Drift-Diffusion in Electrochemistry: Thresholds for Boundary Flux and Discontinuous Optical Generation

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Abstract

We consider an extension of the classical drift-diffusion model, which incorporates thermodynamic switching rules for generation and boundary flux. The motivation is the important case of the splitting of water molecules upon photonic irradiation of a semiconductor electrode located in an electrochemical cell. The solid state electrode forms the spatial domain of the model. The rules are motivated by the fact that the valence band of the semiconductor, which supplies positive charge to solution, has to be located at a lower energy level than the electrochemical potential of O_2 evolution in solution, and the conduction band, which supplies electrons to solution, has to be positioned at a higher energy level than the electrochemical potential of H_2 evolution. This defines thresholds in terms of electrochemical potentials before boundary flux is activated. The optical generation rate is affected, due to increased carrier relaxation time, when these thresholds are crossed, and may be discontinuous. We thus consider a self-consistent model, in which 'switching' occurs only in principal variables. The steady-state model is considered, and trapping regions are derived for the solutions.

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1 Introduction

Electrochemical cells provide examples of electrodiffusion with convection and generation. Recent advanced models at small scale have attempted to model solar 'water splitting' in these cells as sources of energy through creation of hydrogen and oxygen [5, 6, 9]. The cells possess one or more electrodes of porous semiconductor material, which surrender electrons and holes to aqueous solution when light stimulates the electrodes on their contact portions, inducing potential biases and generation of electron/hole pairs. At a semiconductor electrode which functions as an anode (anodic oxidation), oxygen and intermediate hydrogen ions are generated. These recombine in solution (cathodic reduction) with electrons to form hydrogen products. A significant factor in the process [6, p. 35] is that the valence band of the semiconductor has to be located at a lower energy level than the electrochemical potential of O_2 evolution, and the conduction band has to be positioned at a higher energy level than the electrochemical potential of H_2 evolution. One can characterize the electrode interface with solution as inert unless these thermodynamic conditions are satisfied.

We consider a model of drift-diffusion for a semiconductor electrode with anode and cathode interfaces with solution (see [5] for an illustration of such a device) in which 'thermodynamic rules' may be used to establish thresholds or switching for carrier boundary flux and for carrier generation in the conservation subsystem. This is coupled self-consistently to the electrostatic equation. The discontinuous switching requires mathematical tools of analysis, not previously applied to drift-diffusion systems. These include multivalued subdifferential mappings in convex analysis, previously studied for equations. We obtain the system solutions in trapping regions, which constitute generalized maximum principles. Our results are restricted to mathematical well-posedness, and we shall employ the Slotboom variables in the analysis. If the electrode is active as both anode and cathode, then the model reduces to one of standard type.

1.1 The Standard Model

For background, we present the standard isothermal drift-diffusion model employed in solid state physics, the well-known Van Roosbroeck model, introduced in 1950 [8]. However, we describe it in the setting of the electrochemical cell. The pertinent modifications will be presented in the following sections. We denote the region occupied by the electrode as $\bar{\Omega}$, with the boundary partitioned into a section Γ, bounding the aqueous solution, and the section $\partial\Omega \setminus \Gamma$ which forms an electrical contact region for illumination and grounding. In terms of the conduction electron density n, the hole density p, and the electrostatic potential u, the system is given by:

$$-\nabla\cdot[\epsilon\nabla u] + n - p - k_1 = 0, \quad (1)$$
$$-\nabla\cdot[\mu_n n\nabla u - D_n\nabla n] = R - G, \quad (2)$$
$$-\nabla\cdot[\mu_p p\nabla u + D_p\nabla p] = G - R. \quad (3)$$

The function $k_1 = k_1(x)$ denotes the semiconductor doping, and the dielectric satisfies $\epsilon(x) \geq \epsilon_0 > 0$, and is a function of the material and therefore of the position x only. Similar considerations apply to the mobility and diffusion coefficients, and we employ the Einstein relations and units in which the thermal voltage satisfies $kT/e = 1$. Accordingly, the expressions

$$J_n = -\mu_n[n\nabla u - \nabla n], \quad J_p = -\mu_p[p\nabla u + \nabla p],$$

denote the normalized electron and hole current densities, respectively, obtained by division by the charge modulus e, where μ_n, μ_p are mobility coefficients. We have also employed a generation/recombination term, $G - R$, defined below, suited to optical generation. For the model considered here, net recombination is negligible: $R \equiv 0$. The system is augmented by boundary conditions of mixed type, including Robin boundary conditions on $\Gamma \subset \partial\Omega$ and Dirichlet boundary conditions on the contact portions $\partial\Omega \setminus \Gamma$.

The statistical properties of the electron and hole distributions [2] allow exponential representations when Fermi-Dirac statistics are approximated by classical Boltzmann statistics. Typically, when all that is desired is simple mathematical existence for the Van Roosbroeck model, the physical significance of the statistical approximation is unimportant: it defines a change of dependent variable. This was observed in [3], which provides several references for the physical background of the standard model. However, when thermodynamical issues are relevant, the new variables v and w must be interpreted in terms of the conduction and valence band potentials of the semiconductor. We may then express n and p via density of state units, assumed the same here for electrons and holes, as $n = \exp(u - v)$ and $p = \exp(w - u)$. The system (1), (2), and (3) is rewritten:

$$-\nabla\cdot[\epsilon\nabla u] + e^{u-v} - e^{w-u} - k_1 = 0, \quad (4)$$
$$-\nabla\cdot[\mu_n e^{u-v}\nabla v] = -G \quad (5)$$
$$-\nabla\cdot[\mu_p e^{w-u}\nabla w] = G. \quad (6)$$

G is an appropriate positive function, defined by the generation process. Finally, we introduce the new variables, $V = e^{-v}$, $W = e^{w}$, known in the literature as Slotboom variables. Since the mobility functions play no real role in the analysis, we shall assume them to be constant and normalized to one. The system assumes the form,

$$-\nabla\cdot[\epsilon\nabla u] + Ve^{u} - We^{-u} - k_1 = 0, \tag{7}$$

$$-\nabla\cdot[e^{u}\nabla V] - G(x,u,V,W) = 0, \tag{8}$$

$$-\nabla\cdot[e^{-u}\nabla W] - G(x,u,V,W) = 0. \tag{9}$$

We will discuss the form of G in the next section. For simplicity, we take k_1 and ϵ to be bounded measurable functions. Note that

$$J_n = e^{u}\nabla V,\ J_p = -e^{-u}\nabla W, \tag{10}$$

in these variables.

2 Formulation of the Electrode Switching Model

In this model, we incorporate the thermodynamic rules, which impose thresholds on the flux boundary conditions for V and W. We also impose switching regions for generation in the principal variables, i. e. , V in (8) and W in (9). We begin with the boundary conditions.

