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Analysis of a Spin-Polarized Drift-Diffusion Model

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Abstract

We introduce a spin-polarized drift-diffusion model for semiconductor spintronic devices. This coupled system of continuity equations and a Poisson equation with mixed boundary conditions in all equations has to be considered in heterostructures. We give a weak formulation of this problem and prove an existence and uniqueness result for the instationary problem. If the boundary data is compatible with thermodynamic equilibrium the free energy along the solution decays monotonously and exponentially to its equilibrium value. In other cases it may be increasing but we estimate its growth. Moreover we give upper and lower estimates for the solution.

1 Introduction

Active control of spin in semiconductors can lead to significant technological advances, most importantly in digital information storage and processing, magnetic recording and sensing. The use of semiconductors for spintronic applications where spin in addition to charge is manipulated to influence the electric properties promises several advantages.

1.1 Model equations

Spin-polarized drift-diffusion models as proposed in [19, 20, 21, 22] are a generalization of the classical van Roosbroeck equations [16, 17]. There are introduced spin-resolved densities for electrons $n_\uparrow$ and $n_\downarrow$ and holes $p_\uparrow$ and $p_\downarrow$. In the following, we label the spin-resolved quantities (densities, current densities, quasi Fermi energies, band-edges) by $\lambda = 1$ or $\uparrow$ for spin-up and $\lambda = -1$ or $\downarrow$ for spin-down along a chosen quantization axis for the spin angular momentum.

With the spin-resolved densities n_λ and p_λ the total electron and hole densities n and p are given by

$$n = n_\uparrow + n_\downarrow, \quad p = p_\uparrow + p_\downarrow.$$

Moreover, we introduce the spin densities s_n and s_p for electrons and holes by

$$s_n = n_\uparrow - n_\downarrow, \quad s_p = p_\uparrow - p_\downarrow.$$

With these quantities we define the spin polarization of the electron and hole densities

$$P_n = \frac{s_n}{n} = \frac{n_\uparrow - n_\downarrow}{n_\uparrow + n_\downarrow}, \quad P_p = \frac{s_p}{p} = \frac{p_\uparrow - p_\downarrow}{p_\uparrow + p_\downarrow}.$$

A doping with magnetic impurities or the presence of a magnetic field can lead to a spin-splitting of the conduction and the valence bands (see [20]). The splitting ΔE_c and ΔE_v is expressed by qg_c and qg_v, where q is the elementary charge:

$$\Delta E_c = 2qg_c, \quad \Delta E_v = 2qg_v.$$

For the description of the carrier densities we introduce spin-resolved quasi Fermi energies $\varphi_{n\lambda}$ and $\varphi_{p\lambda}$ and formulate the state equations

$$\begin{aligned} n_\lambda &= \frac{N_c}{2}\exp[-(E_{c0} - q\psi - \lambda q g_c - \varphi_{n\lambda})/k_B T], \\ p_\lambda &= \frac{N_v}{2}\exp[-(q\psi + \lambda q g_v + \varphi_{p\lambda} - E_{v0})/k_B T], \end{aligned} \tag{1.1}$$

where E_{c0} and E_{v0} denote the variation of the bulk conduction and valence band-edge energies of the semiconductor material, respectively. N_c and N_v are the corresponding band-edge densities of state defined by

$$N_c = 2\Big(\frac{m_c k_B T}{2\pi\hbar^2}\Big)^{3/2}, \quad N_v = 2\Big(\frac{m_v k_B T}{2\pi\hbar^2}\Big)^{3/2},$$

m_c and m_v are the density of state masses, T is the temperature and k_B is Boltzmann's constant. The electrostatic potential ψ satisfies Poisson's equation

$$-\nabla\cdot(\epsilon\nabla\psi) = q(N_d - N_a - n + p) \tag{1.2}$$

where ϵ is the dielectric permittivity, N_a and N_d are densities of ionized acceptors and donors, respectively. The variation of the net band-edges $E_{c\lambda}$ and $E_{v\lambda}$ than also accounts for the spin-splitting:

$$E_{c\lambda} = E_{c0} - q\psi - \lambda q g_c, \quad E_{v\lambda} = E_{v0} - q\psi - \lambda q g_v.$$

Assuming drift-diffusion transport, the spin-resolved charge current densities for electrons and holes can be expressed by

$$\begin{aligned} j_{n\lambda} &= \mu_{n\lambda} n_\lambda \nabla E_{c\lambda} + q D_{n\lambda} N_c \nabla(n_\lambda/N_c), \\ j_{p\lambda} &= \mu_{p\lambda} p_\lambda \nabla E_{v\lambda} - q D_{p\lambda} N_v \nabla(p_\lambda/N_v). \end{aligned}$$

Using the corresponding Einstein relations for mobility and diffusion coefficient,

$$\mu_{n\lambda} = \frac{q}{k_B T} D_{n\lambda}, \quad \mu_{p\lambda} = \frac{q}{k_B T} D_{p\lambda},$$

we can rewrite the expressions in terms of the gradients of the quasi Fermi energies to

$$j_{n\lambda} = \mu_{n\lambda} n_\lambda \nabla\varphi_{n\lambda}, \quad j_{p\lambda} = \mu_{p\lambda} p_\lambda \nabla\varphi_{p\lambda}. \tag{1.3}$$

The continuity equations for the carrier densities are also a direct generalization of the continuity equations of the unpolarized case complemented by an expression modeling the spin relaxation. The spin relaxation leads to an equilibration of the carrier spin while preserving the nonequilibrium carrier density. For nondegenerate semiconductors the equilibrium spin densities $\widetilde{s}_n$ and $\widetilde{s}_p$ for electrons and holes are related to the equilibrium polarization densities P_{n0} and P_{p0} by the expressions, see [19, 20, 21, 22],

$$\widetilde{s}_n = n P_{n0}, \quad \widetilde{s}_p = p P_{p0},$$

where P_{n0} and P_{p0} are defined by the conduction and valence band spin-splittings

$$P_{n0} = \tanh h_c, \quad P_{p0} = \tanh h_v, \quad h_c = \frac{qg_c}{k_B T}, \quad h_v = -\frac{qg_v}{k_B T}.$$

Then we can write the spin-resolved continuity equations for the carrier densities as, see [19, 20, 21, 22],

$$\begin{aligned}
\frac{\partial n_\lambda}{\partial t} - \nabla\cdot\frac{j_{n\lambda}}{q} &= -R_{n\lambda} - \frac{n_\lambda - n_{-\lambda} - \lambda\widetilde{s}_n}{2\tau_{sn}}, \\
\frac{\partial p_\lambda}{\partial t} + \nabla\cdot\frac{j_{p\lambda}}{q} &= -R_{p\lambda} - \frac{p_\lambda - p_{-\lambda} - \lambda\widetilde{s}_p}{2\tau_{sp}}, \qquad \lambda = \pm 1.
\end{aligned} \tag{1.4}$$

$R_{n\lambda}$, $R_{p\lambda}$ are the recombination/generation rate of electrons and holes with spin polarization λ. τ_{sn} and τ_{sp} are the spin relaxation times for electrons and holes, respectively. Zutic *et al.* [21, 22] suggest the following formal structure for the spin-dependent recombination rates

$$R_{n\lambda} = r(n_\lambda p - n_{\lambda 0} p_0), \quad R_{p\lambda} = r(p_\lambda n - p_{\lambda 0} n_0). \tag{1.5}$$

The system of drift-diffusion equations has to be supplemented with boundary conditions modeling the behavior of the contact regions and with initial conditions.

1.2 A scaled spin-polarized drift-diffusion system

We use a scaling such that potentials and energies are considered in units of $k_B T/q$ and $k_B T$, respectively. We count the four different species in the following order: electrons with spin up, electrons with spin down, holes with spin up and holes with spin down. We introduce the four component vectors $\gamma = (-1,-1,1,1)$ of specific charge numbers, $D = (D_{n\uparrow}, D_{n\downarrow}, D_{p\uparrow}, D_{p\downarrow})$ of diffusion coefficients, and

$$\overline{u} = \Big(\frac{N_c}{2}\exp\big[\frac{-E_{c0}+qg_c}{k_B T}\big], \frac{N_c}{2}\exp\big[\frac{-E_{c0}-qg_c}{k_B T}\big], \frac{N_v}{2}\exp\big[\frac{E_{v0}-qg_v}{k_B T}\big], \frac{N_v}{2}\exp\big[\frac{E_{v0}+qg_v}{k_B T}\big]\Big)$$

of reference densities involving the spin-split band edges. The mass densities are collected in the vector $u = (u_0, \ldots, u_4) = (p_\uparrow + p_\downarrow - n_\uparrow - n_\downarrow, n_\uparrow, n_\downarrow, p_\uparrow, p_\downarrow)$, where the 0-th component denotes the variable charge density, the others are the particle densities. The vector v contains the (scaled) electrostatic potential and chemical potentials, $i = 1, \ldots, 4$,

$$v = (v_0, \ldots, v_4) = \frac{1}{k_B T}\big(q\psi, \varphi_{n\uparrow} + q\psi, \varphi_{n\downarrow} + q\psi, -\varphi_{p\uparrow} - q\psi, -\varphi_{p\downarrow} - q\psi\big).$$

The statistic relations reflecting Boltzmann statistics (1.1) then take the simple form

$$u_i = \overline{u}_i \mathrm{e}^{v_i}, \quad i = 1, \ldots, 4. \tag{1.6}$$

Denoting by ζ_i the (scaled) electrochemical potential of the i-th species we have $\zeta_i = v_i + \gamma_i v_0$ and the particle flux density J_i reads as

$$J_i = -D_i u_i \nabla\zeta_i = -D_i\big(\overline{u}_i \nabla\frac{u_i}{\overline{u}_i} + u_i\gamma_i\nabla v_0\big), \quad i = 1, \ldots, 4.$$

In this notation the spin polarized drift-diffusion model can be written in the form

$$\begin{aligned} -\nabla\cdot(\varepsilon\nabla v_0) &= f+\sum_{i=1}^{4}\gamma_i u_i,\\ \frac{\partial u_i}{\partial t}+\nabla\cdot J_i &= -R_i,\quad i=1,\ldots,4,\quad \text{on } (0,\infty)\times\Omega, \end{aligned}\tag{1.7}$$

where Ω denotes the domain which is occupied by the spintronic device, $\varepsilon=\epsilon k_B T/q^2$ and

$$\begin{aligned} R_1 &= r_{13}(\mathrm{e}^{v_1+v_3}-1)+r_{14}(\mathrm{e}^{v_1+v_4}-1)+r_{12}(\mathrm{e}^{v_1}-\mathrm{e}^{v_2}),\\ R_2 &= r_{23}(\mathrm{e}^{v_2+v_3}-1)+r_{24}(\mathrm{e}^{v_2+v_4}-1)-r_{12}(\mathrm{e}^{v_1}-\mathrm{e}^{v_2}),\\ R_3 &= r_{13}(\mathrm{e}^{v_1+v_3}-1)+r_{23}(\mathrm{e}^{v_2+v_3}-1)+r_{34}(\mathrm{e}^{v_3}-\mathrm{e}^{v_4}),\\ R_4 &= r_{14}(\mathrm{e}^{v_1+v_4}-1)+r_{24}(\mathrm{e}^{v_2+v_4}-1)-r_{34}(\mathrm{e}^{v_3}-\mathrm{e}^{v_4}) \end{aligned}$$

with

$$r_{ij}=r\overline{u}_i\overline{u}_j,\ ij=13,14,23,24,$$
$$r_{12}=\frac{1-\tanh h_c}{2\tau_{sn}}\overline{u}_1,\quad r_{34}=\frac{1-\tanh h_v}{2\tau_{sp}}\overline{u}_3.$$

We split $\partial\Omega$ into the disjoint subsets of Ohmic contacts Γ_D and isolations Γ_N, $\partial\Omega=\Gamma_D\cup\Gamma_N$. We complete the system (1.7) by boundary and initial conditions

$$\begin{aligned} v_i &= v_i^D,\quad i=0,\ldots,4,\quad \text{on } (0,\infty)\times\Gamma_D,\\ \varepsilon\nabla v_0\cdot\nu &= 0,\quad J_i\cdot\nu=0,\quad i=1,\ldots,4,\quad \text{on } (0,\infty)\times\Gamma_N,\\ u_i(0) &= U_i,\quad i=1,\ldots,4,\quad \text{on } \Omega. \end{aligned}\tag{1.8}$$

For a discussion of boundary conditions for semiconductor devices from the physical viewpoint we refer to [17, 15]. Let $v_i^D\colon\Omega\to\mathbb{R}$, $i=0,\ldots,4$, be functions representing the boundary values in (1.8) and $\zeta_i^D=v_i^D+\gamma_i v_0^D$, $i=1,\ldots,4$. We set

$$v^D=(v_0^D,\ldots,v_4^D),\quad \zeta^D=(\zeta_1^D,\ldots,\zeta_4^D).$$

The functions $v-v^D$, $\zeta-\zeta^D$ fulfill homogeneous Dirichlet conditions on Γ_D.

