac{1}{s} \Big\| \Phi_{\mathrm{tr}}(s) - \hat{\Phi}_{\mathrm{tr}} \Big\|^2_{\mathrm{X}_1} = 0; \quad \lim_{s\to 0+0} \frac{1}{s} \Big\| \Phi_{\mathrm{tr}}(s) - \hat{\Phi}_{\mathrm{tr}} \Big\|^2_{\widetilde{\mathrm{X}}_1} = 0; \tag{5.10}$$

$$\lim_{s\to 0+0} \frac{1}{s} \Big\| \Phi_e(s) - \hat{\Phi}_e \Big\|^2_{\mathrm{X}_2} = 0; \tag{5.11}$$

$$\lim_{s\to 0+0} \frac{1}{s} \Big\| W(s) - \hat{W} \Big\|^2_{\mathrm{X}_3} = 0 \quad \textit{and} \quad \lim_{s\to 0+0} \frac{1}{s} \Big\| W(s) - \hat{W} \Big\|^2_{\widetilde{\mathrm{X}}_3} = 0. \tag{5.12}$$

□

Proof. The stability estimate [12], page 7, Theorem 2.7, (2.38), implies

$$\Big\| \Phi_{\mathrm{tr}}(s) - \hat{\Phi}_{\mathrm{tr}} \Big\|^2_{\mathrm{X}_1} = \Big\| \Phi_{\mathrm{tr}}(s) - \hat{\Phi}_{\mathrm{tr}} \Big\|^2_{L^2[(0,T), W^{1,2}(\Omega)]} \leqslant C \cdot \Big\| I_e(s) - \hat{I}_e \Big\|^2_{L^\infty[(0,T), (W^{1,2}(\Omega))^*]}$$

$$\leqslant C \cdot \left\| I_e(s) - \hat{I}_e \right\|^2_{L^\infty\left[\,(0,T),\,L^2(\Omega)\right]} = C\,s^2 \left\| I_e - \hat{I}_e \right\|^2_{L^\infty\left[\,(0,T),\,L^2(\Omega)\right]} \quad \Longrightarrow \tag{5.13}$$

$$\lim_{s\to 0+0} \frac{1}{s} \left\| \Phi_{\mathrm{tr}}(s) - \hat{\Phi}_{\mathrm{tr}} \right\|^2_{\mathrm{X}_1} \leqslant \lim_{s\to 0+0} C\,s \left\| I_e - \hat{I}_e \right\|^2_{L^\infty\left[\,(0,T),\,L^2(\Omega)\right]} = 0 \tag{5.14}$$

as well as

$$\left\| \Phi_e(s) - \hat{\Phi}_e \right\|^2_{\mathrm{X}_2} = \left\| \Phi_e(s) - \hat{\Phi}_e \right\|^2_{L^2\left[\,(0,T),\,W^{1,2}(\Omega)\right]} \leqslant C \cdot \left\| I_e(s) - \hat{I}_e \right\|^2_{L^\infty\left[\,(0,T),\,\left(W^{1,2}(\Omega)\right)^*\right]}$$

$$\leqslant C \cdot \left\| I_e(s) - \hat{I}_e \right\|^2_{L^\infty\left[\,(0,T),\,L^2(\Omega)\right]} = C\,s^2 \left\| I_e - \hat{I}_e \right\|^2_{L^\infty\left[\,(0,T),\,L^2(\Omega)\right]} \quad \Longrightarrow \tag{5.15}$$

$$\lim_{s\to 0+0} \frac{1}{s} \left\| \Phi_e(s) - \hat{\Phi}_e \right\|^2_{\mathrm{X}_2} \leqslant \lim_{s\to 0+0} C\,s \left\| I_e - \hat{I}_e \right\|^2_{L^\infty\left[\,(0,T),\,L^2(\Omega)\right]} = 0 \tag{5.16}$$