2.1 Boundary Conditions

We consider the Dirichlet boundary conditions for the model. We shall initially express these in terms of u, v, w, as is traditional. Let $\Sigma_D = \partial\Omega \setminus \Gamma$. On this set, the potential bias u_D is a state variable, whose value causes the device to assume different possible state configurations. It includes intrinsic contributions which vary according to certain defining properties of the contact. The principal contribution is photonic, i. e. , light induced. The variables v_D and w_D have typically been selected to achieve thermal equilibrium and charge neutrality on ohmic contacts in solid state modeling. Here, however, the constraints required for anodic and cathodic reactions require compatible selection of these values as determined by the trapping region.

On Γ, which includes both the anodic and cathodic interfaces of the electrode, we shall specify a zero electric flux, but we must allow nonzero electron and hole current fluxes J_n, J_p, respectively, expressed in terms of threshold switching values. We assume that the outward normal current densities are proportional to the net charge present, i. e. , proportional to $-(n - n_0)$ and $p - p_0$, respectively, where n_0, p_0 represent stable charge populations, possibly spatially dependent. By (10), we have for the boundary flux expressions:

$$-\frac{\partial V}{\partial \nu} = c_V(V - e^{-u}n_0)(1 - \chi_{\mathcal{E}_V}), \; -\frac{\partial W}{\partial \nu} = c_W(W - e^{u}p_0)(1 - \chi_{\mathcal{E}_W}). \quad (11)$$

Here, c_V, c_W are positive constants, $\mathcal{E}_V = [V_0, \infty)$ and $\mathcal{E}_W = [W_0, \infty)$ are closed interval ranges for V and W, respectively, and $\chi : \mathbb{R} \to \mathbb{R}$ denotes the characteristic function. Since we require the right hand side of both expressions to be monotone in their principal variables, we impose the flux hypotheses:

$$V - e^{-u}n_0 \leq 0, \; V \in [0, V_0], \; W - e^{u}p_0 \leq 0, \; W \in [0, W_0]. \quad (12)$$

Here, $V_0 = \exp(-v_0), W_0 = \exp(w_0)$, for the hydrogen/oxygen evolution potentials v_0, w_0. We assume that v_0, w_0 are given real constants. The inequalities (12) are satisfied if

$$V_0 - e^{-u_{\max}}n_0 \leq 0, \; W_0 - e^{u_{\min}}p_0 \leq 0. \quad (13)$$

Physically, the larger that n_0, p_0 are (relative to unity), the easier it is for the electric potential to be captured in the allowable anodic/cathodic window.

2.2 The System

Prior to displaying the system, we briefly discuss the (optical) generation hypothesis for the rate. The steady state hypothesis [7, pp. 106–109] characterizes the excess electron density δn and excess hole density δp via the simple relations $\delta n = g_{\rm op}\tau_n, \; \delta p = g_{\rm op}\tau_p$, where $g_{\rm op}$ is the steady-state optical generation rate and τ_n, τ_p are carrier relaxation times associated with recombination, and are extended when intermediate carrier trapping occurs. For electrons and holes, we shall permit two different generation rates for the term $g_{\rm op}$, depending on the relation of V, W to the thermodynamic switching levels V_0, W_0. If $V \leq V_0$, electron boundary flux is activated, and we expect reduced trapping of electrons. Similarly for holes if $W \leq W_0$. One expects the relaxation times to be considerably shorter (smaller) than when $V > V_0$ or $W > W_0$. If the respective products representing $\delta n, \delta p$ are to remain invariant as a steady-state hypothesis, the rates must accommodate accordingly. We therefore assume that the optical rate, given by $g_{\rm op} = G > 0$ in the thermodynamic ranges, may *discontinuously* decrease outside the thermodynamic ranges. For mathematical simplicity, we assume that $g_{\rm op}$ discontinuously decreases to zero. The new system becomes

$$\begin{aligned} -\nabla\cdot[\epsilon\nabla u] + Ve^{u} - We^{-u} - k_1 &= 0, && (14)\\ -\nabla\cdot[e^{u}\nabla V] + f_1(u, V, W) &= 0, && (15)\\ -\nabla\cdot[e^{-u}\nabla W] + f_2(u, V, W) &= 0, && (16)\end{aligned}$$

where the generation rates are expressed via

$$f_1(u, V, W) = (\chi_{\mathcal{E}_V} - 1)G(u), \tag{17}$$

$$f_2(u, V, W) = (\chi_{\mathcal{E}_W} - 1)G(u). \tag{18}$$

As expected from physical considerations, G depends on u and is positive; we assume a locally Lipschitz continuous dependence. The discontinuity is expressed by the first factors.

3 Gradient Equations with Nonlinear Flux

Most devices have *piecewise* C^1 boundaries. For simplicity, however, we treat the global C^1 case. This section examines the individual equations of our systems. Thus, let $\Omega \subset \mathbb{R}^N$ be a bounded domain with C^1-boundary $\partial\Omega$, and $\Gamma \subset \partial\Omega$ be such that $\Sigma_D = \partial\Omega \setminus \Gamma$ is a relatively open C^1-portion of $\partial\Omega$ with positive surface measure. Consider the boundary value problem (BVP)

$$-\nabla \cdot [a(x)\nabla u] + f(x, u) \;=\; 0 \;\text{ in }\; \Omega, \tag{19}$$

$$u = u_D \;\text{ on }\Sigma_D, \quad \frac{\partial u}{\partial \nu} + g(x, u) \;=\; 0 \;\text{ on }\; \Gamma, \tag{20}$$

where $a \in L^\infty(\Omega)$ with $a(x) \geq \mu > 0$, and $\partial/\partial\nu$ denotes the outward conormal derivative at Γ. Let $H := W^{1,2}(\Omega)$ denote the usual (real) Sobolev space, and let $H_0 \subset H$ be the subspace of H defined by

$$H_0 = \{u \in H \mid \gamma u = 0 \;\text{ on }\; \Sigma_D\},$$

where $\gamma : H \to L^2(\partial\Omega)$ is the trace operator which is linear and compact. The corresponding dual spaces are denoted by H^* and H_0^*. It is known that $\|u\|_{H_0}^2 = \int_\Omega |\nabla u|^2\, dx$ defines an equivalent norm on the subspace H_0. We introduce the natural partial ordering in $L^2(\Omega)$, that is $u \leq w$ if and only if $w-u$ belongs to the positive cone $L_+^2(\Omega)$ of all nonnegative elements of $L^2(\Omega)$, which also induces a partial ordering in the Sobolev space H. If $u, w \in H$ and $u \leq w$, then $[u, w] = \{v \in H \mid u \leq v \leq w\}$ denotes the order interval formed by u and w. We assume the boundary values u_D to be the restriction of a function $\tilde{u}_D \in H$, i.e., $\tilde{u}_D|_{\Sigma_D} = u_D$. Depending on the regularity of the nonlinearities f and g in (19) and (20), respectively, we treat in the following subsections two cases: Carathéodory type and discontinuous nonlinearities.