Since all occurring reactions are charge conserving, the variable charge density of the spintronic device $u_0=\sum_{i=1}^4\gamma_i u_i$ fulfills

$$\frac{\partial u_0}{\partial t}+\nabla\cdot J_0=0,\quad J_0=\sum_{i=1}^{4}\gamma_i J_i\quad \text{on } (0,\infty)\times\Omega.$$

We use u_0 as one of the unknowns of our problem and work with the vectors $u=(u_0,u_1,\ldots,u_4)$ and $v=(v_0,v_1,\ldots,v_4)$.

Remark 1.1 The system of differential equations (1.7) is a special realization of electro-reaction-diffusion systems which have been investigated in [5, 6, 7, 8, 9]. But in the context of spintronic devices this problem has to be considered under boundary conditions from device simulation. The treatment of electro-reaction-diffusion systems under such mixed boundary conditions for the Poisson equation as well as all for continuity equations, which need not be compatible with thermodynamic equilibrium, is new from an analytical point of view, too. Analytical techniques successfully applied to the van Roosbroeck system (see [3, 4]) will be a further ingredient in the treatment of (1.7), (1.8).

In Section 2 we formulate the assumptions our analytical results are based on, we give a weak formulation (P) of the scaled spin-polarized drift-diffusion model and introduce the energy functionals. Section 3 is devoted to the uniqueness result for (P). Section 4 contains the existence proof. For a regularized problem ($\mathrm{P_M}$) defined in Subsection 4.1 the solvability is shown in Subsection 4.2. Subsection 4.3 provides upper and lower bounds for the solutions to ($\mathrm{P_M}$) which lead to the existence result for (P) in Subsection 4.4. Section 5 deals with the global behavior of solutions to (P) establishing upper and lower bounds (Subsection 5.1) and assertions concerning steady states (Subsection 5.2). Finally, in Subsection 5.3, we prove for boundary data compatible with thermodynamic equilibrium the exponential decay of the free energy, of densities and of potentials to their equilibrium values.

2 Weak formulation of the problem

2.1 Assumptions

At first we collect the general assumptions our analytical investigations are based on.

(A1) $\Omega \subset \mathbb{R}^2$ bounded Lipschitzian domain, Γ_D, Γ_N are disjoint open subsets of $\partial\Omega$, $\partial\Omega = \Gamma_D \cup \Gamma_N \cup (\overline{\Gamma_D} \cap \overline{\Gamma_N})$, mes $\Gamma_D > 0$, $\overline{\Gamma_D} \cap \overline{\Gamma_N}$ consists of finitely many points ($\Omega \cup \Gamma_N$ is regular in the sense of Gröger [12]);

(A2) $D_i \in L^\infty(\Omega)$, $D_i \geq c > 0$ a.e. on Ω, $i = 1, \dots, 4$;

(A3) $r_{ij} : \Omega \times \mathbb{R} \times \mathbb{R}^4_+ \to \mathbb{R}_+$, $r_{ij}(x, \cdot)$ Lipschitzian uniformly w.r.t. $x \in \Omega$, $r_{ij}(\cdot, y)$ measurable for all $y \in \mathbb{R} \times \mathbb{R}^4_+$, $r_{ij}(\cdot, 0) \in L^\infty(\Omega)$, $ij = 13, 14, 23, 24$, $r_{ij} \in L^\infty_+(\Omega)$, $ij = 12, 34$;

(A4) ε, $\overline{u}_i \in L^\infty(\Omega)$, $\varepsilon \geq c > 0$, $\overline{u}_i \geq \underline{c} > 0$ a.e. on Ω, $i = 1, \dots, 4$, $f \in L^2(\Omega)$, $v_i^D \in W^{1,\infty}(\Omega)$, $i = 0, \dots, 4$, $\gamma = (-1, -1, 1, 1)$;

(A5) $u_i^0 \in L^\infty(\Omega)$, $u_i^0 \geq c > 0$ a.e. on Ω, $i = 1, \dots, 4$, $u_0^0 = \sum_{i=1}^4 \gamma_i u_i^0$.

Here and in the following we denote by c (possibly different) positive constants. Moreover, δ indicates small (possibly different) positive constants.

Remark 2.1 The assumptions in (A3) concerning the coefficients r_{ij}, $ij = 13, 14, 23, 24$, are formulated in this weak form to include Shockley-Read-Hall as well as Auger generation/recombination processes. We have $|r_{ij}(\cdot, u)| \leq |r_{ij}(\cdot, 0)| + \sum_{i=1}^4 |u_i|$. Due to (A3), the source terms $-R_i$ in the continuity equations (1.7) can be estimated by $c(1 + \sum_{i=1}^4 |u_i|)$.

2.2 Weak formulation

We work with the vectors $u = (u_0, u_1, \dots, u_4)$ and $v = (v_0, v_1, \dots, v_4)$ and introduce the notation

$$V = H_0^1(\Omega \cup \Gamma_N)^5, \quad H = H^{-1}(\Omega \cup \Gamma_N) \times (L^2(\Omega))^4,$$
$$U = \{u \in H\colon \ \ln u_i \in L^\infty(\Omega),\ i = 1,2,3,4\}$$

and define the operators $E_0 : H_0^1(\Omega \cup \Gamma_N) + v_0^D \to H^{-1}(\Omega \cup \Gamma_N)$ and $E : V + v^D \to V^*$,

$$\langle E_0 v_0, \overline{v}_0\rangle = \int_\Omega \big\{\varepsilon \nabla v_0 \cdot \nabla \overline{v}_0 - f\overline{v}_0\big\}\,\mathrm{d}x, \quad \overline{v}_0 \in H_0^1(\Omega \cup \Gamma_N),$$
$$\langle Ev, \overline{v}\rangle = \langle E_0 v_0, \overline{v}_0\rangle + \int_\Omega \sum_{i=1}^4 \overline{u}_i \mathrm{e}^{v_i} \overline{v}_i \,\mathrm{d}x, \quad \overline{v} \in V.$$

The equation $u = Ev$ is a weak formulation of the Poisson equation in (1.7) and the state equations (1.6). Next, we introduce the operator $A : U \times (V + v^D) \longrightarrow V^*$,

$$\langle A(u,v), \overline{v}\rangle := \int_\Omega \Big\{ \sum_{i=1}^4 D_i u_i \nabla\zeta_i \cdot \nabla\overline{\zeta}_i + \sum_{ij=12,34} r_{ij}(\mathrm{e}^{v_i} - \mathrm{e}^{v_j})(\overline{v}_i - \overline{v}_j)$$
$$+ \sum_{ij=13,14,23,24} r_{ij}(\cdot, u)(\mathrm{e}^{v_i+v_j} - 1)(\overline{v}_i + \overline{v}_j)\Big\}\,\mathrm{d}x, \quad \overline{\zeta}_i = \overline{v}_i + \gamma_i \overline{v}_0,\ \overline{v} \in V.$$

Thus a weak formulation of (1.7), (1.8) is given by

$$\begin{aligned} &u' + A(u,v) = 0, \quad u = Ev \ \text{ a.e. on } \mathbb{R}_+, \quad u(0) = u^0, \\ &u \in H^1_{\mathrm{loc}}(\mathbb{R}_+, V^*), \quad v - v^D \in L^2_{\mathrm{loc}}(\mathbb{R}_+, V) \cap L^\infty_{\mathrm{loc}}(\mathbb{R}_+, L^\infty(\Omega, \mathbb{R}^5)). \end{aligned} \tag{P}$$

2.3 Energy functionals

The operator E is a strict monotone potential operator with potential $G\colon\ V + v^D \to \mathbb{R}$,

$$G(v) = \int_\Omega \Big\{\frac{\varepsilon}{2}|\nabla v_0|^2 - \frac{\varepsilon}{2}|\nabla v_0^D|^2 - f(v_0 - v_0^D) + \sum_{i=1}^4 \overline{u}_i(\mathrm{e}^{v_i} - \mathrm{e}^{v_i^D})\Big\}\mathrm{d}x.$$

Since we work in space dimension two, Trudingers imbedding result (see [18]) implies that dom $G = V$. Moreover, the functional G is continuous, strictly convex, Gateaux differentiable, hence subdifferentiable and $\partial G = E$. According to [2] we introduce the conjugate functional $F : V^* \to \overline{\mathbb{R}}$,

$$F(u) = G^*(u) = \sup_{w \in V} \big\{\langle u, w\rangle - G(w + v^D)\big\}.$$

From standard results of convex analysis it results for $u = Ev$ that $F(u) = \langle u, v - v^D\rangle - G(v)$ and $v - v^D \in \partial F(u)$. The functional F is proper, lower semicontinuous and convex. If $u \in V^*$ and $u_i \in L^2(\Omega)$, $u_i \geq 0$, $i = 1, \dots, 4$, then

$$F(u) = \int_\Omega \Big\{\frac{\varepsilon}{2}|\nabla(v_0 - v_0^D)|^2 + \sum_{i=1}^4 \big\{u_i(\ln\frac{u_i}{\overline{u}_i} - v_i^D - 1) + \overline{u}_i \mathrm{e}^{v_i^D}\big\}\Big\}\mathrm{d}x,$$

where v_0 is the solution to $E_0 v_0 = u_0$. Due to the strong monotonicity of E_0 (given by (A4) and Dirichlet boundary conditions on Γ_D with $\operatorname{mes}\Gamma_D > 0$ (see (A1)) and properties of the ln-function we can estimate the functional F:

$$\begin{aligned} \widehat{c}\Big(\|v_0 - v_0^D\|_{H^1}^2 + \sum_{i=1}^4 \|\sqrt{u_i} - \sqrt{\overline{u}_i \mathrm{e}^{v_i^D}}\|_{L^2}^2\Big) &\le F(u), \\ \sum_{i=1}^4 \|u_i\|_{L^1} &\le F(u) + c. \end{aligned} \tag{2.1}$$

The value $F(u)$ can be interpreted as the free energy of the state u. We show that F is something like a Ljapunov function for solutions (u, v) to (P), namely under special assumptions (see (A6) in Section 5) on the boundary data the function $t \mapsto F(u(t))$ is exponentially decreasing (see Theorem 5.6). Generally, it may be increasing, but its growth can be estimated (see Theorem 5.1). Next, we prove existence and uniqueness results for the spin-polarized drift-diffusion model.

