Institut für Angewandte Analysis und Stochastik

im Forschungsverbund Berlin e.V.

Existence and uniqueness results for equations modelling transport of dopants in semiconductors

A. Glitzky, K. Gröger, R. Hünlich[1]

submitted: 10th April 1995

[1] Institut für Angewandte Analysis
und Stochastik
Hausvogteiplatz 5 – 7
D – O 1086 Berlin
Germany

Preprint No. 29
Berlin 1992

Key words and phrases. Transport of dopants in semiconductors, reaction–diffusion equations, Lyapunov–function, a–priori estimates, global existence, uniqueness, asymptotic behaviour.
This paper is in final form and no version of it will be submitted for publication elsewhere.

Herausgegeben vom
Institut für Angewandte Analysis und Stochastik
Mohrenstraße 39
D — 10117 Berlin

Fax:	+ 49 30 2004975
e–mail (X.400):	c=de;a=d400;p=iaas-berlin;s=preprint
e–mail (Internet):	preprint@iaas-berlin.d400.de

Contents

Abstract. This paper is devoted to the analytical investigation of some nonlinear reaction–diffusion system modelling the transport of dopants in semiconductors. Estimates by the energy functional and L^∞–estimates obtained by a modified De Giorgi method imply global existence and uniqueness as well as results concerning the asymptotic behaviour.

1. Transport of dopants in semiconductors

Modelling the transport of dopant impurities in semiconducting materials is of great interest, both for scientific and technological reasons. It may be rather surprising that given the significance of that phenomenon there exists neither a generally accepted physical model nor a comprehensive mathematical analysis of the various model equations. There have been developed different models from a chemical kinetics viewpoint (see e.g. [5, 14, 15, 17]). More or less simplified models have been used for engineering analysis and computer aided simulation (see e.g. [9, 11, 12, 16]).

This paper is devoted to the mathematical analysis of a relatively simple model which demonstrates typical difficulties arising in attacking such problems. Our aim is to show that the corresponding model equations are well posed from the thermodynamic and the mathematical point of view.

First, we shall shortly explain the physical model which we are going to consider. Let Ω be the domain occupied by the semiconductor. We introduce the following species:

X_0	–	substitutional dopant atoms on lattice sites,
X_1	–	dopant atoms on interstices,
X_2	–	self-interstitial host atoms,
X_3	–	vacancies in the host lattice,
X_4	–	electrons,
X_5	–	holes,

and denote by q_i, u_i, ζ_i, and $j_i, i = 0, \ldots, 5$, their electric charge, concentration, electrochemical potential and flux, respectively. We assume that

$$\begin{aligned} &\zeta_i = \ln \frac{u_i}{u_i^*} + q_i \phi, \; j_i = -D_i u_i \nabla \zeta_i, \; i = 0, \ldots, 5, \\ &q_0 = -1, \, q_1 = q_2 = q_3 = 0, \, q_4 = -1, \, q_5 = +1 \end{aligned} \tag{1.1}$$

where D_i, u_i^* and ϕ denote the diffusivities, the (constant) concentrations of a suitably chosen reference state and the electrostatic potential of the inner electric field. During the diffusion process the host atoms as well as the dopant atoms interchange between substitutional and interstitial sites. This may be understood as a result of chemical reactions of mass action type. We shall take into account the following reactions:

$$\begin{aligned} &X_1 + X_3 \rightleftharpoons X_0 + X_5 && \text{(Frank-Turnbull mechanism)}, \\ &X_2 + X_3 \rightleftharpoons 0 && \text{(defect generation and recombination)}, \\ &X_4 + X_5 \rightleftharpoons 0 && \text{(electron–hole generation and recombination)}. \end{aligned}$$

The corresponding reaction rates are given by

$$\begin{aligned} R_1 &= \tilde{k}_1 (u_1 u_3 - k_1 \, u_0 u_5), \\ R_2 &= \tilde{k}_2 (u_2 u_3 - k_2), \\ R_3 &= \tilde{k}_3 (u_4 u_5 - k_3) \end{aligned} \tag{1.2}$$

with some constants $\tilde{k}_i$, k_i, $i = 1, 2, 3$. Using the local mass conservation law for each species we get the following reaction–diffusion system:

$$\begin{aligned}\frac{\partial u_i}{\partial t} &= -\ \mathrm{div}\ j_i + r_i,\ i = 0,\dots,5, \\ r &= (R_1,\ -R_1,\ -R_2,\ -R_1 - R_2,\ -R_3,\ -R_3 + R_1).\end{aligned} \tag{1.3}$$