3.1 Carathéodory Type Nonlinearities

In this subsection we impose the following regularity and structure conditions on f and g. By a Carathéodory function, we mean measurability in the first argument for each value of the second, and continuity in the second argument for almost all values of the first. This guarantees measurability of superposition with so-called Baire functions.

(C1) $f : \Omega \times \mathbb{R} \to \mathbb{R}$ and $g : \Gamma \times \mathbb{R} \to \mathbb{R}$ are Carathéodory functions in their respective domains of definitions, and the functions $s \mapsto f(x, s)$ and $s \mapsto g(x, s)$ are increasing.

The weak formulation of the BVP (19), (20) reads as follows.

Definition 3.1. *$u \in H$ is called a solution of the BVP (19), (20) if*

(i) $u = u_D$ *on* Σ_D, *and*

(ii) $\int_\Omega a\nabla u\nabla\varphi\, dx + \int_\Gamma g(x, \gamma u)\gamma\varphi\, d\Gamma + \int_\Omega f(x, u)\varphi\, dx = 0,\ \forall\ \varphi \in H_0.$

Let us recall for convenience the notion of (weak) super- and subsolutions.

Definition 3.2. *$\bar{u} \in H$ is called a supersolution of the BVP (19), (20) if*

(i) $\bar{u} \geq u_D$ *on* Σ_D, *and*

(ii) $\int_\Omega a\nabla \bar{u}\nabla\varphi\, dx + \int_\Gamma g(x, \gamma \bar{u})\gamma\varphi\, d\Gamma + \int_\Omega f(x, \bar{u})\varphi\, dx \geq 0,$
$\forall\ \varphi \in H_0 \cap L^2_+(\Omega),$

Similarly, $\underline{u} \in H$ is a *subsolution* if the reversed inequalities in Definition 3.2 hold with $\bar{u}$ replaced by $\underline{u}$. We make the following additional hypotheses.

(C2) There exist a supersolution $\bar{u}$ and a subsolution $\underline{u}$ of the BVP (19), (20) such that $\underline{u} \leq \bar{u}$.

(C3) There is a $p \in L^2_+(\Omega)$ such that $|f(x, s)| \leq p(x)$ for a.e. $x \in \Omega$ and $s \in [\underline{u}(x), \bar{u}(x)]$.

(C4) There is a $q \in L^2_+(\Gamma)$ such that $|g(x, s)| \leq q(x)$ for a.e. $x \in \Gamma$ and $s \in [\gamma\underline{u}(x), \gamma\bar{u}(x)]$.

Remark 3.1. *A linear growth of f and g in the form $|f(x, s)| \leq p(x) + c|s|$, and $|g(x, s)| \leq q(x) + c|s|$ implies (C3) and (C4), respectively.*

The following lemma will later have application to the Poisson equation.

Lemma 3.1. *Under the hypotheses (C1)–(C4), the BVP (19), (20) has a uniquely defined solution u within the order interval $[\underline{u}, \bar{u}]$.*

Proof. To apply functional analytical methods we first transform the BVP (19), (20) to one with homogeneous Dirichlet data on Σ_D by the translation $u = w + \tilde{u}_D$. Thus u is a solution of (19), (20) if and only if $w \in H_0$ satisfies the following relation:

$$\int_\Omega a\nabla w \nabla\varphi\,dx + \int_\Gamma \tilde{g}(x,\gamma w)\gamma\varphi\,d\Gamma + \int_\Omega \tilde{f}(x,w)\varphi\,dx = \langle h,\varphi\rangle, \tag{21}$$

for all $\varphi \in H_0$, where

$$\begin{aligned} \tilde{g}(x,s) &= g(x,\gamma\tilde{u}_D(x)+s), \quad \tilde{f}(x,s) = f(x,\tilde{u}_D(x)+s), \quad \text{and} \\ \langle h,\varphi\rangle &= -\int_\Omega a\nabla\tilde{u}_D\nabla\varphi\,dx. \end{aligned} \tag{22}$$

Obviously, (22) defines a functional on H_0, i.e., $h \in H_0^*$. The transformed nonlinearities $\tilde{f}$ and $\tilde{g}$ preserve the structure and growth conditions of (C3) and (C4) with respect to the shifted order interval $[\underline{w},\bar{w}]$, where $\underline{w} = \underline{u} - \tilde{u}_D$ and $\bar{w} = \bar{u} - \tilde{u}_D$, and $\bar{w}$ and $\underline{w}$ are super- and subsolutions for the BVP in the variable w. Thus the existence of a solution $u \in H$ within $[\underline{u},\bar{u}]$ of the BVP (19), (20) is equivalent to the existence of a solution $w \in H_0$ within $[\underline{w},\bar{w}]$ of the transformed BVP given in its weak formulation by (21). To this end we associate with (21) the following auxiliary truncated problem:

$$\int_\Omega a\nabla w \nabla\varphi\,dx + \int_\Gamma \tilde{g}(x,T\gamma w)\gamma\varphi\,d\Gamma + \int_\Omega \tilde{f}(x,Tw)\varphi\,dx = \langle h,\varphi\rangle, \tag{23}$$

for all $\varphi \in H_0$, where T denotes the truncation operator defined by

$$Tw(x) = \begin{cases} \bar{w}(x), & w(x) > \bar{w}(x), \\ w(x), & \underline{w}(x) \le w(x) \le \bar{w}(x), \\ \underline{w}(x), & w(x) < \underline{w}(x). \end{cases} \tag{24}$$

Defining operators A, $\tilde{G}$, and $\tilde{F}$ as follows:

$$\begin{aligned} \langle Aw,\varphi\rangle &= \int_\Omega a\nabla w\nabla\varphi\,dx, \quad \langle \tilde{G}w,\varphi\rangle = \int_\Gamma \tilde{g}(x,T\gamma w)\gamma\varphi\,d\Gamma, \quad \text{and} \\ \langle \tilde{F}w,\varphi\rangle &= \int_\Omega \tilde{f}(x,Tw)\varphi\,dx, \quad \varphi \in H_0, \end{aligned}$$

we can rewrite the truncated problem (23) in the operator format,

$$\text{Find } w \in H_0: \quad \langle (A+\tilde{G}+\tilde{F})w,\varphi\rangle = \langle h,\varphi\rangle, \ \forall\, \varphi \in H_0. \tag{25}$$