and

$$\left\| W(s) - \hat{W} \right\|^2_{\mathrm{X}_3} = \left\| W(s) - \hat{W} \right\|^2_{L^2(\Omega_T)} \leqslant C \cdot \left\| I_e(s) - \hat{I}_e \right\|^2_{L^\infty\left[\,(0,T),\,\left(W^{1,2}(\Omega)\right)^*\right]}$$

$$\leqslant C \cdot \left\| I_e(s) - \hat{I}_e \right\|^2_{L^\infty\left[\,(0,T),\,L^2(\Omega)\right]} = C\,s^2 \left\| I_e - \hat{I}_e \right\|^2_{L^\infty\left[\,(0,T),\,L^2(\Omega)\right]} \quad \Longrightarrow \tag{5.17}$$

$$\lim_{s\to 0+0} \frac{1}{s} \left\| W(s) - \hat{W} \right\|^2_{\mathrm{X}_3} \leqslant \lim_{s\to 0+0} C\,s \left\| I_e - \hat{I}_e \right\|^2_{L^\infty\left[\,(0,T),\,L^2(\Omega)\right]} = 0. \tag{5.18}$$

In an analogous manner, the relation with $\left\| W(s) - \hat{W} \right\|^2_{\tilde{\mathrm{X}}_3}$ can be confirmed. In order to establish the relation with $\left\| \Phi_{\mathrm{tr}}(s) - \hat{\Phi}_{\mathrm{tr}} \right\|^2_{\tilde{\mathrm{X}}_1}$, we rely on [12], page 7, Theorem 2.7, (2.39), which leads to

$$\left\| \Phi_{\mathrm{tr}}(s) - \hat{\Phi}_{\mathrm{tr}} \right\|^2_{\tilde{\mathrm{X}}_1} = \left\| \Phi_{\mathrm{tr}}(s) - \hat{\Phi}_{\mathrm{tr}} \right\|^2_{W^{1,4/3}\left[\,(0,T),\,\left(W^{1,2}(\Omega)\right)^*\right]} \tag{5.19}$$

$$\leqslant C^2 \cdot \mathrm{Max}\left(\left\| I_e(s) - \hat{I}_e \right\|^2_{L^\infty\left[\,(0,T),\,\left(W^{1,2}(\Omega)\right)^*\right]},\ \left\| I_e(s) - \hat{I}_e \right\|^4_{L^\infty\left[\,(0,T),\,\left(W^{1,2}(\Omega)\right)^*\right]} \right) \tag{5.20}$$

$$\leqslant C \cdot \mathrm{Max}\left(s^2 \left\| I_e - \hat{I}_e \right\|^2_{L^\infty\left[\,(0,T),\,L^2(\Omega)\right]},\ s^4 \left\| I_e - \hat{I}_e \right\|^4_{L^\infty\left[\,(0,T),\,L^2(\Omega)\right]} \right) \quad \Longrightarrow \tag{5.21}$$

$$\lim_{s\to 0+0} \frac{1}{s} \left\| \Phi_{\mathrm{tr}}(s) - \hat{\Phi}_{\mathrm{tr}} \right\|^2_{\tilde{X}_1} \tag{5.22}$$

$$\leqslant \lim_{s\to 0+0} C \cdot \mathrm{Max}\left(s \left\| I_e - \hat{I}_e \right\|^2_{L^\infty\left[\,(0,T),\,L^2(\Omega)\right]},\ s^3 \left\| I_e - \hat{I}_e \right\|^4_{L^\infty\left[\,(0,T),\,L^2(\Omega)\right]} \right) = 0.$$

□

• **Step 3.** By Theorems 4.1 and 4.2, in correspondence to $(\hat{\Phi}_{\mathrm{tr}}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)$, there exist functions $P_1 \in \left(L^{4/3}\left[\,(0,T),\,\left(W^{1,2}(\Omega)\right)^*\right]\right)^* = L^4\left[\,(0,T),\,W^{1,2}(\Omega)\right]$, $P_2 \in \left(L^2\left[\,(0,T),\,W^{1,2}(\Omega)\right]\right)^* = L^2\left[\,(0,T),\,W^{1,2}(\Omega)\right]$ with $\int_\Omega P_2(x,t)\,\mathrm{d}x = 0$ for almost all $t \in (0,T)$ and $P_3 \in \left(L^2\left[\,(0,T),\,\left(L^2(\Omega)\right)^*\right]\right)^* = L^2(\Omega_T)$ satisfying the system (4.8)–(4.10) as weak solutions. Consequently, P_1, P_2 and P_3 solve the adjoint equations (4.5)–(4.7) together with $P_4 = -P_1(\,\cdot\,,0)$ and $P_5 = -P_3(\,\cdot\,,0)$. With these functions, we may derive the following estimates:

Lemma 5.7. *The following estimates hold true:*

$$\lim_{s\to 0+0} \frac{1}{s} \Big\langle\, P_1\,,\, D_{\Phi_{\rm tr}}\, E_1(\hat{\Phi}_{\rm tr},\hat{\Phi}_e,\hat{W})\,(\Phi_{\rm tr}(s)-\hat{\Phi}_{\rm tr}) + D_{\Phi_e}\, E_1(\hat{\Phi}_{\rm tr},\hat{\Phi}_e,\hat{W})\,(\Phi_e(s)-\hat{\Phi}_e) + D_W\, E_1(\hat{\Phi}_{\rm tr},\hat{\Phi}_e,\hat{W})\,(W(s)-\hat{W})\,\Big\rangle \,=\, 0\,; \tag{5.23}$$

$$\lim_{s\to 0+0} \frac{1}{s} \Big\langle\, P_2\,,\, D_{\Phi_{\rm tr}}\, E_2(\hat{\Phi}_{\rm tr},\hat{\Phi}_e,\hat{I}_e)\,(\Phi_{\rm tr}(s)-\hat{\Phi}_{\rm tr}) + D_{\Phi_e}\, E_2(\hat{\Phi}_{\rm tr},\hat{\Phi}_e,\hat{I}_e)\,(\Phi_e(s)-\hat{\Phi}_e) + \Big\langle\, P_2\,,\, D_{I_e}\, E_2(\hat{\Phi}_{\rm tr},\hat{\Phi}_e,\hat{I}_e)\,(I_e-\hat{I}_e)\,\Big\rangle \,=\, 0\,; \tag{5.24}$$

$$\lim_{s\to 0+0} \frac{1}{s} \Big\langle\, P_3\,,\, D_{\Phi_{\rm tr}}\, E_3(\hat{\Phi}_{\rm tr},\hat{W})\,(\Phi_{\rm tr}(s)-\hat{\Phi}_{\rm tr}) + D_W\, E_3(\hat{\Phi}_{\rm tr},\hat{W})\,(W(s)-\hat{W})\,\Big\rangle \,=\, 0. \tag{5.25}$$

Proof. We restrict ourselves to the proof of (5.23), noting that (5.24) and (5.25) can be confirmed in a completely analogous manner. Due to our assumptions on the differentiability of r, the principal theorem of calculus in its Bochner integral version is applicable, *cf.* [3], page 68, (2.1.11). For the feasible solutions $(\Phi_{\rm tr}(s),\Phi_e(s),W(s),I_e(s))$ and $(\hat{\Phi}_{\rm tr},\hat{\Phi}_e,\hat{W},\hat{I}_e)$, we get from the first state equation in (P), (3.12):

$$\begin{aligned}
\mathfrak{o} \,=\, & E_1(\Phi_{\rm tr}(s),\Phi_e(s),W(s)) - E_1(\hat{\Phi}_{\rm tr},\hat{\Phi}_e,\hat{W}) \,=\, \int_0^1 D_{(\Phi_{\rm tr},\Phi_e,W)}\, E_1\big(\hat{\Phi}_{\rm tr}+\tau\,(\Phi_{\rm tr}(s)-\hat{\Phi}_{\rm tr})\,,\\
& \hat{\Phi}_e+\tau\,(\Phi_e(s)-\hat{\Phi}_e)\,,\, \hat{W}+\tau\,(W(s)-\hat{W})\big)\,(\Phi_{\rm tr}(s)-\hat{\Phi}_{\rm tr},\Phi_e(s)-\hat{\Phi}_e,W(s)-\hat{W})\,{\rm d}\tau \quad\Longrightarrow
\end{aligned} \tag{5.26}$$