Next, we have to prescribe some boundary conditions. We assume that one part of the boundary is masked so that there all fluxes vanish. The remaining part Γ shall be in contact with a gas phase containing uncharged dopant atoms X with concentrations u on Γ and $\hat{u} = \text{const}$ far away from Γ. On high process temperatures one may assume the transport in the gas phase to be so fast such that approximately $u = \hat{u}$. The processes on Γ will be interpreted as chemical reactions, too. Let us regard the following ones:

$$\begin{aligned} X_0 + X_5 &\rightleftharpoons X_3 && \text{(infiltration of dopants to substitutional sites),} \\ X_1 &\rightleftharpoons 0 && \text{(infiltration of dopants to interstitial sites),} \\ X_2 &\rightleftharpoons 0 && \text{(surface recombination of self–interstitials),} \\ X_3 &\rightleftharpoons 0 && \text{(surface recombination of vacancies).} \end{aligned}$$

The reaction rates are given by

$$\begin{aligned} R_4 &= \tilde{k}_4(u_0 u_5 - k_4\, u_3), \\ R_5 &= \tilde{k}_5(u_1 - k_5), \\ R_6 &= \tilde{k}_6(u_2 - k_6), \\ R_7 &= \tilde{k}_7(u_3 - k_7) \end{aligned} \tag{1.4}$$

with some constants $\tilde{k}_i$, k_i, $i = 4,\dots,7$. Then, the boundary conditions read as follows:

$$\begin{aligned} j_{i,\nu} &= \begin{cases} 0 & \text{on } \partial\Omega \setminus \Gamma \\ b_i & \text{on } \Gamma \end{cases},\ i = 0,\dots,5, \\ b &= (R_4,\ R_5,\ R_6,\ -R_4 + R_7,\ 0,\ R_4). \end{aligned} \tag{1.5}$$

If there exists a simultaneous equilibrium of all volume and surface reactions then necessarily $k_1\, k_4 = k_5$, $k_6\, k_7 = k_2$.

Next, let us introduce the charge density ϱ and the current density j. According to our assumptions on the charge states we have

$$\varrho = -u_0 - u_4 + u_5,\ j = -j_0 - j_4 + j_5.$$

By (1.3), (1.5) the continuity equation

$$\frac{\partial \varrho}{\partial t} = -\ \mathrm{div}\ j,\ j_\nu|_{\partial\Omega} = 0$$

follows, and we get

$$\int_\Omega \varrho \,\mathrm{d}x = 0 \tag{1.6}$$

for all the time if in the initial state this condition is fulfilled. Then, the semiconductor structure as a whole will be electrically neutral but there exists an inner electric field the potential of which has to be determined in a selfconsistent way by means of the Poisson equation:

$$-\operatorname{div}(\varepsilon\nabla\phi) = \varrho,\ \nabla\phi\cdot\nu|_{\partial\Omega} = 0 \tag{1.7}$$

where ε denotes the dielectric permittivity.

Finally, we have to impose initial conditions which are compatible with (1.6):

$$u_i(0,x) = U_i(x),\ x\in\Omega,\ i=0,\ldots,5, \qquad \int_\Omega(-U_0-U_4+U_5)\,\mathrm{d}x = 0. \tag{1.8}$$

Corresponding to the chosen physical model we have found the initial boundary value problem (1.3), (1.5), (1.7), (1.8) which should be used for further mathematical analysis. Let us mention that the equations for the dopants and defects and those for the electrons and holes are coupled. With respect to applications in the field of numerical simulation it seems to be useful to remove this coupling in some approximation. This may be done under additional assumptions which are satisfied on sufficiently high process temperatures.

i) Let $D_4, D_5 \to \infty$. If we want the fluxes j_4, j_5 to remain bounded we have to require that $\zeta_4, \zeta_5 = \mathrm{const}$.