One readily verifies that $A : H_0 \to H_0^*$ is continuous, bounded and strongly monotone. The continuity of the truncation operator $T : L^2(\Omega) \to [\underline{w},\bar{w}]$

and the compact embedding $H_0 \subset L^2(\Omega)$ imply that the superposition operator $w \mapsto \tilde{f}(\cdot, Tw)$ is a uniformly bounded and compact mapping from H_0 into $L^2(\Omega)$, and hence by the monotonicity of $s \mapsto \tilde{f}(x,s)$, it follows that $\tilde{F} : H_0 \to H_0^*$ is monotone, compact and uniformly bounded. The compactness of the trace operator γ together with continuity and boundedness of the truncation T considered as a mapping $T : L^2(\Gamma) \to [\gamma \underline{w}, \gamma \bar{w}]$, and the monotonicity of $s \mapsto \tilde{g}(x,s)$ imply that $\tilde{G} : H_0 \to H_0^*$ is monotone, compact and uniformly bounded. Thus $A + \tilde{G} + \tilde{F} : H_0 \to H_0^*$ is strongly monotone, continuous and bounded, which, by applying the main theorem on monotone operators (see, e.g., [11, Theorem 26.A]), yields the existence of a uniquely defined solution u of (25), and thus of the auxiliary problem (23). To complete the proof of the lemma, we need only show that the solution w of (23) lies within the order interval $[\underline{w}, \bar{w}]$, because then we have $Tw = w$, and thus $\tilde{f}(\cdot, Tw) = f(\cdot, w)$, and $\tilde{g}(\cdot, T\gamma w) = g(\cdot, \gamma w)$, which shows that w is in fact a solution of the transformed problem (21) within $[\underline{w}, \bar{w}]$. We shall show that $w \le \bar{w}$ only, since the proof of $\underline{w} \le w$ is similar. By assumption, $\bar{w}$ is a supersolution for (21), that is, $\bar{w} \ge 0$ on Σ_D, and the following inequality is satisfied:

$$\int_\Omega a \nabla \bar{w} \nabla \varphi \, dx + \int_\Gamma \tilde{g}(x, \gamma \bar{w}) \gamma \varphi \, d\Gamma + \int_\Omega \tilde{f}(x, \bar{w}) \varphi \, dx \ge \langle h, \varphi \rangle, \tag{26}$$

for all $\varphi \in H_0 \cap L_+^2(\Omega)$. Subtracting (26) from (23), and taking as special nonnegative testfunction $\varphi = (w - \bar{w})^+ := \max\{(w - \bar{w})^+, 0\}$, we obtain

$$\begin{aligned} &\textstyle\int_\Omega a \nabla (w - \bar{w}) \nabla (w - \bar{w})^+ \, dx \\ &+ \textstyle\int_\Gamma \left(\tilde{g}(x, T\gamma w) - \tilde{g}(x, \gamma \bar{w}) \right) \gamma (w - \bar{w})^+ \, d\Gamma \\ &+ \textstyle\int_\Omega \left(\tilde{f}(x, Tw) - \tilde{f}(x, \bar{w}) \right) (w - \bar{w})^+ \, dx \le 0. \end{aligned} \tag{27}$$

By using the truncation property of T, we see that the second and third integrals on the left-hand side of (27) are zero, so that we obtain

$$\mu \int_\Omega |\nabla (w - \bar{w})^+|^2 \, dx \le \int_\Omega a \, \nabla (w - \bar{w}) \nabla (w - \bar{w})^+ \, dx \le 0, \tag{28}$$

which yields $(w - \bar{w})^+ = 0$, and thus $w \le \bar{w}$. □

3.2 Discontinuous Nonlinearities

Motivated by the discontinuous BVP for V and W, we consider in this subsection the BVP (19), (20) under the following regularity, structure and growth conditions on f and g.

(D1) There exist super - and subsolutions $\bar{u}$ and $\underline{u}$ in the sense of Definition 3.2 such that $\underline{u} \leq \bar{u}$.

(D2) $f : \Omega \times \mathbb{R} \to \mathbb{R}$ and $g : \Gamma \times \mathbb{R} \to \mathbb{R}$ are Baire measurable in their respective domains of definitions, and the functions $s \mapsto f(x,s)$ and $s \mapsto g(x,s)$ are increasing.

(D3) There there exist functions $p \in L^2_+(\Omega)$ and $q \in L^2_+(\Gamma)$ such that $|f(x,s)| \leq p(x) + c_f|s|$, for all $(x,s) \in \Omega \times \mathbb{R}$,

$|g(x,s)| \leq q(x) + c_g|s|$, for all $(x,s) \in \Gamma \times \mathbb{R}$,

where c_f and c_g are some nonnegative constants.

Our goal is to prove a similar enclosure result as in the Carathéodory case. However, simple examples show that even monotonicity as assumed in (D2) does not ensure existence of solutions in the sense of Definition 3.1 within the order interval $[\underline{u}, \bar{u}]$. Therefore, we extend the notion of solution and instead of the BVP (19), (20) we consider its multivalued version in the form

$$-\nabla \cdot [a(x)\nabla u] + \alpha(x,u) \ni 0 \quad \text{in } \Omega, \tag{29}$$

$$u = u_D \quad \text{on } \Sigma_D, \qquad \frac{\partial u}{\partial \nu} + \beta(x,u) \ni 0 \quad \text{on } \Gamma, \tag{30}$$

where $\alpha : \Omega \times \mathbb{R} \to 2^{\mathbb{R}} \setminus \emptyset$ and $\beta : \Gamma \times \mathbb{R} \to 2^{\mathbb{R}} \setminus \emptyset$ denote the maximal monotone graphs generated by f and g, respectively, given by

$$\alpha(x,s) = [f(x,s-), f(x,s+)], \quad \beta(x,s) = [g(x,s-), g(x,s+)],$$

with $f(x,s\pm)$ and $g(x,s\pm)$ denoting the one-sided limits at s.

Definition 3.3. *The function $u \in H$ is a solution of the BVP (29), (30) if there is an $\xi \in L^2(\Omega)$ and an $\eta \in L^2(\Gamma)$ such that $u = u_D$ on Σ_D and*

(i) $\xi(x) \in \alpha(x, u(x))$ *for a.e.* $x \in \Omega$, $\eta(x) \in \beta(x, \gamma u(x))$ *for a.e.* $x \in \Gamma$,

(ii) $\langle Au + \xi + \gamma^*\eta, \varphi \rangle = 0, \ \forall \ \varphi \in H_0$,

where $\gamma^* : L^2(\Gamma) \to H_0^*$ denotes the adjoint operator to γ, and

$$\langle \xi, \varphi \rangle = \int_\Omega \xi(x)\, \varphi(x)\, dx, \quad \langle \gamma^*\eta, \varphi \rangle = \int_\Gamma \eta(x)\, \gamma\varphi(x)\, d\Gamma, \quad \varphi \in H_0.$$