3 Uniqueness

According to Grögers regularity result for elliptic equations [12, Theorem 1] and (A4), (A1) we we can fix a $q = q(\Omega, \varepsilon) > 2$ such that, if

$$\forall \overline{y} \in H_0^1(\Omega \cup \Gamma_N): \int_\Omega \varepsilon \nabla y \cdot \nabla \overline{y}\, \mathrm{d}x = \langle g, \overline{y}\rangle, \quad g \in W^{-1,q}(\Omega \cup \Gamma_N), y \in H_0^1(\Omega \cup \Gamma_N)$$

then $y \in W_0^{1,q}(\Omega \cup \Gamma_N)$ and $\|y\|_{W_0^{1,q}} \le c\|g\|_{W^{-1,q}}$. Here $W^{-1,q}(\Omega \cup \Gamma_N)$ means the dual of $W_0^{1,q'}(\Omega \cup \Gamma_N)$, where q' denotes the dual exponent to q. Moreover, let r, r' be defined by

$$r = \frac{2q}{q-2}, \quad r' = \frac{2q}{q+2}. \tag{3.1}$$

Setting

$$\langle g, \overline{y}\rangle = \int_\Omega \Big\{\big(f + \sum_{i=1}^4 \gamma_i u_i\big)\overline{y} - \varepsilon \nabla v_0^D \cdot \nabla \overline{y}\Big\}\, \mathrm{d}x, \quad \overline{y} \in H_0^1(\Omega \cup \Gamma_N),$$

using (A4) we find from the Poisson equation that $v_0 - v_0^D \in L^\infty(S, W_0^{1,q}(\Omega \cup \Gamma_N))$ and

$$\|v_0(t) - v_0^D\|_{W_0^{1,q}} \le c\|g(t)\|_{W^{-1,q}} \le c(1 + \sum_{i=1}^4 \|u_i\|_{L^{r'}}) \quad \forall t \in S.$$

Especially, due to (A4) we can estimate

$$\|\nabla v_0(t)\|_{L^q} \le \|v_0(t) - v_0^D\|_{W_0^{1,q}} + \|\nabla v_0^D\|_{L^q} \le c(1 + \sum_{i=1}^4 \|u_i(t)\|_{L^{r'}}) \quad \forall t \in S. \tag{3.2}$$

Theorem 3.1 *Under the assumptions* (A1) – (A5) *there exists at most one solution to* (P).

Proof. It suffices to prove uniqueness on every finite time interval $S := [0,T]$. Let (u^j, v^j), $j = 1,2$, be solutions to (P). Then there exists a constant c such that

$$\|u^j(t)\|_{L^\infty},\ \|v^j(t)\|_{L^\infty},\ \|\nabla v_0^j(t)\|_{L^q} \le c \text{ f.a.a. } t \in S\,,\ j = 1,2,$$

where $q > 2$ (cf. (3.2)). Let $\widetilde{v} := v^1 - v^2$. Testing $E_0 v_0^1(t) - E_0 v_0^2(t) = u^1(t) - u^2(t)$ by $\widetilde{v}_0(t)$ we obtain by the strong monotonicity of E_0 that

$$\|\widetilde{v}_0(t)\|_{H^1} \le c \sum_{i=1}^4 \|u_i^1(t) - u_i^2(t)\|_{L^2} \text{ f.a.a. } t \in S. \tag{3.3}$$

Let $z_i := (u_i^1 - u_i^2)/\overline{u}_i$, $i = 1, \dots, 4$. We use $(0, z_1, \dots, z_4) \in L^2(S, V)$ as test function for (P) and take into account that the reaction rates are uniformly (w.r.t. x) locally Lipschitz continuous in the state variable and can be estimated by the corresponding norms of z_i. With the Gagliardo-Nirenberg inequality $\|z_i\|_{L^r} \le \|z_i\|_{L^2}^{2/r} \|z_i\|_{H^1}^{1-2/r}$ for r from (3.1), with inequality (3.3), and with Youngs inequality we conclude as follows

$$\begin{aligned}
\sum_{i=1}^4 \Big\{ \|z_i(t)\|_{L^2}^2 + \int_0^t \|z_i\|_{H^1}^2 \mathrm{d}s \Big\} &\le c \int_0^t \sum_{i=1}^4 \Big\{ \|z_i\|_{L^r} \|\nabla v_0^1\|_{L^q} \|\nabla z_i\|_{L^2} \\
&\quad + \|\nabla \widetilde{v}_0\|_{L^2} \|\nabla z_i\|_{L^2} + \|z_i\|_{L^2}^2 \Big\} \mathrm{d}s \\
&\le \int_0^t \sum_{i=1}^4 \Big\{ \tfrac{1}{4} \|z_i\|_{H^1}^2 + c\big(\|z_i\|_{L^2}^{2/r} \|\nabla v_0^1\|_{L^q} \|z_i\|_{H^1}^{2-2/r} + \|z_i\|_{L^2}^2 \big) \Big\} \mathrm{d}s \\
&\le \int_0^t \sum_{i=1}^4 \Big\{ \tfrac{1}{2} \|z_i\|_{H^1}^2 + c\big(\|\nabla v_0^1\|_{L^q}^r \|z_i\|_{L^2}^2 + \|z_i\|_{L^2}^2 \big) \Big\} \mathrm{d}s \\
&\le \int_0^t \sum_{i=1}^4 \Big\{ \tfrac{1}{2} \|z_i\|_{H^1}^2 + c \|z_i\|_{L^2}^2 \Big\} \mathrm{d}s \quad \forall t \in S.
\end{aligned}$$

Gronwall's lemma yields $z_i = 0$ on S, $i = 1, \dots, 4$. With (3.3) the assertion follows. □

4 Existence

The guideline for the existence proof is the following: First we discuss a regularized problem ($\mathrm{P_M}$) on an arbitrarily chosen finite time interval $S = [0,T]$, where the state equations and reaction terms are regularized (parameter M). We prove solvability of ($\mathrm{P_M}$) by time discretization and passing to the limit. Then we provide a priori estimates for solutions to ($\mathrm{P_M}$) which are independent of M. (Here we use energy estimates and Moser techniques to get upper and lower bounds.) Thus a solution to ($\mathrm{P_M}$) is a solution to (P), if M is chosen sufficiently large.

4.1 A regularized problem ($\mathrm{P_M}$)

We introduce the convex projection

$$P_k(y) = \begin{cases} k, & \text{if } y > k \\ y, & \text{if } |y| \le k \\ -k, & \text{if } y < k \end{cases}.$$

Let $v^0 = E^{-1}u^0$ and $M > \max_{i=1,\dots,4} \|v_i^0\|_{L^\infty}$. We define operators $E_M\colon V + v^D \to V^*$, $A_M\colon U \times (V + v^D) \to V^*$

$$\langle E_M v, \overline{v}\rangle = \langle E_0 v_0, \overline{v}_0\rangle + \int_\Omega \sum_{i=1}^4 \overline{u}_i \mathrm{e}^{P_M v_i} \overline{v}_i \,\mathrm{d}x, \quad \overline{v} \in V,$$

$$\begin{aligned}\langle A_M(u,v), \overline{v}\rangle = \int_\Omega \Big\{ \sum_{i=1}^4 D_i u_i \nabla\zeta_i \cdot \nabla\overline{\zeta}_i + \sum_{ij=12,34} r_{ij} \Big[\big(\mathrm{e}^{P_M v_i} - \frac{u_j}{\overline{u}_j}\big)\overline{v}_i - \big(\frac{u_i}{\overline{u}_i} - \mathrm{e}^{P_M v_j}\big)\overline{v}_j \Big] \\ + \sum_{ij=13,14,23,24} r_{ij}(\cdot, u)\big(\mathrm{e}^{P_{2M}(v_i+v_j)} - 1\big)(\overline{v}_i + \overline{v}_j) \Big\} \,\mathrm{d}x, \quad \overline{v} \in V,\end{aligned}$$

where $\zeta_i = v_i + \gamma_i v_0$, $\overline{\zeta}_i = \overline{v}_i + \gamma_i \overline{v}_0$. We prove for arbitrarily fixed time intervals $S = [0, T]$ the solvability of

$$\begin{aligned} &u' + A_M(u, v) = 0, \quad u = E_M v \ \text{ f.a.a. } t \in S, \\ &u(0) = u^0, \quad v - v^D \in L^2(S, V), \quad u \in H^1(S, V^*). \end{aligned} \tag{$\mathrm{P_M}$}$$

The regularized energy functionals are $G_M : V + v^D \to \mathbb{R}$,

$$\begin{aligned} G_M(v) &= \int_\Omega \Big\{ \frac{\varepsilon}{2}|\nabla v_0|^2 - \frac{\varepsilon}{2}|\nabla v_0^D|^2 - f(v_0 - v_0^D) + \sum_{i=1}^4 \overline{u}_i \int_{v_i^D}^{v_i} \mathrm{e}^{P_M y}\,\mathrm{d}y \Big\} \mathrm{d}x, \\ F_M(u) &= G_M^*(u) = \sup_{w\in V} \big\{ \langle u, w\rangle - G_M(w + v^D) \big\}. \end{aligned} \tag{4.1}$$

Then $\partial G_M(v) = E_M v$ and results from convex analysis guarantee that for $u = E_M v$ we have $v - v^D \in \partial F_M(u)$ and $\langle u, v - v^D\rangle = G_M(v) + F_M(u)$, and therefore

$$\begin{aligned} F_M(u) &= \langle u, v - v^D\rangle - G_M(v) \\ &= \int_\Omega \Big\{ \frac{\varepsilon}{2}|\nabla(v_0 - v_0^D)|^2 + \sum_{i=1}^4 \int_{v_i^D}^{v_i} \big(u_i - \overline{u}_i \mathrm{e}^{P_M y}\big)\,\mathrm{d}y \Big\} \mathrm{d}x \\ &= \int_\Omega \Big\{ \frac{\varepsilon}{2}|\nabla(v_0 - v_0^D)|^2 + \sum_{i=1}^4 \big\{ u_i\big(\ln\frac{u_i}{\overline{u}_i} - v_i^D - 1\big) + \overline{u}_i \mathrm{e}^{v_i^D} \big\} \Big\} \mathrm{d}x = F(u) \end{aligned} \tag{4.2}$$

for $u = E_M v$.