ii) Let $\tilde{k}_3 \to \infty$. If the reaction rate R_3 remains bounded then in the limit the relation

$$u_4\,u_5 = k_3 \tag{1.9}$$

is fulfilled. Suppose that $u_4^*\,u_5^* = k_3$, too. Because of (1.1) we get $\zeta_4+\zeta_5=0$, and without any loss of generality we may assume that $\zeta_4=\zeta_5=0$. Once more by (1.1) we find

$$\phi = -\ln\frac{u_5}{u_5^*}. \tag{1.10}$$

iii) After scaling the Poisson equation (1.7) one gets

$$-\Delta\phi = \frac{1}{\lambda^2}(-u_0-u_4+u_5)$$

where λ denotes the Debye length. Let $\lambda\to 0$. If the scaled charge density remains bounded then in the limit

$$-u_0-u_4+u_5 = 0. \tag{1.11}$$

Suppose $-u_0^*-u_4^*+u_5^*=0$, too.

By (1.9), (1.10), (1.11) the variables u_4, u_5, ϕ can be expressed in terms of u_0. It holds

$$u_0\,u_5 = g(u_0),\ \zeta_0 = \ln\frac{g(u_0)}{g(u_0^*)}$$

where

$$g(y) := \frac{1}{2}y\left(y+\sqrt{y^2+4\,k_3}\right). \tag{1.12}$$

Taking into account only the corresponding components of the equations (1.3), (1.5), (1.7), (1.8) we get an initial boundary value problem for the variables u_0, u_1, u_2, u_3. Now the field induced convective part in the flux j_0 is transformed to a pure diffusion term which contains a diffusivity depending on the concentration u_0. Further nonlinearities the growth of which is of at most second order occur in the volume as well as in the surface reactions.

Here we shall not write down all equations in their final form. After changing the notation in a suitable way this will be done in the following section. There we also summarize all our assumptions with respect to the data. Because of the second order terms in the boundary conditions we have to restrict ourselves to two–dimensional domains. It is worth noting that we do not use the concrete form of the function g (see (1.12)), only some properties of this function are important. Furthermore, in Section 2 the weak formulation of the reaction–diffusion system is given globally with respect to time (see problem (P)). Finally, some basic results concerned with imbedding as well as interpolation theorems are listed.

With the exception of the last theorem in Section 8 we impose conditions such that in the reaction–diffusion system under consideration there exits a unique thermodynamic equilibrium state. In Section 3 we introduce the free energy of the system. It will be shown that the free energy represents a Lyapunov function. More precisely, along any solution to (P) the free energy decays monotonously and exponentially to its equilibrium value as time tends to infinity (cf. [6], too). Thus, our problem is well posed from the point of view of thermodynamic principles. Moreover, based on estimates of the free energy first global a–priori estimates for solutions to (P) are obtained.

Section 4 is devoted to further upper a–priori estimates for solutions u to (P). By the fact that terms of second order occur in the boundary conditions we had to develop a special technique: As test functions we use simultaneously different powers of the components of u. Thus we obtain global L^∞–estimates.

In Section 5, the existence of solutions to (P) is proved by means of the Schauder Fixed Point Theorem. Using results of [7], in Section 6 we derive further regularity properties of solutions to (P) which enable us to prove uniqueness in Section 7.

Section 8 contains some additional results. First, it is shown that any solution to (P) approaches its equilibrium value exponentially in each L^p–norm, $p \in [1, \infty)$, as time tends to infinity. Next, global lower bounds for solutions to (P) are obtained. At last we consider the more general situation where a thermodynamic equilibrium does not exist. By a slightly modified technique we obtain existence as well as uniqueness results on finite time intervals.

2. The reaction-diffusion system

Let $\Omega \subset \mathbb{R}^2$ be a bounded Lipschitz domain and $u = (u_0, u_1, u_2, u_3)\colon \mathbb{R}_+ \times \Omega \longrightarrow \mathbb{R}^4_+$ the vector of concentrations. We consider the system of differential equations

$$\begin{aligned} \frac{\partial u_0}{\partial t} &= -\operatorname{div}\ j_0 + R_1(u), \\ \frac{\partial u_1}{\partial t} &= -\operatorname{div}\ j_1 - R_1(u), \\ \frac{\partial u_2}{\partial t} &= -\operatorname{div}\ j_2 - R_2(u), \\ \frac{\partial u_3}{\partial t} &= -\operatorname{div}\ j_3 - R_1(u) - R_2(u), \end{aligned} \tag{2.1}$$