To solve the BVP (29), (30) we again perform the translation $u = w + \tilde{u}_D$ to get homogeneous boundary values on Σ_D, which yields

$$-\nabla \cdot [a(x)\nabla w] + \tilde{\alpha}(x, w) \ \ni \ h \ \text{ in } \ \Omega, \tag{31}$$

$$w = 0 \ \text{ on } \Sigma_D, \quad \frac{\partial(w + \tilde{u}_D)}{\partial \nu} + \tilde{\beta}(x, w) \ \ni \ 0 \ \text{ on } \ \Gamma, \tag{32}$$

where $h \in H_0^*$ is given by $\langle h, \varphi\rangle = -\langle A\tilde{u}_D, \varphi\rangle$, and $\tilde{\alpha}$, $\tilde{\beta}$ are the shifted maximal monotone graphs. By using convex analysis calculus, one can show that the BVP (31), (32) is equivalent to the following variational inequality: Find $w \in H_0$ such that for all $\varphi \in H_0$ the following holds

$$\langle Aw, \varphi - w\rangle + J(\varphi) - J(w) + (\Phi \circ \gamma)(\varphi) - (\Phi \circ \gamma)(w) \geq \langle h, \varphi - w\rangle, \tag{33}$$

where the functionals $J : L^2(\Omega) \to \mathbb{R}$ and $\Phi : L^2(\Gamma) \to \mathbb{R}$ given by,

$$J(w) = \int_\Omega \Big(\int_0^{w(x)} \tilde{f}(x, s)\, ds \Big) dx, \quad \Phi(w) = \int_\Gamma \Big(\int_0^{w(x)} \tilde{g}(x, s)\, ds \Big) d\Gamma,$$

are convex and locally Lipschitz continuous. The existence of a unique solution of the variational inequality (33), and thus of the BVP (29), (30), is an immediate consequence of the strong monotonicity of the operator $A : H_0 \to H_0^*$ in the sense of Browder and the fact that $w \mapsto J(w) + (\Phi\circ\gamma)(w)$ is convex and continuous. Hypothesis (D1) permits the following comparison result.

Lemma 3.2. *Let hypotheses (D1)–(D3) be satisfied. Then the uniquely defined solution u of the multivalued BVP (29), (30) satisfies $\underline{u} \leq u \leq \bar{u}$.*

Proof. We shall show $u \leq \bar{u}$ only, since the inequality $\underline{u} \leq u$ can be proved similarly. Denote $\bar{\xi} = f(\cdot, \bar{u})$ and $\bar{\eta} = g(\cdot, \gamma\bar{u})$. Then by Definition 3.2 the supersolution $\bar{u}$ satisfies $\bar{u} \geq u_D$ on Σ_D and

$$\langle A\bar{u} + \bar{\xi} + \gamma^*\bar{\eta}, \varphi\rangle \geq 0, \ \forall \ \varphi \in H_0 \cap L_+^2(\Omega). \tag{34}$$

In particular, we have $\bar{\xi}(x) \in \alpha(x, \bar{u}(x))$ and $\bar{\eta}(x) \in \beta(x, \gamma\bar{u}(x))$ so that by subtracting (34) from relation (ii) of Definition 3.3 we get

$$\langle A(u - \bar{u}) + (\xi - \bar{\xi}) + (\gamma^*\eta - \gamma^*\bar{\eta}, \varphi\rangle \leq 0, \ \forall \ \varphi \in H_0 \cap L_+^2(\Omega). \tag{35}$$

With the nonnegative testfunction $\varphi = (u - \bar{u})^+$ in (35), we obtain via the maximal monotonicity of α and β,

$$0 \leq \mu \|(u - \bar{u})^+\|_{H_0} \leq \langle A(u - \bar{u}), (u - \bar{u})^+\rangle \leq 0,$$

which implies $(u - \bar{u})^+ = 0$, and thus $u \leq \bar{u}$. $\square$

4 System Analysis for the Model

If $U = (u_0, u_1, u_2) := (u, V, W)$, and $U_D = (u_{0,D}, u_{1,D}, u_{2,D} := (u_D, e^{-v_D}, e^{w_D})$, then the BVP for the model can be written in a unified way as ($k = 0, 1, 2$):

$$-\nabla \cdot [a_k(x, u_0)\nabla u_k] + f_k(x, U) \;=\; 0, \quad \text{in} \quad \Omega, \tag{36}$$

$$u_k = u_{k,D} \quad \text{on} \quad \Sigma_D, \; \frac{\partial u_k}{\partial \nu} + g_k(x, U) \;=\; 0, \quad \text{on} \quad \Gamma, \tag{37}$$

where $f_0(x, U) = u_1 e^{u_0} - u_2 e^{-u_0} - k_1(x)$ is a Carathéodory function and increasing in u_0 for nonnegative u_1, and u_2. Because $G(u) > 0$ the functions f_1 and f_2 given by (17) and (18) are discontinuous and increasing with respect to their principal argument. We further have $g_0 = 0$, and $g_1,\; g_2$ as given by (11) are discontinuous with respect to their principal argument and are monotone provided the following flux hypothesis holds.

Flux hypothesis

$$u_1 - e^{-u_0} n_0 \le 0, \text{ if } u_1 \le V_0; \; u_2 - e^{u_0} p_0 \le 0, \text{ if } u_2 \le W_0.$$

Later, we will give conditions, which very naturally imply this hypothesis, in terms of the trapping region. The coefficients of the elliptic operators are given by $a_0(x, u_0) = \epsilon(x),\; a_1(x, u_0) = e^{u_0}$, and $\; a_2(x, u_0) = e^{-u_0}$. We note that the coefficient a_0 does not depend on the unknown u_0 which stands for the potential u. Let $X = [H]^3$, $X_0 = [H_0]^3$, and $Y = (L^2(\Omega))^3$ be equipped with componentwise partial ordering. Define the following operators for $k = 0, 1, 2$:

$$\begin{aligned}
A_k(u_0) \;&:\; H \to H_0^*, \;\; \langle A_k(u_0)u_k, \varphi\rangle = \int_\Omega a_k(x, u_0)\nabla u_k \,\nabla\varphi \, dx, \\
F_k(U) \;&:\; Y \to H_0^*, \;\; \langle F_k(U), \varphi\rangle = \int_\Omega f_k(x, U)\, \varphi \, dx, \\
(G_k \circ \gamma)(U) \;&:\; X \to H_0^*, \;\; \langle (G_k \circ \gamma)(U), \varphi\rangle = \int_\Gamma g_k(x, \gamma u_0, \gamma u_k)\gamma\varphi \, d\Gamma,
\end{aligned}$$

for $\varphi \in H_0$. We denote $A(U) = (A_0(u_0)u_0, A_1(u_0)u_1, A_2(u_0)u_2)$ and accordingly the vector operators $F(U)$ and $(G \circ \gamma)(U)$, where $\gamma U = (\gamma u_0, \gamma u_1, \gamma u_2)$. The weak formulation of the system (36), (37), describing our model, then reads as follows.