4.2 Solvability of problem ($\mathrm{P_M}$)

We use a time discretization scheme to prove solvability of problem ($\mathrm{P_M}$). For $n \in \mathbb{N}$ let $h_n := \frac{T}{n}$ and $S_n^k := \big((k-1)h_n, kh_n\big]$. If X is a Banach space, we denote by $C_n(S,X)$ the space of all functions $u : (0,T] \to X$, which are constant on S_n^k, $k = 1, ..., n$. The value of $u \in C_n(S,X)$ on S_n^k is denoted by u^k. We define operators Δ_n, $\sigma_n : C_n(S,V^*) \to C_n(S,V^*)$ and $K_n : C_n(S,V^*) \to C(S,V^*)$

$$(\Delta_n u)^k := \frac{1}{h_n}(u^k - u^{k-1}), \quad (\sigma_n u)^k := u_n^{k-1}, \quad k = 1, \dots, n,$$
$$(K_n u)(t) := u^0 + \int_0^t (\Delta_n u)(s)\,\mathrm{d}s,$$

where u^0 is the initial value to (P). Obviously, $(K_n u)' = \Delta_n u$. For $n \in \mathbb{N}$ investigate the discrete time problem

$$\Delta_n u_n + A_M(\sigma_n u_n, v_n) = 0, \quad u_n = E_M v_n, \quad v_n - v^D \in C_n(S,V). \tag{$\mathrm{P_{Mn}}$}$$

More explicitely this reads as

$$\frac{1}{h_n}(u_n^k - u_n^{k-1}) + A_M(u_n^{k-1}, v_n^k) = 0, \quad u_n^k = E_M v_n^k, \quad k = 1, \dots, n, \quad u_n^0 = u^0. \tag{4.3}$$

Lemma 4.1 *Let* (A1) – (A5) *be satisfied. Then, for every $n \in \mathbb{N}$ there exists a unique solution (u_n, v_n) to* ($\mathrm{P_{Mn}}$)*, and there exists a number $n_0 = n_0(T) \in \mathbb{N}$ such that*

$$\sup_{n \in \mathbb{N},\, n \geq n_0} \big\{ \|v_n - v^D\|_{L^2(S,V)} + \|\Delta_n u_n\|_{L^2(S,V^*)} + \|K_n u_n\|_{C(S,H)} \big\} < \infty.$$

Proof. 1. Let $n \in \mathbb{N}$. For fixed $u \in U$ the map $\frac{1}{h_n} E_M(\cdot + v^D) + A_M(u, \cdot + v^D) : V \to V^*$ is strongly monotone. Thus, equations (4.3) considered as equations w.r.t. v_n^k for given u_n^{k-1} are uniquely solvable. And we obtain unique solvability of ($\mathrm{P_{Mn}}$).

2. We use (4.1), (4.2), note that $u_n^k = E_M v_n^k$ holds. Due to the choice of M we have $F_M(u^0) = F(u^0)$, too. For $l = 1, \dots, n$ we estimate

$$\begin{aligned} F(u_n^l) - F(u^0) &= \sum_{k=1}^{l} \big(F(u_n^k) - F(u_n^{k-1})\big) \leq \sum_{j=1}^{l} \langle u_n^k - u_n^{k-1}, v_n^k - v^D \rangle \\ &= -h_n \sum_{j=1}^{l} \langle A_M(u_n^{k-1}, v_n^k), v_n^k - v^D \rangle. \end{aligned} \tag{4.4}$$

With

$$\langle A_M(u_n^{k-1}, v_n^k), v_n^k - v^D \rangle = \langle A_M(u_n^{k-1}, v_n^k) - A_M(u_n^{k-1}, v^D), v_n^k - v^D \rangle + \langle A_M(u_n^{k-1}, v^D), v_n^k - v^D \rangle,$$

$$\langle A_M(u_n^{k-1}, v_n^k) - A_M(u_n^{k-1}, v^D), v_n^k - v^D \rangle \geq 2\delta \mathrm{e}^{-M} \sum_{i=1}^{4} \|\zeta_{ni}^k - \zeta_i^D\|_{H^1}^2,$$

$$|\langle A_M(u_n^{k-1}, v^D), v_n^k - v^D\rangle| \le c(M)\Big(\sum_{i=1}^4 \|\zeta_{ni}^k - \zeta_i^D\|_{H^1} + \|v_{n0}^k - v_0^D\|_{H^1}\Big),$$

and Youngs inequality we continue the estimate (4.4)

$$F(u_n^l) + h_n\delta \mathrm{e}^{-M}\sum_{k=1}^l\sum_{i=1}^4 \|\zeta_{ni}^k - \zeta_i^D\|_{H^1}^2 \le h_n\Big(\sum_{k=1}^l (\|v_{n0}^k - v_0^D\|_{H^1}^2 + c(M))\Big) + F(u^0).$$

According to (2.1) we have $\widehat{c}\|v_{n0}^l - v_0^D\|_{H^1}^2 \le F(u_n^l)$. Setting

$$a_n^l := \widehat{c}\|v_{n0}^l - v_0^D\|_{H^1}^2 + h_n\delta \mathrm{e}^{-M}\sum_{k=1}^l\sum_{i=1}^4 \|\zeta_{ni}^k - \zeta_i^D\|_{H^1}^2,$$

we obtain

$$a_n^l \le \frac{h_n}{\widehat{c}}\sum_{k=1}^l a_n^k + lh_n c(M) + F(u^0).$$

We choose $n_0 \in \mathbb{N}$ such that $2h_n < \widehat{c}$ for all $n \ge n_0$ and find

$$a_n^l \le 2\frac{h_n}{\widehat{c}}\sum_{k=1}^{l-1} a_n^k + 2(lh_n c(M) + F(u^0))$$

for $n \ge n_0$, $l = 1, \dots, n$. Thus a discrete version of Gronwalls Lemma (cf. [13, Lemma 2]) yields $a_n^l \le c(M,T)$, $l = 1, \dots, n$, $n \ge n_0$, and we conclude that

$$\sup_{n\in\mathbb{N},\, n\ge n_0} \Big\{\|v_{n0} - v_0^D\|_{L^\infty(S,H^1(\Omega))} + \|v_n - v^D\|_{L^2(S,V)}\Big\} < \infty.$$

Therefore

$$\sup_{n\in\mathbb{N},\, n\ge n_0} \|\Delta_n u_n\|_{L^2(S,V^*)} = \sup_{n\in\mathbb{N},\, n\ge n_0} \|A_M(\sigma_n u_n, v_n)\|_{L^2(S,V^*)} < \infty.$$

From $u_{n0} = E_0 v_{n0}$ and $\underline{c}\mathrm{e}^{-M} \le u_{ni} \le \overline{c}\mathrm{e}^{M}$, $i = 1, \dots, 4$, we obtain finally

$$K_n u_n \in C(S,H), \qquad \sup_{n\in\mathbb{N},\, n\ge n_0} \|K_n u_n\|_{C(S,H)} < \infty. \qquad \square$$

Lemma 4.2 *Under the assumptions* (A1) – (A5) *there exists a solution* (u,v) *to* ($\mathrm{P_M}$).

Proof. For $n \in \mathbb{N}$, let (u_n, v_n) be the solution to ($\mathrm{P_{Mn}}$). Due to Lemma 4.1 we obtain for subsequences (again index n) the weak convergences

$$v_n - v^D \rightharpoonup v - v^D \text{ in } L^2(S,V),$$
$$K_n u_n \rightharpoonup u \text{ in } L^2(S,H) \text{ and } H^1(S,V^*).$$

The idea of the proof now is the same as in [4, Lemma 3.2]. But in our situation we have four species, $u_0 = \sum_{i=1}^4 \gamma_i u_i$, and additional spin relaxation reactions. Therefore we have to adapt the arguments in step 5 of that proof. We find: $u_{ni} \to u_i$ in $L^2(S, L^2(\Omega))$, $i = 1, \dots, 4$, implies $\sigma_n u_n \to u$ in $L^2(S,H)$, and $A_M(\sigma_n u_n, v) \to A_M(u,v)$ in $L^2(S,V^*)$ also with our spin relaxation reactions. Thus we obtain $\langle A_M(\sigma_n u_n, v), v_n - v\rangle \to 0$ in our case and can then argue similar to the estimates in step 5 of the proof of [4, Lemma 3.2]. Note that in step 6 then $A_M(\sigma_n u_n, v_n) \to A_M(u,v)$ in $L^2(S,V^*)$ is guaranteed also with our additional reaction terms. $\square$

4.3 A priori estimates for the regularized problem

In proofs of this subsection c denotes (possibly different) positive constants which do not depend on M and T.

Lemma 4.3 *Let* (A1) – (A5) *be satisfied. Then there exists a constant* $c_1 > 0$ *depending only on the data* (*but not on* M, T) *such that*

$$F(u(t)) \le (F(u^0)+1)e^{c_1 t} \qquad \forall t \in S$$

for any solution (u, v) *to* $(\mathrm{P_M})$.

Proof. We use $v - v^D \in L^2(S, V)$ as test function for $u' + A_M(u, v) = 0$. Since $u(t) = E_M(v(t))$ a.e. on S we have $v(t) - v^D \in \partial F_M(u(t))$ a.e. on S and the Brézis formula (cf. [1, Lemma 3.3]) yields

$$\begin{aligned}
F(u(t)) - F(u_0) &= \int_0^t \langle u'(s), v(s) - v^D\rangle \,\mathrm{d}s = -\int_0^t \langle A_M(u,v), v(s) - v^D\rangle \,\mathrm{d}s \\
&= -\int_0^t\int_\Omega \Big\{ \sum_{k=1}^4 D_k u_k \nabla\zeta_k \cdot \nabla(\zeta_k - \zeta_k^D) + \sum_{ij=12,34} r_{ij}(\mathrm{e}^{P_M v_i} - \mathrm{e}^{P_M v_j})(v_i - v_j - (v_i^D - v_j^D)) \\
&\qquad + \sum_{ij=13,14,23,24} r_{ij}(\cdot, u)(\mathrm{e}^{P_{2M}(v_i+v_j)} - 1)(v_i + v_j - (v_i^D + v_j^D))\Big\} \,\mathrm{d}x\,\mathrm{d}s \\
&\le \int_0^t\int_\Omega \sum_{k=1}^4 \Big\{ u_k\Big(-\delta|\nabla(\zeta_k - \zeta_k^D)|^2 + c|\nabla\zeta_k^D||\nabla(\zeta_k - \zeta_k^D)| + c\sum_{ij=12,34}|v_i^D - v_j^D|\Big) \\
&\qquad + c(u_k + 1)\sum_{ij=13,14,23,24}|v_i^D + v_j^D|\Big\}\mathrm{d}x\,\mathrm{d}s \\
&\le c\int_0^t \sum_{k=1}^4 (\|u_k\|_{L^1} + 1)\Big\{ \|\nabla\zeta_k^D\|^2_{L^\infty} + \sum_{ij=12,34}\|v_i^D - v_j^D\|_{L^\infty} + \sum_{ij=13,14,23,24}\|v_i^D + v_j^D\|_{L^\infty}\Big\} \,\mathrm{d}s.
\end{aligned}$$

Taking into account that $\|u_k\|_{L^1} \le F(u) + c$ (see (2.1)) and using Gronwalls lemma we find $F(u(t)) \le (F(u^0) + ct)\,\mathrm{e}^{ct}$ which proves the lemma. □

Remark 4.1 If (u, v) is a solution to $(\mathrm{P_M})$, then by Lemma 4.3 and (2.1), $\|v_0(t) - v_0^D\|_{H^1}$ and $\|u_i(t)\|_{L^1}$, $i = 1, \dots, 4$, are bounded for all $t \in S$.

Lemma 4.4 *Let* (A1) – (A5) *be satisfied. Then there exists a monotonous function* $d : \mathbb{R}_+ \to \mathbb{R}_+$ *depending only on the data* (*but not on* M, T) *such that*

$$\sum_{i=1}^4 \|u_i(t)\|_{L^2} \le d(\|F(u)\|_{C(S)}) \quad \forall t \in S$$

for any solution (u, v) *to* $(\mathrm{P_M})$.