$$\begin{aligned}
0 \,=\, & \Big\langle\, P_1\,,\, \int_0^1 \Big(D_{(\Phi_{\rm tr},\Phi_e,W)}\, E_1\big(\hat{\Phi}_{\rm tr}+\tau\,(\Phi_{\rm tr}(s)-\hat{\Phi}_{\rm tr})\,,\, \hat{\Phi}_e+\tau(\Phi_e(s)-\hat{\Phi}_e)\,,\, \hat{W}+\tau\,(W(s)-\hat{W})\big)\\
& \qquad (\Phi_{\rm tr}(s)-\hat{\Phi}_{\rm tr},\Phi_e(s)-\hat{\Phi}_e,W(s)-\hat{W})\\
& -\, D_{(\Phi_{\rm tr},\Phi_e,W)}\, E_1(\hat{\Phi}_{\rm tr},\hat{\Phi}_e,\hat{W})\,(\Phi_{\rm tr}(s)-\hat{\Phi}_{\rm tr},\Phi_e(s)-\hat{\Phi}_e,W(s)-\hat{W})\Big)\,{\rm d}\tau\,\Big\rangle\\
& +\, \Big\langle\, P_1\,,\, D_{(\Phi_{\rm tr},\Phi_e,W)}\, E_1(\hat{\Phi}_{\rm tr},\hat{\Phi}_e,\hat{W})\,(\Phi_{\rm tr}(s)-\hat{\Phi}_{\rm tr},\Phi_e(s)-\hat{\Phi}_e,W(s)-\hat{W})\,\Big\rangle
\end{aligned} \tag{5.27}$$

$$\begin{aligned}
& = \Big\langle\, P_1\,,\, \int_0^1 \Big(D_{\Phi_{\rm tr}}\, E_1(\hat{\Phi}_{\rm tr}+\tau\ldots,\hat{\Phi}_e+\tau\ldots,\hat{W}+\tau\ldots)\,(\Phi_{\rm tr}(s)-\hat{\Phi}_{\rm tr}) - D_{\Phi_{\rm tr}}\, E_1(\hat{\Phi}_{\rm tr},\hat{\Phi}_e,\hat{W})\,(\Phi_{\rm tr}(s)-\hat{\Phi}_{\rm tr})\\
& +\, D_{\Phi_e}\, E_1(\hat{\Phi}_{\rm tr}+\tau\ldots,\hat{\Phi}_e+\tau\ldots,\hat{W}+\tau\ldots)\,(\Phi_e(s)-\hat{\Phi}_e) - D_{\Phi_e}\, E_1(\hat{\Phi}_{\rm tr},\hat{\Phi}_e,\hat{W})\,(\Phi_e(s)-\hat{\Phi}_e)\\
& +\, D_W\, E_1(\hat{\Phi}_{\rm tr}+\tau\ldots,\hat{\Phi}_e+\tau\ldots,\hat{W}+\tau\ldots)\,(W(s)-\hat{W}) - D_W\, E_1(\hat{\Phi}_{\rm tr},\hat{\Phi}_e,\hat{W})\,(W(s)-\hat{W})\Big)\,{\rm d}\tau\,\Big\rangle\\
& +\, \Big\langle\, P_1\,,\, D_{\Phi_{\rm tr}}\, E_1(\hat{\Phi}_{\rm tr},\hat{\Phi}_e,\hat{W})(\Phi_{\rm tr}(s)-\hat{\Phi}_{\rm tr}) + D_{\Phi_e}\, E_1(\hat{\Phi}_{\rm tr},\hat{\Phi}_e,\hat{W})(\Phi_e(s)-\hat{\Phi}_e)\\
& \qquad + D_W\, E_1(\hat{\Phi}_{\rm tr},\hat{\Phi}_e,\hat{W})(W(s)-\hat{W})\,\Big\rangle.
\end{aligned} \tag{5.28}$$