Definition 4.1. *$U \in X$ is a weak solution of (36), (37) if it satisfies*

$$U = U_D \;\; \textit{on} \;\; \Sigma_D, \quad \textit{and} \;\; A(U) + (G \circ \gamma)(U) + F(U) = 0 \quad \textit{in} \;\; X_0^*.$$

Let $\mathcal{R} = [\underline{U}, \overline{U}] \subset X$ be the rectangle formed by the ordered pair $\underline{U} = (\underline{u}_0, \underline{u}_1, \underline{u}_2)$ and $\overline{U} = (\bar{u}_0, \bar{u}_1, \bar{u}_2)$. In the following two definitions we extend in an appropriate way the notion of super- and subsolutions known for scalar equations to systems.

Definition 4.2. *The vector $A(U) + (G \circ \gamma)(U) + F(U)$ is called a generalized outward pointing vector on the boundary $\partial\mathcal{R}$ of the rectangle $\mathcal{R}$ if the following inequalities hold for all $\varphi \in H_0 \cap L^2_+(\Omega)$:*

$$\begin{aligned} \langle A_k(u_0)\underline{u_k} + F_k(\underline{U_k}) + (G_k \circ \gamma)(\underline{U}_k), \varphi\rangle &\leq 0, \ \forall\ \underline{U_k} \in [\underline{U}, \bar{U}], \\ \langle A_k(u_0)\bar{u}_k) + F_k(\overline{U_k}) + (G_k \circ \gamma)(\overline{U}_k), \varphi\rangle &\geq 0, \ \forall\ \overline{U_k} \in [\underline{U}, \bar{U}], \end{aligned}$$

where $\underline{U_k} = (u_0, u_1, u_2)|_{u_k = \underline{u}_k}$, $\overline{U_k} = (u_0, u_1, u_2)|_{u_k = \bar{u}_k}$ and $k = 0, 1, 2$.

Definition 4.3. *Let $\underline{U}$, $\overline{U} \in X$ be an ordered pair satisfying $\underline{U} \leq U_D \leq \overline{U}$ on Σ_D, where U_D is the vector of the boundary values. Then $\mathcal{R} = [\underline{U}, \overline{U}]$ is called a trapping region of the system (36), (37) if $A(U) + (G \circ \gamma)(U) + F(U)$ is a generalized outward pointing vector on $\partial\mathcal{R}$.*

Due to the discontinuous nonlinearities f_1, f_2 and g_1, g_2, we consider the following multivalued version of system (36), (37):

$$A_0(u_0)u_0 + f_0(\cdot, U) = 0, \tag{38}$$

$$A_j(u_0)u_j + \alpha_j(\cdot, U) \ni 0, \tag{39}$$

$$U = U_D \ \text{ on } \Sigma_D, \ \frac{\partial u_0}{\partial \nu} = 0, \ \ \frac{\partial u_j}{\partial \nu} + \beta_j(\cdot, U) \ni 0, \ \text{ on } \ \Gamma, \tag{40}$$

where α_j and β_j are the maximal monotone graphs of f_j and g_j, respectively, with respect to their principal argument, for $j = 1, 2$.

Theorem 4.1. *Let $[\underline{U}, \overline{U}]$ be a trapping region in the sense of Definition 4.3, such that the flux hypothesis is satisfied in the trapping region, and assume $\underline{u}_0$, $\bar{u}_0 \in L^\infty(\Omega)$, and $\underline{U} \geq 0$. Then system (38), (39), (40), which is the multi-valued formulation of system (36), (37), has a solution within $[\underline{U}, \overline{U}]$.*

Proof. Our approach will be an extension of the approach introduced in [3] and discussed extensively in [4]. To this end let us first consider the following auxiliary, truncated system:

$$A_0(u_0)u_0 + f_0(\cdot, T_0u_0, T_1u_1, T_2u_2) = 0, \tag{41}$$

$$A_1(T_0u_0)u_1 + \alpha_1(\cdot, T_0u_0, u_1) \ni 0, \tag{42}$$

$$A_2(T_0u_0)u_2 + \alpha_2(\cdot, T_0u_0, u_2) \ni 0, \tag{43}$$

under the following boundary conditions

$$U = U_D \text{ on } \Sigma_D, \ \frac{\partial u_0}{\partial \nu} = 0 \text{ on } \Gamma, \tag{44}$$

$$\frac{\partial u_1}{\partial \nu} + \beta_1(\cdot, T_0 u_0, u_1) \ni 0, \quad \frac{\partial u_2}{\partial \nu} + \beta_2(\cdot, T_0 u_0, u_2) \ni 0 \text{ on } \Gamma, \tag{45}$$

where T_k is the truncation between $\underline{u}_k$ and $\bar{u}_k$, which is defined analogously to (24). The existence of solutions for the auxiliary system (41), (42), (43) is based on Schauder's fixed point theorem. To this end for fixed $(u_1, u_2) \in [L^2(\Omega)]^2$ we first solve equation (41) under the given boundary condition for u_0. From the trapping region we infer that $\underline{u}_0$ and $\bar{u}_0$ are sub-supersolutions, respectively, for (41), which by Lemma 3.1 implies the existence of a uniquely defined solution z_0 within the interval $[\underline{u}_0, \bar{u}_0]$. Thus the following mapping is well defined:

$$[L^2(\Omega)]^2 \ni (u_1, u_2) \mapsto z_0 := P(u_1, u_2) \in H. \tag{46}$$

Next we decouple 42), (43) by the substitution $z_0 = P(u_1, u_2)$ in each equation which results in the decoupled system:

$$A_1(z_0)u_1 + \alpha_1(\cdot, z_0, u_1) \ni 0, \tag{47}$$

$$A_2(z_0)u_2 + \alpha_2(\cdot, z_0, u_2) \ni 0, \tag{48}$$

under the boundary conditions

$$u_1 = u_{1,D} \text{ on } \Sigma_D, \ \frac{\partial u_1}{\partial \nu} + \beta_1(\cdot, z_0, u_1) \ni 0 \text{ on } \Gamma, \tag{49}$$

$$u_2 = u_{2,D} \text{ on } \Sigma_D, \ \frac{\partial u_2}{\partial \nu} + \beta_2(\cdot, z_0, u_2) \ni 0 \text{ on } \Gamma. \tag{50}$$

By Lemma 3.2 the above uncoupled gradient equations (47),(49) and (48),(50) are uniquely solvable, and in view of the assumption on the trappping region we have, in addition, for the unique solutions z_j, $j = 1, 2$, the following comparison:

$$\underline{u}_j \le z_j \le \bar{u}_j, \quad \text{for } j = 1, 2. \tag{51}$$

Define a mapping $S : H \to [H]^2$ by

$$H \ni z_0 \mapsto (z_1, z_2) =: Sz_0 \in [H]^2. \tag{52}$$

Set $Z = S \circ P : [L^2(\Omega)]^2 \to [H]^2 \subset [L^2(\Omega)]^2$. Then a fixed point (u_1^*, u_2^*) of Z defines a solution of the original coupled system (38), (39), (40) via (u_0^*, u_1^*, u_2^*), where $u_0^* = P(u_1^*, u_2^*)$. To prove the existence of a fixed point of