Proof. We use the test function $\mathrm{e}^{2t}(0, z_1, z_2, z_3, z_4)$,

$$z_i := \Big(\frac{u_i}{\overline{u}_i} - K\Big)^+, \quad \text{where } K \geq \widehat{K} := \max\Big(1, \mathrm{e}^{\max_{i=1,\dots,4}\|v_i^D\|_{L^\infty}}, \max_{i=1,\dots,4}\|\frac{u_i^0}{\overline{u}_i}\|_{L^\infty}\Big) \tag{4.5}$$

will be fixed later. (Due to the choice of $\widehat{K}$ we have $z_i(0) = 0$, $z_i|_{\Gamma_D} = 0$, $z_i \in H_0^1(\Omega \cup \Gamma_N)$.)

$$\begin{aligned}
&\frac{\mathrm{e}^{2t}}{2}\,\underline{c}\sum_{i=1}^4 \|z_i(t)\|_{L^2}^2 \\
&= \int_0^t \mathrm{e}^{2s}\int_\Omega \Big\{\sum_{i=1}^4 \overline{u}_i z_i^2 - D_i u_i\Big(\frac{\overline{u}_i}{u_i}\nabla z_i + \gamma_i \nabla v_0\Big)\cdot\nabla z_i + \sum_{ij=12,34} r_{ij}\big(\mathrm{e}^{P_M v_j} - \mathrm{e}^{P_M v_i}\big)(z_i - z_j) \\
&\qquad + \sum_{ij=13,14,23,24} r_{ij}(\cdot,u)\big(1 - \mathrm{e}^{P_{2M}(v_i+v_j)}\big)(z_i + z_j)\Big\}\,\mathrm{d}x\,\mathrm{d}s \\
&\leq \int_0^t \mathrm{e}^{2s}\sum_{i=1}^4 \Big\{ -\delta\|z_i\|_{H^1}^2 + c\|u_i\|_{L^r}\big(\|\nabla(v_0 - v_0^D)\|_{L^q} + 1\big)\|z_i\|_{H^1} + c\|z_i\|_{L^2}^2 + cK^2\Big\}\,\mathrm{d}s.
\end{aligned}$$

Concerning the reaction terms we refer to Remark 2.1. Now we use (3.2) and the three variants of Gagliardo-Nirenberg estimates

$$\|z_i\|_{L^2}^2 \leq \|z_i\|_{L^1}\|z_i\|_{H^1}, \qquad \|z_i\|_{L^r} \leq \|z_i\|_{L^1}^{1/r}\|z_i\|_{H^1}^{1/r'}, \qquad \|z_i\|_{L^{r'}} \leq \|z_i\|_{L^1}^{1/r'}\|z_i\|_{H^1}^{1/r}.$$

Then Youngs inequality leads to

$$\begin{aligned}
\frac{e^{2t}}{2}\,\underline{c}\sum_{i=1}^4 \|z_i(t)\|_{L^2}^2 \leq \int_0^t e^{2s}\sum_{i=1}^4 \Big\{\Big(-\frac{\delta}{2} + \widehat{c}\sum_{j=1}^4 \|z_j\|_{L^1}\Big)\|z_i\|_{H^1}^2 \\
+ c(K)\big(\|z_i\|_{L^1}^2 + 1\big)\Big\}\mathrm{d}s
\end{aligned} \tag{4.6}$$

for all $t \in S$ with a monotonous increasing function $c(K)$. For $\ln K > 1$ we can estimate

$$\begin{aligned}
F(u) &\geq \sum_{i=1}^4 \int_\Omega \Big\{u_i\Big(\ln\frac{u_i}{\overline{u}_i} - 1\Big) + \overline{u}_i\Big\}\,\mathrm{d}x \\
&\geq \sum_{i=1}^4 \int_{\{x: z_i = (u_i/\overline{u}_i - K)^+ > 0\}} \Big\{u_i\Big(\ln\frac{u_i}{\overline{u}_i} - 1\Big) + \overline{u}_i\Big\}\,\mathrm{d}x \geq (\ln K - 1)\underline{c}\sum_{i=1}^4 \|z_i\|_{L^1}
\end{aligned}$$

with $\underline{c}$ from (A4). Fixing now $K \geq \widehat{K}$ as a monotonous increasing function of $\|F(u)\|_{C(S)}$ fulfilling

$$\Big(\widehat{c}\sum_{i=1}^4 \|z_i\|_{L^1} \leq\Big) \quad \frac{\widehat{c}\|F(u)\|_{C(S)}}{\underline{c}(\ln K - 1)} < \frac{\delta}{2}$$

(see Lemma 4.3), the term infront of the H^1-norm in (4.6) is negative. We obtain

$$e^{2t}\sum_{i=1}^4 \|z_i(t)\|_{L^2}^2 \leq e^{2t}\,c\,c(K)(\|F(u)\|_{C(S)}^2 + 1)$$

which together with $u_i \le \overline{u}_i(z_i + K)$ proves the Lemma. $\square$

According to Lemma 4.4, (3.2) and (A4), $\|\nabla v_0\|_{L^\infty(S,L^q(\Omega))}$ is bounded by a continuous function of $\|F(u)\|_{C(S)}$ depending on the data but not on M and T (for any solution (u, v) to $(\mathrm{P_M})$). We define

$$\kappa = \Big(\|\nabla v_0\|_{L^\infty(S,L^q(\Omega))} + 1\Big)^{2r}. \tag{4.7}$$

Theorem 4.1 *Let* (A1) – (A5) *be satisfied. Then there exists a* $c_3 > 0$ *depending only on the data* (*but not on* M, T) *such that*

$$\sum_{i=1}^{4} \|u_i(t)\|_{L^\infty} \le c_3\, \kappa \sum_{i=1}^{4} \Big(\sup_{s\in S} \|u_i(s)\|_{L^1} + 1\Big) \qquad \forall t \in S$$

for any solution (u, v) *to* $(\mathrm{P_M})$.

Proof. The proof is based on Moser iteration. In [4] such techniques are applied to the van Roosbroeck equations, in [11] to problems from semiconductor technology. Let $z_i := \big(\frac{u_i}{\overline{u}_i} - \widehat{K}\big)^+$, $i = 1, \dots, 4$, with $\widehat{K}$ from (4.5). Using the test functions

$$p\, e^{pt} \left(0, z_1^{p-1}, z_2^{p-1}, z_3^{p-1}, z_4^{p-1}\right) \in L^2(S, V), \quad p = 2^n, \quad n \ge 1,$$

taking into account Remark 2.1, applying Hölders, Gagliardo-Nirenbergs and Youngs inequality we obtain

$$\begin{aligned}
\underline{c}\, e^{pt} \sum_{i=1}^{4} \|z_i(t)\|_{L^p}^p &\le \int_0^t e^{ps} \int_\Omega \sum_{i=1}^{4} \Big\{ cp\big(u_i |\nabla v_0||\nabla z_i^{p-1}| + |z_i|^p + (u_i + 1) z_i^{p-1}\big) \\
&\qquad\qquad - \delta |\nabla z_i^{p/2}|^2 \Big\}\, dx\, ds \\
&\le \int_0^t e^{ps} \sum_{i=1}^{4} \Big\{ cp\big(\|\nabla v_0\|_{L^q} (\|z_i^{p/2}\|_{L^r} + 1)\|z_i^{p/2}\|_{H^1} \\
&\qquad\qquad + cp\big(\|z_i^{p/2}\|_{L^2}^2 + 1\big) - \delta \|z_i^{p/2}\|_{H^1}^2 \Big\}\, ds \\
&\le \int_0^t e^{ps} \Big\{ \kappa\, c\, p^{2r} \sum_{i=1}^{4} (\|z_i^{p/2}\|_{L^1}^2 + 1)\, ds \Big\}.
\end{aligned}$$

This guarantees the estimate

$$\sum_{i=1}^{4} \|z_i(t)\|_{L^p}^p \le c p^{2r} \kappa \sum_{i=1}^{4} \sup_{s\in S} (\|z_i(s)\|_{L^{p/2}}^p + 1) \qquad \forall t \in S. \tag{4.8}$$

Defining

$$\omega_n = \sum_{i=1}^{4} \Big\{ \sup_{s\in S} \|z_i(s)\|_{L^{2^n}}^{2^n} + 1 \Big\}, \quad n = 0, 1, \dots$$

inequality (4.8) leads to

$$\omega_n \le c^n\, \kappa\, \omega_{n-1}^2 \le c^{n+2(n-1)}\, \kappa^{1+2}\, \omega_{n-2}^4 \le \cdots \le c^{2^{n+1}-2-n}\, \kappa^{2^n-1}\, \omega_0^{2^n},$$

and we can continue estimate (4.8) by

$$\sum_{i=1}^{4} \|z_i(t)\|_{L^{2^n}} \le c\kappa \sum_{i=1}^{4} \Big\{ \sup_{s\in S} \|z_i(s)\|_{L^1} + 1 \Big\}.$$

Taking the limit $n \to \infty$, we find

$$\sum_{i=1}^{4} \|z_i(t)\|_{L^\infty} \le c\kappa \sum_{i=1}^{4} \Big\{ \sup_{s\in S} \|z_i(s)\|_{L^1} + 1 \Big\} \qquad \forall t \in S.$$

Since $u_i \le \overline{u}_i(z_i + \widehat{K})$ this supplies the desired estimate for the densities u_i. □

Theorem 4.2 *Let* (A1) – (A5) *be satisfied and let*

$$M \ge K := \sum_{i=1}^{4} \Big(\|\ln\big(\frac{u_i}{\overline{u}_i} + 1\big)\|_{L^\infty(S,L^\infty)} + \|v_i^D\|_{L^\infty} \Big) + \max_{i=1,\dots,4} \|\big(\ln \frac{u_i^0}{\overline{u}_i}\big)^-\|_{L^\infty}.$$

Then there exists a $c_4 > 0$ *depending only on the data* (*but not on* M, T) *such that*

$$-\ln \frac{u_i(t)}{\overline{u}_i} \le K + c_4\, \kappa^{5/2} \quad \forall t \in S,\ i = 1,\dots,4,$$

for any solution (u,v) *to* $(\mathrm{P_M})$.

Proof. Let (u,v) be a solution to $(\mathrm{P_M})$. The choice $M \ge K$ ensures that $v_i \le P_M v_i$. Our choice of K guarantees that $\big(\ln \frac{u_i}{\overline{u}_i} + K\big)^-(0) = 0$ and $\big(\ln \frac{u_i}{\overline{u}_i} + K\big)^- \in L^2(S, H_0^1(\Omega \cup \Gamma_N))$, $i = 1,\dots,4$. We fix some $i \in \{1,2,3,4\}$ and use test functions

$$-p\, e^{pt}\big(0,\dots,0, z^{p-1}\frac{\overline{u}_i}{u_i}, 0,\dots,0\big) \in L^2(S,V), \quad p \ge 2, \quad z := \big(\ln \frac{u_i}{\overline{u}_i} + K\big)^-.$$