By [24], page 133, Corollary 1, we have

$$\big|\,\Big\langle\, P_1\,,\, \int_0^1 (\ldots)\,{\rm d}\tau\,\Big\rangle\,\big| \,\leqslant\, \|\,P_1\,\|_{{\rm Z}_1^*}\cdot \Big\|\int_0^1 (\ldots)\,{\rm d}\tau\,\Big\|_{{\rm Z}_1} \,\leqslant\, \|\,P_1\,\|_{{\rm Z}_1^*}\cdot \int_0^1 \|\ldots\|_{{\rm Z}_1}\,{\rm d}\tau. \tag{5.29}$$

Consequently, for the first summand within (5.28), it holds that

$$\lim_{s\to 0+0} \frac{1}{s} \left| \left\langle P_1\,,\, \int_0^1 (\ldots)\,\mathrm{d}\tau \right\rangle \right| \leqslant \lim_{s\to 0+0} \| P_1 \|_{Z_1^*} \Big(\int_0^1 \| D_{\Phi_{\rm tr}} E_1(\hat\Phi_{\rm tr}+\tau\ldots, \hat\Phi_e+\tau\ldots, \hat W+\tau\ldots) \tag{5.30}$$

$$- D_{\Phi_{\rm tr}} E_1(\hat\Phi_{\rm tr}, \hat\Phi_e, \hat W) \|_{\mathcal{L}(\widetilde{X}_1, Z_1)} \frac{1}{s} \Big\| \Phi_{\rm tr}(s) - \hat\Phi_{\rm tr} \Big\|_{\widetilde{X}_1} \mathrm{d}\tau$$

$$+ \int_0^1 \Big\| D_{\Phi_e} E_1(\hat\Phi_{\rm tr}+\tau\ldots, \hat\Phi_e+\tau\ldots, \hat W+\tau\ldots,) - D_{\Phi_e} E_1(\hat\Phi_{\rm tr}, \hat\Phi_e, \hat W) \Big\|_{\mathcal{L}(X_2, Z_1)} \frac{1}{s} \Big\| \Phi_e(s) - \hat\Phi_e \Big\|_{X_2} \mathrm{d}\tau$$

$$+ \int_0^1 \Big\| D_W E_1(\hat\Phi_{\rm tr}+\tau\ldots, \hat\Phi_e+\tau\ldots, \hat W+\tau\ldots,) - D_W E_1(\hat\Phi_{\rm tr}, \hat\Phi_e, \hat W) \Big\|_{\mathcal{L}(\widetilde{X}_3, Z_1)} \frac{1}{s} \Big\| W(s) - \hat W \Big\|_{\widetilde{X}_3} \mathrm{d}\tau \Big)$$

$$\leqslant \lim_{s\to 0+0} \| P_1 \|_{Z_1^*} \Big(\int_0^1 L_1\,\tau \Big(\Big\| \Phi_{\rm tr}(s) - \hat\Phi_{\rm tr} \Big\|_{\widetilde{X}_1} + \Big\| \Phi_e(s) - \hat\Phi_e \Big\|_{X_2} + \Big\| W(s) - \hat W \Big\|_{\widetilde{X}_3} \Big) \frac{1}{s} \Big\| \Phi_{\rm tr}(s) - \hat\Phi_{\rm tr} \Big\|_{\widetilde{X}_1} \mathrm{d}\tau$$

$$+ \int_0^1 L_2\,\tau \Big(\Big\| \Phi_{\rm tr}(s) - \hat\Phi_{\rm tr} \Big\|_{\widetilde{X}_1} + \Big\| \Phi_e(s) - \hat\Phi_e \Big\|_{X_2} + \Big\| W(s) - \hat W \Big\|_{\widetilde{X}_3} \Big) \frac{1}{s} \Big\| \Phi_e(s) - \hat\Phi_e \Big\|_{X_2} \mathrm{d}\tau$$