Z we study next the mappings P and S. By inspection of the nonlinearity f_0 and taking the uniform boundedness of the truncations $T_k : L^2(\Omega) \to L^2(\Omega)$ into account, one can see that $(u_1, u_2) \mapsto f_0(\cdot, T_0 u_0, T_1 u_1, T_2 u_2)$ is uniformly bounded for any $u_0 \in L^2(\Omega)$ from $[L^2(\Omega)]^2$ to $L^2(\Omega)$. Thus by definition of the operator P from (41) we obtain by standard estimate

$$\|P(u_1, u_2)\|_H \leq C, \quad \text{for all} \;\; (u_1, u_2) \in [L^2(\Omega)]^2. \tag{53}$$

Moreover, the mapping $P : [L^2(\Omega)]^2 \to H$ is continuous, which can be seen as follows. Let $z_0 = P(u_1, u_2)$ and $\hat{z}_0 = P(\hat{u}_1, \hat{u}_2)$; then due to $P(u_1, u_2) \in [\underline{u}_0, \bar{u}_0]$ for any $(u_1, u_2) \in [L^2(\Omega)]^2$, from the weak formulation of (41), with $\varphi = z_0 - \hat{z}_0 \in H_0$ as special testfunction, we obtain ($\epsilon(x) \geq \epsilon_0 > 0$):

$$\begin{aligned} &\epsilon_0 \|z_0 - \hat{z}_0\|_{H_0}^2 \\ &+ \textstyle\int_\Omega \left(f_0(\cdot, z_0, T_1 u_1, T_2 u_2) - f_0(\cdot, \hat{z}_0, T_1 u_1, T_2 u_2)\right)(z_0 - \hat{z}_0) dx \\ &\leq \textstyle\int_\Omega \left(f_0(\cdot, \hat{z}_0, T_1 \hat{u}_1, T_2 \hat{u}_2) - f_0(\cdot, \hat{z}_0, T_1 u_1, T_2 \hat{u}_2)\right)(z_0 - \hat{z}_0) dx \\ &+ \textstyle\int_\Omega \left(f_0(\cdot, \hat{z}_0, T_1 u_1, T_2 \hat{u}_2) - f_0(\cdot, \hat{z}_0, T_1 u_1, T_2 u_2)\right)(z_0 - \hat{z}_0) dx. \end{aligned} \tag{54}$$

The integral on the left-hand side of (54) is nonnegative due to the monotonicity of f_0 in u_0. Applying the Lipschitz continuity of $f_0(\cdot, s_0, s_1, s_2)$ in s_1 and s_2, we get from (54) the continuity of $(u_1, u_2) \mapsto P(u_1, u_2)$. Next, we show that $S : [H] \to [H]^2$ is continuous and bounded. To this end let $S z_0 = (z_1, z_2)$ and and $S \hat{z}_0 = (\hat{z}_1, \hat{z}_2)$, where $S z_0$ and $S \hat{z}_0$ are given by the unique solution of the uncoupled system (47)–(50) for fixed z_0 and $\hat{z}_0$, respectively. Consider the inclusion (47) under the boundary condition (49) for given z_0 and $\hat{z}_0$, whose unique solution is denoted by z_1 and $\hat{z}_1$, respectively, which, e.g., for z_1 is equivalent to the following variational inequality: Find $z_1 \in \tilde{u}_{1,D} + H_0$ such that for all $\varphi \in \tilde{u}_{1,D} + H_0$:

$$\begin{aligned} &\int_\Omega a_1(z_0) \nabla z_1 \nabla(\varphi - z_1)\, dx + J_1(z_0, \varphi) - J_1(z_0, z_1) \\ &+ (\Phi_1 \circ \gamma)(z_0, \varphi) - (\Phi_1 \circ \gamma)(z_0, z_1) \geq 0, \end{aligned} \tag{55}$$

where the functionals are given by

$$\begin{aligned} J_1(z_0, \varphi) &= \textstyle\int_\Omega \left(\int_0^{\varphi(x)} f_1(x, z_0(x), s)\, ds \right) dx, \\ (\Phi_1 \circ \gamma)(z_0, \varphi) &= \textstyle\int_\Gamma \left(\int_0^{\gamma\varphi(x)} g_1(x, \gamma z_0(x), s)\, ds \right) d\Gamma. \end{aligned} \tag{56}$$

A corresponding variational inequality holds for $\hat{z}_1$. Specializing $\varphi = \hat{z}_1$ in (55) and using $\varphi = z_1$ in the variational inequality for $\hat{z}_1$, we obtain by adding the resulting inequalities the following one:

$$
\begin{aligned}
\int_\Omega a_1(\hat z_0)|\nabla(\hat z_1 - z_1)|^2\,dx \le &\int_\Omega (a_1(z_0)-a_1(\hat z_0))\nabla z_1 \nabla(\hat z_1 - z_1)\,dx \\
&+ \int_\Omega \left(\int_{z_1(x)}^{\hat z_1(x)} (f_1(x,z_0(x),s) - f_1(x,\hat z_0(x),s))ds \right) dx \\
&+ \int_\Gamma \left(\int_{\gamma z_1(x)}^{\gamma \hat z_1(x)} (g_1(x,\gamma z_0(x),s) - g_1(x,\gamma \hat z_0(x),s))ds \right) d\Gamma \qquad (57)
\end{aligned}
$$

By using the formulas for f_1 and g_1 given by (17) and (11), respectively, we get the following estimate:

$$
\begin{aligned}
|f_1(x,z_0(x),s) - f_1(x,\hat z_0(x),s)| &= |(\chi_{\mathcal{E}_s} - 1)(G(z_0(x) - G(\hat z_0(x))| \\
&\le C\,|z_0(x) - \hat z_0(x)|, \quad (58) \\
|g_1(x,\gamma z_0(x),s) - g_1(x,\gamma \hat z_0(x),s)| &\le |c_1(1-\chi_{\mathcal{E}_s})n_0||e^{-\gamma \hat z_0(x)} - e^{-\gamma z_0(x)}| \\
&\le C\,|\gamma z_0(x) - \gamma \hat z_0(x)|, \quad (59)
\end{aligned}
$$

where $C > 0$ is some generic constant. For the estimate (58), (59) we have used that the function $t \mapsto G(t)$ is locally Lipschitz, and the image of the operator P is contained in the interval $[\underline{u}_0, \bar u_0] \subset L^\infty(\Omega)$. Denoting the three integral terms on the right-hand side of inequality (57) by I_1, I_2, I_3 and applying estimates (58), (59) one gets the following:

$$
\begin{aligned}
&|I_1| \le C\,\|(a_1(z_0) - a_1(\hat z_0))\nabla z_1\|_{L^2(\Omega)} \|\nabla(z_1 - \hat z_1)\|_{L^2(\Omega)}, \\
&|I_2| \le C\,\|z_0 - \hat z_0\|_{L^2(\Omega)} \|z_1 - \hat z_1\|_{L^2(\Omega)}, \\
&|I_3| \le C\,\|\gamma z_0 - \gamma \hat z_0\|_{L^2(\Gamma)} \|\gamma z_1 - \gamma \hat z_1\|_{L^2(\Gamma)}. \qquad (60)
\end{aligned}
$$