(Analogously this can be done for the other components $j \ne i$.) If $z > 0$ then $v_i \le P_M v_i < -K$ and $v_i + v_j \le -K + \ln \frac{u_j}{\overline{u}_j} \le 0$, thus $(\mathrm{e}^{P_{2M}(v_i+v_j)} - 1)z \le 0$ for $ij = 13, 14, 23, 24$. Therefore the generation/recombination reactions give no contribution for our estimate. Moreover, for the spin relaxation reactions we can estimate from above $(\mathrm{e}^{P_M v_i} - \mathrm{e}^{P_M v_j})\frac{\overline{u}_i}{u_i} z \le z$. In summary we obtain

$$\begin{aligned}
&\underline{c}\, \mathrm{e}^{pt}\|z(t)\|_{L^p}^p \\
&\le \int_0^t \mathrm{e}^{ps} p \int_\Omega \Big\{ D_i u_i \nabla\zeta_i \cdot \nabla\Big(\frac{\overline{u}_i}{u_i} z^{p-1}\Big) + c(z^p + z^{p-1}) \Big\}\, \mathrm{d}x\, \mathrm{d}s \\
&\le \int_0^t \mathrm{e}^{ps} p \int_\Omega D_i \overline{u}_i (-\nabla z + \gamma_i \nabla v_0)(z^{p-1} + (p-1)z^{p-2}) \cdot \nabla z + c(z^p + 1) \Big\}\, \mathrm{d}x\, \mathrm{d}s \\
&\le \int_0^t \mathrm{e}^{ps} \Big\{ -\frac{\delta}{p} \|z^{(p+1)/2}\|_{H^1}^2 - \delta \|z^{p/2}\|_{H^1}^2 \\
&\qquad + cp\|\nabla v_0\|_{L^q}(\|z^{p/2}\|_{L^r} + 1)\|z^{p/2}\|_{H^1} + cp(\|z^{p/2}\|_{L^2}^2 + 1) \Big\}\, \mathrm{d}s \\
&\le \int_0^t \mathrm{e}^{ps} \Big\{ -\frac{\delta}{p} \|z^{(p+1)/2}\|_{H^1}^2 + cp^{2r}\kappa(\|z^{p/2}\|_{L^1}^2 + 1) \Big\}\, \mathrm{d}s.
\end{aligned} \tag{4.9}$$

Here we used Hölders, Gagliardo-Nirenbergs and Youngs inequality and (4.7). Setting

$$\omega_n = \sup_{s\in S} \|z(s)\|_{L^{2^n}}^{2^n} + 1, \quad n = 0, 1, 2, \ldots$$

we find $\omega_n \le c^n \kappa \omega_{n-1}^2$ and $\omega_n \le (c\kappa\,\omega_0)^{2^n}$ which means $\|z(t)\|_{L^{2^n}} \le c\kappa(\sup_{s\in S}\|z(s)\|_{L^1} + 1)$, and leads in the limit $n \to \infty$ to

$$\|z(t)\|_{L^\infty} \le c\kappa(\sup_{s\in S}\|z(s)\|_{L^1} + 1) \quad \forall t \in S. \tag{4.10}$$

Considering the inequality (4.9) for $p = 2$ and estimating for $d \in \mathbb{R}_+$, $z \in H_0^1(\Omega \cup \Gamma_N)$

$$d\|z\|_{L^1}^2 \le dc\,\|z\|_{L^{3/2}}^2 = dc\,\|z^{3/2}\|_{L^1}^{4/3} \le dc\,\|z^{3/2}\|_{H^1}^{4/3} \le \frac{\delta}{2}\|\nabla z^{3/2}\|_{L^2}^2 + cd^3,$$

we get $\|z(t)\|_{L^2}^2 \le c\kappa^3$ for all $t \in S$. Therefore $\|z(t)\|_{L^1} \le c\|z(t)\|_{L^2} \le c\kappa^{3/2}$ for all $t \in S$ and together with (4.10) we obtain $\|z(t)\|_{L^\infty} \le c\kappa^{5/2}$ for all $t \in S$. This ensures

$$-\ln\frac{u_i(t)}{\overline{u}_i} \le K + c_4\kappa^{5/2} \quad \text{a.e. in } \Omega \quad \forall t \in S. \qquad \square$$

4.4 Solvability of problem (P)

Theorem 4.3 *Under the assumptions* (A1) – (A5) *there exists a* (*unique*) *solution to problem* (P)*.*

Proof. It suffices to prove that for every $T > 0$, $S = [0, T]$ the problem

$$\begin{aligned} &u' + A(u, v) = 0, \quad u = Ev \text{ a.e. on } S, \quad u(0) = u^0, \\ &u \in H^1(S, V^*), \quad v - v^D \in L^2(S, V) \cap L^\infty(S, L^\infty(\Omega, \mathbb{R}^5)) \end{aligned} \tag{4.11}$$

is solvable. The a priori estimates for $(\mathrm{P_M})$ in Theorem 4.1 and Theorem 4.2 guarantee that if we choose M sufficiently large, then for every solution (u, v) to $(\mathrm{P_M})$ the equalities

$$P_M v_i = v_i,\ i = 1, \ldots, 4, \quad P_{2M}(v_i + v_j) = v_i + v_j,\ ij = 13, 14, 23, 24,$$

hold. Therefore we have $E_M v = Ev$, $A_M(u, v) = A(u, v)$ and the pair (u, v) is a solution to (4.11), too. Uniqueness is given by Theorem 3.1. $\square$

5 Global behavior of solutions to (P)

5.1 Boundedness of solutions to (P)

The estimates for solutions to $(\mathrm{P_M})$ in the proofs of Lemma 4.3, Lemma 4.4, Theorem 4.1 and Theorem 4.2 are done in such a way that they can be applied to Problem (P), too. Especially, since $u(t) = Ev(t)$ a.e. we have $v(t) - v^D \in \partial F(u(t))$ a.e. and Brézis formula is applicable to obtain the estimate for the free energy. By discussing the different cases we here find

$$r_{ij}(\cdot,u)(1-\mathrm{e}^{v_i+v_j})(v_i+v_j-(v_i^D+v_j^D)) \le c\sum_{k=1}^4 (u_k+1)|v_i^D+v_j^D|, \quad ij=13,14,23,24.$$

Generally, where we in the proofs substituted $\mathrm{e}^{P_M v_i}$ by $u_i/\overline{u}_i$ we now have to substitute e^{v_i} by $u_i/\overline{u}_i$. And in the proof of Theorem 4.2 we argue: If $z>0$ then

$$v_i+v_j \le -K+\ln\frac{u_i}{\overline{u}_i} \le 0 \quad \text{and} \quad (\mathrm{e}^{v_i+v_j}-1)z \le 0, \quad ij=13,14,23,24,$$

$$(\mathrm{e}^{v_i}-\mathrm{e}^{v_j})\frac{\overline{u}_i}{u_i}z \le z, \quad ij=12,34.$$

We summerize the results in two theorems.

Theorem 5.1 *Let* (A1) – (A5) *be satisfied and let* $T>0$ *be arbitrarily given. Then there exists a constant* $c_1>0$ *depending only on the data* (*but not on* T) *such that*

$$F(u(t)) \le (F(u^0)+1)e^{c_1 t} \qquad \forall t\in S=[0,T]$$

for the solution (u,v) *to* (P).

Theorem 5.2 *Let* (A1) – (A5) *be satisfied and let* $T>0$ *be arbitrarily given. Then there exist constants* $c_3, c_4>0$ *depending only on the data* (*but not on* T) *such that*

$$\sum_{i=1}^4 \|u_i(t)\|_{L^\infty} \le c_3\,\kappa \sum_{i=1}^4 \Big(\sup_{s\in S}\|u_i(s)\|_{L^1}+1\Big),$$

$$-v_i(t) \le \sum_{k=1}^4 \Big(\|\ln(\frac{u_k}{\overline{u}_k}+1)\|_{L^\infty(S,L^\infty)}+\|v_k^D\|_{L^\infty}\Big)+\max_{i=1,\dots,4}\|\big(\ln\frac{u_i^0}{\overline{u}_i}\big)^-\|_{L^\infty}+c_4\kappa^{5/2},$$

$i=1,\dots,4$, *for all* $t\in S=[0,T]$ *for the solution* (u,v) *to* (P).

Some of the results of this section are obtained under the additional assumption

(A6) $\nabla(v_k^D+\gamma_k v_0^D)=0, \quad k=1,\dots,4,$

$v_i^D=v_j^D,\ ij=12,34, \quad v_i^D+v_j^D=0,\ ij=13,14,23,24.$

These conditions mean that the prescribed boundary values are compatible with thermodynamic equilibrium which is a state with vanishing flows of the carriers, and with vanishing reaction rates. (A6) implies that $\zeta^D\in$ span γ.

Theorem 5.3 *Under the assumptions* (A1) – (A6) *the following global estimates for the solution* (u,v) *to* (P) *are satisfied*

$$F(u(t_2)) \le F(u(t_1)) \le F(u^0) \quad \forall t_2\ge t_1\ge 0,$$
$$\sum_{i=1}^4\|u_i(t)\|_{L^\infty}\le c, \quad \sum_{i=1}^4\|v_i(t)^-\|_{L^\infty}\le c \quad \forall t>0. \tag{5.1}$$

Proof. Using (A6), $\gamma = (-1,-1,1,1)$ and the techniques of Lemma 4.3 we obtain

$$F(u(t_2)) - F(u(t_1)) = -\int_0^t \int_\Omega \Big\{ \sum_{k=1}^4 D_k u_k |\nabla \zeta_k|^2 + \sum_{ij=12,34} r_{ij} (\mathrm{e}^{v_i} - \mathrm{e}^{v_j})(v_i - v_j) + \sum_{ij=13,14,23,24} r_{ij}(\cdot,u)(\mathrm{e}^{v_i+v_j} - 1)(v_i + v_j) \Big\} \,\mathrm{d}x\,\mathrm{d}s \le 0,$$

and the monotone decay of the free energy follows. Especially $F(u(t)) \le F(u^0)$ for all $t > 0$. Thus by (2.1), $\|u_i(t)\|_{L^1} \le F(u(t)) + c \le F(u^0) + c$ for all $t > 0$. Moreover $\|\nabla v_0(t)\|_{L^q} \le c$ for all $t > 0$. Having in mind (4.7), Theorem 5.2 yields a uniform upper bound for the densities u_i on $\mathbb{R}_+$. Therefore $\|\ln(\frac{u_i}{\overline{u}_i} + 1)\|_{L^\infty(\mathbb{R}_+,L^\infty)} \le c$, and Theorem 5.2 supplies that $\|v_i^-\|_{L^\infty(\mathbb{R}_+,L^\infty)} \le c$. $\square$

5.2 Steady states

Remember that for solutions (u, v) to (P)

$$u_0(t) = \sum_{i=1}^4 \gamma_i u_i(t), \quad t > 0.$$

(This follows easily from $u' + A(u, v) = 0$ by test functions (w, qw), $w \in H_0^1(\Omega \cup \Gamma_N)$.) Therefore we would expect also for stationary solutions (u, v) to (P) that $u_0 = \sum_{i=1}^4 \gamma_i u_i$. We look at the stationary problem

$$A(u^*, v^*) = 0, \quad u^* = Ev^*, \quad u_0 = \textstyle\sum_{i=1}^4 \gamma_i u_i, \quad (u^*, v^*) \in U \times (V + v^D). \tag{S}$$

We give an existence result for steady states (S) which is obtained similarly to the corresponding result for the van Roosbroeck system in [15, 4] by Schauder's Fixed Point Theorem. We need two preparatory lemmas. The first lemma can be found in [14].

Lemma 5.1 *Let $\widetilde{k} > 0$, $s > 1$. Furthermore, let $\phi : [\widetilde{k}, \infty) \to \mathbb{R}_+$ be a nonincreasing function such that, for $h \ge k \ge \widetilde{k}$:*

$$(h - k)\phi(h) \le c_1 \phi(k)^s.$$

Then $\phi(k) = 0$ if $k \ge \widetilde{k} + 2^{-s/(s-1)} c_1\, \phi(\widetilde{k})^{s-1}$.

Let $M := \max\big\{\|v_0^D\|_{L^\infty}, \max_{i=1,2,3,4} \|\zeta_i^D\|_{L^\infty}\big\}$.