$$+ \int_0^1 L_3\,\tau \Big(\Big\| \Phi_{\rm tr}(s) - \hat\Phi_{\rm tr} \Big\|_{\widetilde{X}_1} + \Big\| \Phi_e(s) - \hat\Phi_e \Big\|_{X_2} + \Big\| W(s) - \hat W \Big\|_{\widetilde{X}_3} \Big) \frac{1}{s} \Big\| W(s) - \hat W \Big\|_{\widetilde{X}_3} \mathrm{d}\tau \tag{5.31}$$

with Lipschitz constants L_1, L_2, L_3, whose existence is ensured by the twice continuous Fréchet differentiability of E_1 with respect to $\Phi_{\rm tr}$, Φ_e and W. With reference to Lemma 5.6, the estimate (5.31) may be continued as follows:

$$\lim_{s\to 0+0} \frac{1}{s} \left| \left\langle P_1\,,\, \int_0^1 (\ldots)\,\mathrm{d}\tau \right\rangle \right|$$

$$\leqslant \lim_{s\to 0+0} \| P_1 \|_{Z_1^*} \frac{1}{2} \big(L_1 + L_2 + L_3 \big) \frac{1}{s} \Big(\Big\| \Phi_{\rm tr}(s) - \hat\Phi_{\rm tr} \Big\|_{\widetilde{X}_1} + \Big\| \Phi_e(s) - \hat\Phi_e \Big\|_{X_2} + \Big\| W(s) - \hat W \Big\|_{\widetilde{X}_3} \Big)^2 \tag{5.32}$$

$$\leqslant \lim_{s\to 0+0} \| P_1 \|_{Z_1^*} C \Big(\frac{1}{s} \Big\| \Phi_{\rm tr}(s) - \hat\Phi_{\rm tr} \Big\|_{\widetilde{X}_1}^2 + \frac{1}{s} \Big\| \Phi_e(s) - \hat\Phi_e \Big\|_{X_2}^2 + \frac{1}{s} \Big\| W(s) - \hat W \Big\|_{\widetilde{X}_3}^2 \Big) = 0\,, \tag{5.33}$$

and this implies the first of the claimed relations, namely

$$\lim_{s\to 0+0} \frac{1}{s} \Big\langle P_1\,,\, D_{\Phi_{\rm tr}} E_1(\hat\Phi_{\rm tr}, \hat\Phi_e, \hat W)\,(\Phi_{\rm tr}(s) - \hat\Phi_{\rm tr}) + D_{\Phi_e} E_1(\hat\Phi_{\rm tr}, \hat\Phi_e, \hat W)\,(\Phi_e(s) - \hat\Phi_e) \tag{5.34}$$

$$+ D_W E_1(\hat\Phi_{\rm tr}, \hat\Phi_e, \hat W)\,(W(s) - \hat W) \Big\rangle = 0.$$

From the second and third state equations (3.13) and (3.14), the limit relations (5.24) and (5.25) can be derived in a completely analogous way. □

Since $\Phi_{\rm tr}(s)$ and $W(s)$ take the same initial values as $\hat\Phi_{\rm tr}$ and $\hat W$, respectively, it holds further that

$$\lim_{s\to 0+0} \frac{1}{s} \Big\langle P_4\,,\, D_{\Phi_{\rm tr}} E_4(\hat\Phi_{\rm tr})\,(\Phi_{\rm tr}(s) - \hat\Phi_{\rm tr}) \Big\rangle = \lim_{s\to 0+0} \frac{1}{s} \Big\langle P_5\,,\, D_W E_5(\hat W)\,(W(s) - \hat W) \Big\rangle = 0. \tag{5.35}$$