Since $a_1(t) = e^t \ge e^{\underline{u}_0} > 0$ for all $t \in [\underline{u}_0, \bar u_0]$, and $u \mapsto (\int_\Omega |\nabla u|^2\,dx)^{1/2}$ defines an equivalent norm in H_0, we obtain from (57) and (60)

$$
\begin{aligned}
\|\hat z_1 - z_1\|_H \;\le\; & C\Big(\|(a_1(z_0) - a_1(\hat z_0))\nabla z_1\|_{L^2(\Omega)} \\
& + \|z_0 - \hat z_0\|_{L^2(\Omega)} + \|\gamma z_0 - \gamma \hat z_0\|_{L^2(\Gamma)}\Big). \qquad (61)
\end{aligned}
$$

In just the same way one obtains the following estimate

$$
\begin{aligned}
\|\hat z_2 - z_2\|_H \;\le\; & C\Big(\|(a_2(z_0) - a_2(\hat z_0))\nabla z_2\|_{L^2(\Omega)} \\
& + \|z_0 - \hat z_0\|_{L^2(\Omega)} + \|\gamma z_0 - \gamma \hat z_0\|_{L^2(\Gamma)}\Big). \qquad (62)
\end{aligned}
$$

Taking into account that the trace operator $\gamma : H \to L^2(\partial\Omega)$ is linear and continuous (even compact) from (61) and (62) we readily see that the operator $S : H \to [H^2]$ is continuous. To prove the boundedness of $z_0 \mapsto S(z_0) = (z_1, z_2)$ we use the variational inequality (55) with the special test function $\varphi = \tilde{u}_{1,D}$ which yields the estimate

$$\int_\Omega a_1(z_0)|\nabla z_1|^2\,dx \;\leq\; \int_\Omega a_1(z_0)\nabla z_1 \nabla \tilde{u}_{1,D}\,dx + J_1(z_0,\tilde{u}_{1,D}) - J_1(z_0,z_1) + (\Phi_1\circ\gamma)(z_0,\tilde{u}_{1,D}) - (\Phi_1\circ\gamma)(z_0,z_1). \tag{63}$$

By means of the trapping region we already know that $z_0 \in [\underline{u}_0, \bar{u}_0]$ for any image z_0 of P, and that the following enclosure for $S(z_0) = (z_1, z_2)$ holds:

$$(\underline{u}_1, \underline{u}_2) \leq (z_1, z_2) \leq (\bar{u}_1, \bar{u}_2). \tag{64}$$

Due to $z_0 \in [\underline{u}_0, \bar{u}_0]$ there exist positive constants $\underline{a}_1, \bar{a}_1$ such that

$$0 < \underline{a}_1 \leq a_1(z_0) \leq \bar{a}_1 \quad \text{for all} \quad z_0 \in [\underline{u}_0, \bar{u}_0]. \tag{65}$$

By using (64), (65) from (63) we obtain an estimate in the form

$$\underline{a}_1 \int_\Omega |\nabla z_1|^2\,dx \leq C(\tilde{u}_{1,D}, \underline{u}_1, \bar{u}_1) + C(\bar{a}_1, \varepsilon) + \varepsilon\,\|\nabla z_1\|^2_{L^2(\Omega)}, \tag{66}$$

for any $\varepsilon > 0$. Selecting $\varepsilon < \underline{a}_1$ there exists a constant $R_1 > 0$ depending only on the data of the original problem and the trapping region such that $\|z_1\|_H \leq R_1$. In a similar way one shows the existence of a constant R_2 such that $\|z_2\|_H \leq R_2$. Thus with $R = \max\{R_1, R_2\}$ we have proved:

$$\|S(z_0)\|_{[H]^2} = \|(z_1, z_2)\|_{[H]^2} \leq R \quad \text{for all} \quad z_0 = P(u_1, u_2). \tag{67}$$

Due to the compact embedding $[H]^2 \subset [L^2(\Omega)]^2$ the operator

$$Z = S \circ P : \overline{B(0,R)} \to \overline{B(0,R)}$$

provides a continuous and compact mapping of the closed ball $\overline{B(0,R)} \subset [L^2(\Omega)]^2$ into itself. Schauder's fixed point theorem then completes the proof. □

Construction of a trapping region

It remains to construct a trapping region $\mathcal{R} = [\underline{U}, \overline{U}]$ for the model. We do this in terms of constant vectors $\overline{U} = (\bar{u}_0, \bar{u}_1, \bar{u}_2) := (\bar{u}, \overline{V}, \overline{W})$, $\underline{U} =$

$(\underline{u}_0, \underline{u}_1, \underline{u}_2) := (\underline{u}, \underline{V}, \underline{W})$. We begin with the boundary values for the variables v, w. Set

$$\varrho_v = \inf_{\Sigma_D} v_D,\ \ \varrho_w = \inf_{\Sigma_D} w_D, \kappa_v = \sup_{\Sigma_D} v_D,\ \ \kappa_w = \sup_{\Sigma_D} w_D, \tag{68}$$

Then we require

$$0 < \underline{V} < \min(V_0, \exp(-\kappa_v)),\ \overline{V} > \max(V_0, \exp(-\varrho_v)), \tag{69}$$
$$0 < \underline{W} < \min(W_0, \exp(\varrho_w)),\ \overline{W} > \max(W_0, \exp(\kappa_w)), \tag{70}$$

and

$$\underline{u} = \min(\inf_{\Sigma_D} u_D,\ \underline{\delta}),\ \bar{u} = \max(\sup_{\Sigma_D} u_D,\ \bar{\delta}), \tag{71}$$

where $\underline{\delta}$ and $\bar{\delta}$ are any solutions of the inequalities:

$$\begin{array}{ll} \bar{\delta}: & \underline{V}\exp(\bar{\delta}) - \overline{W}\exp(-\bar{\delta}) \geq \sup_\Omega k_1, \\ \underline{\delta}: & \overline{V}\exp(\underline{\delta}) - \underline{W}\exp(-\underline{\delta}) \leq \inf_\Omega k_1. \end{array} \tag{72}$$

One easily verifies that the so obtained constant vectors $\overline{U}$ and $\underline{U}$ form a trapping region in the sense of Definition 4.3 if the boundary flux hypothesis holds. This is implied by the inequalities,

$$V_0 - \exp(-\overline{u}) \inf_\Omega n_0 \leq 0,\ W_0 - \exp(\underline{u}) \inf_\Omega p_0 \leq 0. \tag{73}$$

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