Lemma 5.2 *We assume* (A1) *and* (A4)*. Let $v_0 \in v_0^D + H_0^1(\Omega \cup \Gamma_N)$ be the solution to*

$$\widehat{E}_0 v_0 = 0, \quad \langle \widehat{E}_0 v_0, \overline{v}_0 \rangle := \langle E_0 v_0, \overline{v}_0 \rangle - \sum_{i=1}^4 \int_\Omega \gamma_i \overline{u}_i e^{P_M \zeta_i - \gamma_i P_N v_0} \overline{v}_0 \, dx, \tag{5.2}$$

for all $\overline{v}_0 \in H_0^1(\Omega \cup \Gamma_N)$, with arbitrarily given $\zeta_i \in L^2(\Omega)$, $i = 1,2,3,4$, and some constant $N > M$. Then there exists a $K_0 > 0$ not depending on M, N, ζ_i, $i = 1,2,3,4$, such that $\|v_0\|_{L^\infty} \le M + K_0$.

Proof. $\widehat{E}_0(\cdot + v_0^D) : H_0^1(\Omega \cup \Gamma_N) \to H^{-1}(\Omega \cup \Gamma_N)$ is strongly monotone and Lipschitz continuous. Thus, for arbitrarily given $\zeta_i \in L^2(\Omega)$, $i = 1,2,3,4$, the equation $\widehat{E}_0 v_0 = 0$ has exactly one solution. If $k \geq M$ then $(v_0 - k)^+ \in H_0^1(\Omega \cup \Gamma_N)$. We use it as test function for (5.2). Since $P_M\zeta_i - \gamma_i P_N v_0 < 0$ for $v_0 > k$ and $\gamma_i > 0$ we obtain

$$\|(v_0-k)^+\|_{H^1}^2 \leq c\|(v_0-k)^+\|_{W^{1,q'}} \leq c\|(v_0-k)^+\|_{H^1}\mathrm{mes}\{v_0 > k\}^{1/r}$$

with the exponents from (3.1) and constants c not depending on M, N, ζ_i, $i = 1,2,3,4$. Therefore, for $p > r$ it results $\|(v_0-k)^+\|_{L^p} \leq \mathrm{mes}\{v_0 > k\}^{1/r}$. Because of

$$\|(v_0-k)^+\|_p \geq (h-k)\,\mathrm{mes}\{v_0 > h\}^{1/p}$$

the last estimates guarantee for $h \geq k \geq M$ that

$$(h-k)\phi(h) \leq c\phi(k)^s \quad \text{with } \phi(h) = \mathrm{mes}\{v_0 > h\}^{1/r},\ s = \frac{p}{r}.$$

Thus Lemma 5.1 ensures a $K_0 > M$ such that $v_0 \leq k$ for all $k \geq M + K_0$. Testing (5.2) by $-(v_0+K)^-$, we prove that $v_0 \geq -(M+K_0)$. □

Theorem 5.4 *Under the assumptions* (A1) – (A5) *there exists a solution to* (S).

Proof. 1. We use M and K_0 from Lemma 5.2. For arbitrarily given $(v_0, \zeta_1, \ldots, \zeta_4) \in L^2(\Omega)^5$ we define $u_i = \overline{u}_i \mathrm{e}^{P_M\zeta_i - \gamma_i P_{M+K_0}v_0}$, $i = 1,2,3,4$. Let $\widetilde{v}_0 \in v_0^D + H_0^1(\Omega \cup \Gamma_N)$, $\widetilde{\zeta}_i \in \zeta_i^D + H_0^1(\Omega \cup \Gamma_N)$, $i = 1,2,3,4$, be the solution of the system

$$\langle E_0\widetilde{v}_0, \overline{v}_0\rangle = \sum_{i=1}^4 \int_\Omega \gamma_i u_i \overline{v}_0 \,\mathrm{d}x, \quad \forall \overline{v}_0 \in H_0^1(\Omega \cup \Gamma_N), \tag{5.3}$$

$$\begin{aligned}\int_\Omega \Big\{ \sum_{k=1}^4 D_k u_k \nabla\widetilde{\zeta}_k \cdot \nabla\overline{\zeta}_k + \sum_{ij=12,34} r_{ij} \mathrm{e}^{\frac{5-i-j}{2}P_{M+K_0}v_0}(\mathrm{e}^{P_M\zeta_i} - \mathrm{e}^{P_M\zeta_j})(\overline{\zeta}_i - \overline{\zeta}_j) \\ + \sum_{ij=13,14,23,24} r_{ij}(\cdot,u)(\mathrm{e}^{P_M\zeta_i + P_M\zeta_j} - 1)(\overline{\zeta}_i + \overline{\zeta}_j)\Big\}\,\mathrm{d}x = 0 \quad \forall\overline{\zeta} \in H_0^1(\Omega\cup\Gamma_N)^4.\end{aligned} \tag{5.4}$$

2. Due to our assumptions concerning the data, the test of (5.3) by $\widetilde{v}_0 - v_0^D$ and the test of (5.4) by $\widetilde{\zeta} - \zeta^D$ we find that $\|\widetilde{v}_0 - v_0^D\|_{H^1}$ and $\|\widetilde{\zeta}_i - \zeta_i^D\|_{H^1}$, $i = 1,2,3,4$, are bounded by a constant which depends on M and K_0 but which does not depend on $v_0, \zeta_1, \ldots, \zeta_4$. Thus the same is true for $\|\widetilde{v}_0\|_{H^1}$ and $\|\widetilde{\zeta}_i\|_{H^1}$, Sobolev's imbedding result gives $\|\widetilde{v}_0\|_{L^2} \leq \widetilde{c}$, $\|\widetilde{\zeta}_i\|_{L^2} \leq \widetilde{c}$. We define

$$\mathcal{A} = \{y \in L^2(\Omega)^5 : \|y_i\|_{L^2} \leq \widetilde{c}, i = 1,\ldots,5\}.$$

3. Let $\mathcal{T}$ denote the operator which assigns to $(v_0, \zeta_1, \ldots, \zeta_4)$ the solution $(\widetilde{v}_0, \widetilde{\zeta}_1, \ldots, \widetilde{\zeta}_4)$ of (5.3), (5.4), $\mathcal{T}(v_0, \zeta_1, \ldots, \zeta_4) = (\widetilde{v}_0, \widetilde{\zeta}_1, \ldots, \widetilde{\zeta}_4)$. We consider $\mathcal{T}$ as mapping from $L^2(\Omega)^5$ into itself and verify the assumptions of Schauder's Fixed Point Theorem. $\mathcal{T}$ maps the convex, closed set $\mathcal{A}$ into itself. Due to step 2 and the Rellich-Kondrachov imbedding Theorem, $\mathcal{T}(\mathcal{A})$ is precompact in $L^2(\Omega)^5$. The continuity of $\mathcal{T}$ is guaranteed by continuity properties of Nemyckij operators. Thus $\mathcal{T}$ possesses at least one fixed point.

4. Let $(v_0,\zeta_1,\dots,\zeta_4)$ be a fixed point of $\mathcal{T}$. Due to Lemma 5.2 we have $\|v_0\|_{L^\infty}\le M+K_0$. On the one hand, testing (5.4) (for $\widetilde{\zeta}=\zeta$) by $(\zeta-M)^+\in H_0^1(\Omega\cup\Gamma_N)^4$ we obtain

$$c\sum_{k=1}^4\|(\zeta_k-M)^+\|_{H^1}^2$$
$$\le\int_\Omega\Big\{\sum_{k=1}^4 D_k|\nabla(\zeta_i-M)^+|^2+\sum_{ij=13,14,23,24}r_{ij}(\cdot,u)(\mathrm{e}^{P_M\zeta_i+P_M\zeta_j}-1)((\zeta_i-M)^++(\zeta_j-M)^+)$$
$$+\sum_{ij=12,34}r_{ij}\mathrm{e}^{\frac{5-i-j}{2}P_{M+K_0}v_0}(\mathrm{e}^{P_M\zeta_i}-\mathrm{e}^{P_M\zeta_j})((\zeta_i-M)^+-(\zeta_j-M)^+)\Big\}\,\mathrm{d}x=0.$$

Here we used that the expressions $(\mathrm{e}^M-\mathrm{e}^{P_M\zeta_j})(\zeta_i-M)^+$ and $(\mathrm{e}^{M+P_M\zeta_j}-1)(\zeta_i-M)^+$ for $\zeta_i>M$ are nonnegative and can be omitted in the estimate. On the other hand, the test function $(\zeta+M)^-$ supplies that $\zeta_i\ge -M$, $i=1,2,3,4$. Consequently, $P_M\zeta_i=\zeta_i$ and $u_i=\overline{u}_i\mathrm{e}^{\zeta_i-\gamma_i v_0}$, $i=1,2,3,4$. Defining $u=(E_0v_0,u_1,\dots,u_4)$, $v=(v_0,\zeta_1+v_0,\zeta_2+v_0,\zeta_3-v_0,\zeta_4-v_0)$, we obtain from a fixed point $(v_0,\zeta_1,\dots,\zeta_4)$ of $\mathcal{T}$ a solution (u,v) to (S). □

Theorem 5.5 *Let the assumptions* (A1) – (A6) *be satisfied. Then there exists a unique solution* (u^*,v^*) *to* (S). *Moreover,* $\nabla\zeta_i^*=0$, $i=1,\dots,4$, *and* $\zeta^*=(\zeta_1^*,\zeta_2^*,\zeta_3^*,\zeta_4^*)=\zeta^D$.

Proof. 1. If (u^*,v^*) is a solution to (S) then we have $\langle A(u^*,v^*),v^*-v^D\rangle=0$. Since (A6) is fulfilled this implies $\nabla(v_i^*+\gamma_i v_0^*)=0$, $i=1,\dots,4$, $v_i^*=v_j^*$, $ij=12,34$, $v_i^*+v_j^*=0$, $ij=13,14,23,24$. Let $h^*:=v_0^*-v_0^D$. The boundary conditions enforce $v_i^*+\gamma_i v_0^*=v_i^D+\gamma_i v_0^D$, $i=1,\dots,4$. Therefore we would have

$$u_i^*=\overline{u}_i\mathrm{e}^{v_i^D+\gamma_i v_0^D-\gamma_i(h^*+v_0^D)}=\overline{u}_i\mathrm{e}^{v_i^D-\gamma_i h^*},\quad i=1,\dots,4.$$

Moreover, the requirements from (S) that $u_0^*=\sum_{i=1}^4\gamma_i u_i^*=E_0v_0^*$ lead to

$$\langle\widetilde{E}_0h^*,\overline{y}\rangle:=\int_\Omega\Big\{\varepsilon\nabla(h^*+v_0^D)\cdot\nabla\overline{y}-f\overline{y}-\sum_{i=1}^4\gamma_i\overline{u}_i\mathrm{e}^{v_i^D-\gamma_i h^*}\overline{y}\Big\}\,\mathrm{d}x=0\quad\forall\overline{y}\in H_0^1(\Omega\cup\Gamma_N).$$

Due to (A1) and (A4), the operator $\widetilde{E}_0\colon H_0^1(\Omega\cup\Gamma_N)\to H^{-1}(\Omega\cup\Gamma_N)$ is strongly monotone. Using Trudingers imbedding theorem [18], the hemicontinuity of this operator can be shown. Therefore there exists a unique solution $h^*\in H_0^1(\Omega\cup\Gamma_N)$ of $\widetilde{E}_0h^*=0$. Now we improve the regularity of h^*. Due to (A4) and Trudingers imbedding theorem $\sum_{i=1}^4\gamma_i\overline{u}_i\mathrm{e}^{v_i^D+\gamma_i h^*}\in L^2(\Omega)$. For

$$\langle\mathcal{E}_0h,\overline{y}\rangle=\int_\Omega\varepsilon\nabla h\cdot\nabla\overline{y}\,\mathrm{d}x,\quad\langle g,\overline{y}\rangle=\int_\Omega\Big\{f+\sum_{i=1}^4\gamma_i\overline{u}_i\mathrm{e}^{v_i^D-\gamma_i h^*}\Big\}\overline{y}\,\mathrm{d}x,\quad\overline{y}\in H_0^1(\Omega\cup\Gamma_N),$$

we have $g\in W^{-1,q}(\Omega\cup\Gamma_N)$, and $\widetilde{E}_0h^*=0$ is equivalent to $\mathcal{E}_0h^*=g$. Thus the regularity result of Gröger [12, Theorem 1] for linear elliptic equations ensures $h^*\in W_0^{1,q}(\Omega\cup\Gamma_N)$, for our $q>2$. Therefore $h^*\in L^\infty(\Omega)$, too.