• **Step 4.** *The first variation of the objective.* Choose now $\varepsilon > 0$ small enough in order to ensure that the difference $F(\Phi_{\rm tr}(s), \Phi_e(s), W(s), I_e(s)) - F(\hat\Phi_{\rm tr}, \hat\Phi_e, \hat W, \hat I_e)$ of the objective values is nonnegative for all quadruples $(\Phi_{\rm tr}(s), \Phi_e(s), W(s), I_e(s))$ belonging to the closed ball $U_\varepsilon(\hat\Phi_{\rm tr}, \hat\Phi_e, \hat W, \hat I_e)$ defined in (5.9). As a consequence of our assumptions about the integrand r, the first variation may be written as

$$\begin{aligned} 0 &\leqslant \delta^+ F(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)\,(\Phi_{\rm tr}(1) - \hat{\Phi}_{\rm tr}, \Phi_e(1) - \hat{\Phi}_e, W(1) - \hat{W}, I_e - \hat{I}_e) \\ &= \lim_{s\to 0+0} \frac{1}{s} \Big(F(\Phi_{\rm tr}(s), \Phi_e(s), W(s), I_e(s)) - F(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e) \Big) \qquad (5.36) \\ &= \lim_{s\to 0+0} \frac{1}{s} \Big(D_{\Phi_{\rm tr}} F(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)\,(\Phi_{\rm tr}(s) - \hat{\Phi}_{\rm tr}) + D_{\Phi_e} F(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)\,(\Phi_e(s) - \hat{\Phi}_e) \qquad (5.37) \\ &\qquad + D_W F(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)\,(W(s) - \hat{W}) + D_{I_e} F(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)\,(I_e(s) - \hat{I}_e) \Big). \end{aligned}$$

Together with Lemma 5.7 and (5.35), we obtain

$$\begin{aligned} 0 \leqslant \lim_{s\to 0+0} \frac{1}{s} \Big(& D_{\Phi_{\rm tr}} F(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)\,(\Phi_{\rm tr}(s) - \hat{\Phi}_{\rm tr}) \qquad (5.38) \\ & + \big\langle P_1\,,\, D_{\Phi_{\rm tr}} E_1(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W})\,(\Phi_{\rm tr}(s) - \hat{\Phi}_{\rm tr}) \big\rangle + \big\langle P_2\,,\, D_{\Phi_{\rm tr}} E_2(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{I}_e)\,(\Phi_{\rm tr}(s) - \hat{\Phi}_{\rm tr}) \big\rangle \\ & + \big\langle P_3\,,\, D_{\Phi_{\rm tr}} E_3(\hat{\Phi}_{\rm tr}, \hat{W})\,(\Phi_{\rm tr}(s) - \hat{\Phi}_{\rm tr}) \big\rangle + \big\langle P_4\,,\, D_{\Phi_{\rm tr}} E_4(\hat{\Phi}_{\rm tr})\,(\Phi_{\rm tr}(s) - \hat{\Phi}_{\rm tr}) \big\rangle \\ & + D_{\Phi_e} F(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)\,(\Phi_e(s) - \hat{\Phi}_e) \\ & + \big\langle P_1\,,\, D_{\Phi_e} E_1(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W})\,(\Phi_e(s) - \hat{\Phi}_e) \big\rangle + \big\langle P_2\,,\, D_{\Phi_e} E_2(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{I}_e)\,(\Phi_e(s) - \hat{\Phi}_e) \big\rangle \\ & + D_W F(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)\,(W(s) - \hat{W}) \\ & + \big\langle P_1\,,\, D_W E_1(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W})\,(W(s) - \hat{W}) \big\rangle + \big\langle P_2\,,\, D_W E_2(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{I}_e)\,(W(s) - \hat{W}) \big\rangle \\ & + \big\langle P_3\,,\, D_W E_3(\hat{\Phi}_{\rm tr}, \hat{W})\,(W(s) - \hat{W}) \big\rangle + \big\langle P_5\,,\, D_W E_5(\hat{W})\,(W(s) - \hat{W}) \big\rangle \\ & + D_{I_e} F(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)\,(I_e(s) - \hat{I}_e) + \big\langle P_2\,,\, D_{I_e} E_2(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{I}_e)\,(I_e - \hat{I}_e) \big\rangle \Big) \end{aligned}$$

where the first three parts vanish since P_1, P_2, P_3 together with $P_4 = -P_1(\,\cdot\,,0)$ and $P_5 = -P_3(\,\cdot\,,0)$ solve the adjoint equations (4.5)–(4.7). Note that, by Section 4.1. above, these equations take the claimed form. Consequently, we arrive at

$$\begin{aligned} 0 &\leqslant \lim_{s\to 0+0} \frac{1}{s} \Big(D_{I_e} F(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)\,(I_e(s) - \hat{I}_e) + \big\langle P_2\,,\, D_{I_e} E_2(\hat{\Phi}_{\rm tr}, \hat{\Phi}_e, \hat{I}_e)\,(I_e - \hat{I}_e) \big\rangle \Big) \qquad (5.39) \\ &= \int_0^T \int_\Omega \Big(\mu\,\hat{I}_e - P_2 \Big) \cdot \big(I_e - \hat{I}_e \big)\,{\rm d}x\,{\rm d}t = \int_0^T \int_\Omega \Big(\mu\,\hat{I}_e - Q\,P_2 \Big) \cdot \big(I_e - \hat{I}_e \big)\,{\rm d}x\,{\rm d}t \qquad (5.40) \end{aligned}$$

for arbitrary $I_e \in \mathcal{C}$. Since I_e and $\hat{I}_e$ vanish outside $\Omega_{\rm con} \times [\,0\,,\,T\,]$, this confirms the claimed optimality condition (5.3), and the proof is complete.

Proof of Corollary 5.3. Using the representations $I_e = Q\,I$ and $\hat{I}_e = Q\,\hat{I}$, inequality (5.40) may be rewritten as

$$\begin{aligned} 0 &\leqslant \int_0^T \int_\Omega \Big(\mu \cdot Q\,\hat{I} - Q\,P_2 \Big) \cdot \big(Q\,I - Q\,\hat{I} \big)\,{\rm d}x\,{\rm d}t = \int_0^T \int_\Omega \Big(\mu \cdot Q\,\hat{I} - Q\,P_2 \Big) \cdot \big(I - \hat{I} \big)\,{\rm d}x\,{\rm d}t \qquad (5.41) \\ &= \int_0^T \int_{\Omega_{\rm con}} \Big(\mu \cdot Q\,\hat{I} - Q\,P_2 \Big) \cdot \big(I - \hat{I} \big)\,{\rm d}x\,{\rm d}t \qquad (5.42) \\ &\qquad \forall\, I \in L^\infty\big[\,(\,0\,,\,T\,)\,,\,L^2(\Omega)\,\big] \ \textit{with} \ {\rm supp}\,(I) \subseteq \Omega_{\rm con} \times [\,0\,,\,T\,] \ \textit{and} \ |\,I(x,t)\,| \leqslant R \ \ (\forall)\,(x,t) \in \Omega_T. \end{aligned}$$

To (5.42), we may apply a Lebesgue point argument analogous to [11], page 1541, Proof of Corollary 3.6., in order to get

$$\Big(\mu \cdot Q\,\hat{I}(x_0,t_0) - Q\,P_2(x_0,t_0) \Big) \cdot \big(\eta_0 - \hat{I}(x_0,t_0) \big) \geqslant 0 \ \ \forall\, \eta_0 \in [\,-R\,,\,R\,] \ \ (\forall)\,(x_0,t_0) \in \Omega_{\rm con} \times [\,0\,,\,T\,], \qquad (5.43)$$

and this implies the conditions (5.4) and (5.5). □

Proof of Corollary 5.4. This is implied by (5.5) since $Q\,P_2\,\big|\,\Omega_{\rm con} \in L^2\big[\,(\,0\,,\,T\,)\,,\,W^{1,2}(\Omega_{\rm con})\,\big]$ together with $P_2 \in L^2\big[\,(\,0\,,\,T\,)\,,\,W^{1,2}(\Omega)\,\big]$. □

Proof of Corollary 5.5. We can follow the Proof of Theorem 5.2 where only in (5.36), (5.38) and (5.39) the minorization by 0 must be deleted. □

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