2. We construct the unique solution to (S) now as follows: We solve $\widetilde{E}_0h^*=0$, obtain a unique solution $h^*\in H_0^1(\Omega\cup\Gamma_N)\cap L^\infty(\Omega)$. Setting $v_0^*:=h^*+v_0^D\in L^\infty(\Omega)$, $v_i^*:=v_i^D+\gamma_i v_0^D-\gamma_i v_0^*\in L^\infty(\Omega)$, $u_i^*:=\overline{u}_i\mathrm{e}^{v_i^*}\in L^\infty(\Omega)$, $i=1,\dots,4$, $u_0^*:=\sum_{i=1}^4\gamma_i u_i^*$. □

Remark 5.1 Theorem 5.5 says that if the boundary conditions are compatible with thermodynamic equilibrium then (S) is uniquely solvable and the solution is a thermodynamic equilibrium. In addition let us remark that local existence and uniqueness for (S) can be proved for data v^D "nearly" fulfilling (A6) by methods we used in [10] for stationary energy models with multiple species. (In the present model we have no energy balance equation and consider the temperature as a constant parameter.) The stationary problem (S) has to be formulated in a $W^{1,p}$ setting, $p > 2$, where the homogeneous part and the Dirichlet boundary functions of the potentials are considered as two different arguments. Then the linearization of the problem with respect to the homogeneous part of the potentials taken in the thermodynamic equilibrium turns out to be an injective Fredholm operator of index zero. Thus the Implicit Function Theorem supplies a unique solution to the stationary problem (S) provided that

$$\|\nabla\zeta_k^D\|_{L^p(\Omega)},\ k=1,2,3,4, \quad \|v_i^D - v_j^D\|_{L^1(\Gamma_D)},\ ij=12,34,$$

$$\|v_i^D + v_j^D\|_{L^1(\Gamma_D)},\ ij=13,14,23,24,$$

are sufficiently small (see [10, Theorem 2, Corollary 2]).

5.3 Exponential decay of the free energy

Theorem 5.6 *We assume* (A1) – (A6)*. Let* (u^*, v^*) *be the thermodynamic equilibrium according to Theorem 5.5. Then the solution* (u, v) *to* (P) *possesses the following asymptotics. There exist constants* c, $\lambda, \lambda_p > 0$ *such that*

$$F(u(t)) - F(u^*) \le e^{-\lambda t}(F(u^0) - F(u^*)) \quad \forall t \in \mathbb{R}_+, \tag{5.5}$$

$$\sum_{i=0}^4 \|u_i(t) - u_i^*\|_{L^p},\ \sum_{i=0}^4 \|v_i(t) - v_i^*\|_{L^p} \le ce^{-\lambda_p t} \quad \forall t \in \mathbb{R}_+ \quad \textit{where } p \in [1,\infty). \tag{5.6}$$

Proof. 1. Let (u, v) be the solution to (P). The next considerations we do f.a.a. $t \in \mathbb{R}_+$ and leave the argument t. Defining $\overline{v}_0 := v_0 - v_0^*$, $w_i := \mathrm{e}^{(\zeta_i - \zeta_i^*)/2} - 1$ we have $w_i|_{\Gamma_D} = 0$ and

$$\sqrt{u_i/u_i^*} - 1 = w_i \mathrm{e}^{-\gamma_i \overline{v}_0/2} + \mathrm{e}^{-\gamma_i \overline{v}_0/2} - 1. \tag{5.7}$$

Since $\|v_0\|_{L^\infty(\mathbb{R},L^\infty)}$, $\|v_0^*\|_{L^\infty} \le c$ we conclude that

$$\|\sqrt{u_i/u_i^*} - 1\|_{L^4} \le c(\|w_i\|_{L^4} + \|\overline{v}_0\|_{L^4}), \quad i = 1, \dots, 4. \tag{5.8}$$

Testing the equation $E_0 v_0 - E_0 v_0^* = u_u - u_0^*$ with $\overline{v}_0$, using the strong monotonicity of E_0

and (5.7) we obtain

$$
\begin{aligned}
c\|\overline{v}_0\|_{H^1}^2 &\le \int_\Omega \sum_{i=1}^4 \gamma_i \sqrt{u_i^*}(\sqrt{u_i} + \sqrt{u_i^*})(\sqrt{u_i/u_i^*} - 1)\overline{v}_0 \,\mathrm{d}x \\
&\le \int_\Omega \sum_{i=1}^4 \gamma_i \sqrt{u_i^*}(\sqrt{u_i} + \sqrt{u_i^*})\Big(w_i \mathrm{e}^{-\gamma_i \overline{v}_0/2} + \mathrm{e}^{-\gamma_i \overline{v}_0/2} - 1\Big)\overline{v}_0 \,\mathrm{d}x \\
&\le c\sum_{i=1}^4 \|w_i\|_{L^2}\|\overline{v}_0\|_{L^2} + \int_\Omega \sum_{i=1}^4 \sqrt{u_i^*}(\sqrt{u_i} + \sqrt{u_i^*})\gamma_i \overline{v}_0(\mathrm{e}^{-\gamma_i \overline{v}_0/2} - 1)\,\mathrm{d}x \\
&\le c\sum_{i=1}^4 \|w_i\|_{L^2}\|\overline{v}_0\|_{L^2}.
\end{aligned}
$$

Here we used that $z(\mathrm{e}^{-z} - 1) \le 0$ for $z \in \mathbb{R}$. In summary we find that

$$
\|\overline{v}_0\|_{H^1} \le c\sum_{i=1}^4 \|w_i\|_{L^2}. \tag{5.9}
$$

Since $\zeta^* = \zeta^D$ we have $\langle u - u^*, v^* - v^D\rangle = 0$. Using additionally (5.1) in Theorem 5.3, (5.8), (5.9) we estimate

$$
\begin{aligned}
\Psi(u) &:= F(u) - F(u^*) \\
&= \int_\Omega \Big\{\frac{\varepsilon}{2}|\nabla \overline{v}_0|^2 + \sum_{i=1}^4 \Big[u_i \ln \frac{u_i}{u_i^*} - u_i + u_i^*\Big]\Big\}\,\mathrm{d}x + \langle u - u^*, v^* - v^D\rangle \\
&\le c\Big(\|\overline{v}_0\|_{L^2}^2 + \sum_{i=1}^4 \|u_i - u_i^*\|_{L^2}^2\Big) \le c\Big(\|\overline{v}_0\|_{L^2}^2 + \sum_{i=1}^4 \|\sqrt{u_i/u_i^*} - 1\|_{L^4}^2\Big) \\
&\le c\Big(\|\overline{v}_0\|_{L^2}^2 + \sum_{i=1}^4 \|w_i\|_{L^4}^2 + \|\overline{v}_0\|_{L^4}^2\Big) \le c\sum_{i=1}^4 \|w_i\|_{H^1}^2.
\end{aligned} \tag{5.10}
$$

Because of $\|v_0\|_{L^\infty(\mathbb{R},L^\infty)}$, $\|v_0^*\|_{L^\infty} \le c$, under assumption (A6) the following inequality holds true

$$
\langle A(u(s), v(s)), v(s) - v^*\rangle \ge c\sum_{i=1}^4 \|w_i\|_{H^1}^2. \tag{5.11}
$$

2. If (u, v) is a solution to (P) then $v(t) - v^* \in \partial\Psi(u(t))$ f.a.a. $t \in \mathbb{R}_+$, and for $\lambda \in \mathbb{R}$ we obtain (cf. [1])

$$
\begin{aligned}
\mathrm{e}^{\lambda t_2}\Psi(u(t_2)) - \mathrm{e}^{\lambda t_1}\Psi(u(t_1)) &= \int_{t_1}^{t_2} \mathrm{e}^{\lambda s}\big\{\lambda\Psi(u(s)) + \langle u'(s), v(s) - v^*\rangle\big\}\,\mathrm{d}s \\
&= \int_{t_1}^{t_2} \mathrm{e}^{\lambda s}\big\{\lambda\Psi(u(s)) - \langle A(u(s), v(s)), v(s) - v^*\rangle\big\}\,\mathrm{d}s.
\end{aligned}
$$

Combining (5.10) and (5.11) we find a constant $\lambda > 0$ depending only on the data such that $\lambda\Psi(u(s)) \le \langle A(u(s), v(s)), v(s) - v^*\rangle$ f.a.a. $t \in \mathbb{R}_+$. Therefore the previous inequality and (5.10) supply the exponential decay of the free energy to its equilibrium value (5.5).

3. Since $\Psi(u) \geq c(\|\overline{v}_0\|_{H^1}^2 + \sum_{i=1}^4 \|\sqrt{u_i/u_i^*} - 1\|_{L^2}^2)$ and u_i and u_i^* are bounded, it results

$$\|\overline{v}_0(t)\|_{H^1},\ \|\sqrt{u_i(t)/u_i^*} - 1\|_{L^2},\ \|u_i(t) - u_i^*\|_{L^1} \leq c\mathrm{e}^{\lambda t/2} \quad \forall t \in \mathbb{R}_+.$$

For $p \in [1, \infty)$ and $i = 1, \dots, 4$, we obtain

$$\|u_i(t) - u_i^*\|_{L^p}^p \leq \|u_i(t) - u_i^*\|_{L^1} \|u_i(t) - u_i^*\|_{L^\infty}^{p-1} \leq c^p\, \mathrm{e}^{-\lambda t/2} \quad \forall t \in \mathbb{R}_+. \tag{5.12}$$

For $i = 0$ we get the corresponding result from $u_0 = \sum_{k=1}^4 \gamma_k u_k$, $u_0^* = \sum_{k=1}^4 \gamma_k u_k^*$ by the previous arguments.

4. From $\|\overline{v}_0(t)\|_{H^1} \leq c\mathrm{e}^{\lambda t/2}$ and $\|\overline{v}_0(t)\|_{L^\infty} \leq c$ we conclude

$$\|\overline{v}_0(t)\|_{L^p}^p \leq \|\overline{v}_0(t)\|_{L^1} \|\overline{v}_0(t)\|_{L^\infty}^{p-1} \leq c^{p-1} \|\overline{v}_0(t)\|_{H^1} \leq c^p\, \mathrm{e}^{-\lambda t/2} \quad \forall t \in \mathbb{R}_+.$$

Finally,

$$\|v_i(t) - v_i^*\|_{L^1} \leq \|\ln u_i - \ln u_i^*\|_{L^1} \leq c \|u_i(t) - u_i^*\|_{L^1} \quad \forall t \in \mathbb{R}_+, \quad i = 1, \dots, 4,$$

which analogously to (5.12) leads to the exponential decay of $\|v_i(t) - v_i^*\|_{L^p}$. □

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