$$j_0 = -D_0\, u_0 \nabla \ln g(u_0),\ \ j_i = -D_i\, u_i \nabla \ln u_i,\ \ i = 1, 2, 3,$$

$$R_1(u) = \tilde{k}_1(u_1 u_3 - k_1\, g(u_0)),\ \ R_2(u) = \tilde{k}_2(u_2 u_3 - k_2)$$

in $\mathbb{R}_+ \times \Omega$, the boundary conditions

$$\begin{aligned} j_{0,\nu} &= h_0(g(u_0) - u_3), \\ j_{i,\nu} &= h_i(u_i - \hat{u}_i),\ \ i = 1, 2, \\ j_{3,\nu} &= h_3(u_3 - \hat{u}_3) - h_0(g(u_0) - u_3) \end{aligned} \tag{2.2}$$

on $\mathbb{R}_+ \times \partial\Omega$ as well as the initial condition

$$u(0, \cdot) = U \tag{2.3}$$

on Ω.

Let us put together the assumptions concerning the data in the equations formulated above, which will be used during the following sections.

Assumptions:

$$\begin{aligned} &D_j = \text{const} > 0,\ \ j = 0, \ldots, 3, \\ &h_j \in L^\infty_+(\partial\Omega),\ \ j = 0, 1, 2, 3, \\ &k_1, k_2 = \text{const} > 0, \\ &\tilde{k}_1, \tilde{k}_2 \in L^\infty_+(\Omega), \\ &\hat{u}_j \in L^\infty_+(\partial\Omega),\ \ j = 1, 2, 3, \\ &U \in L^\infty_+(\Omega, \mathbb{R}^4); \end{aligned} \tag{2.4}$$

$$\begin{aligned} &\Gamma \subset \partial\Omega,\ \ \text{mes}\ \Gamma > 0, \\ &h_j = 0 \text{ on } \partial\Omega \backslash \Gamma,\ \ h_j \geq \text{const} > 0 \text{ on } \Gamma,\ \ j = 0, 1, 2, 3, \\ &\hat{u}_1 = k_1,\ \ \hat{u}_2, \hat{u}_3 = \text{const},\ \ \hat{u}_2\, \hat{u}_3 = k_2; \end{aligned} \tag{2.5}$$

$$
\begin{aligned}
&g \in C^1(\mathbb{R}_+),\\
&\varphi(y) := \frac{g'(y)\,y}{g(y)},\ \psi(y) := \frac{g(y)}{y},\ y > 0,\ \text{are such that}\\
&\psi(y) \geq \tau_1,\ |\psi(y_1) - \psi(y_2)| \leq \tau_2 |y_1 - y_2|,\ y, y_1, y_2 > 0,\\
&\tau_3 \leq \varphi(y) \leq \tau_4,\ y > 0;\ \tau_i = \text{const} > 0,\ i = 1, ..., 4;
\end{aligned}
\tag{2.6}
$$

$$
\begin{aligned}
&U_j \in W^{1,p}(\Omega),\ j = 0, ..., 3, \quad \text{for some } p > 2,\\
&\varphi \text{ locally Lipschitz continuous;}
\end{aligned}
\tag{2.7}
$$

$$
U_j \geq \text{const} > 0,\ j = 0, ..., 3. \tag{2.8}
$$

Throughout this paper we assume the conditions (2.4), (2.5) and (2.6) to be satisfied.

Remark 2.1.

i) (2.6) implies that $\varphi, \psi \in C([0, +\infty))$ and the inequalities in (2.6) are satisfied for $y = 0$, too. We have $g(0) = 0,\ \psi(0) = g'(0) > 0,\ \varphi(0) = 1$.

ii) There exists a positive constant τ_0 with $\psi(y) \leq \tau_0(1 + y)$ for $y \in \mathbb{R}_+$.

iii) There exists a constant $\tau_5 > 0$ such that

$$
g(y_1) - g(y_2) \geq \tau_5(y_1 - y_2),\ y_1 \geq y_2 \geq 0.
$$

iv) There exists $g^{-1}\colon [0, +\infty) \longrightarrow [0, +\infty)$.

v) With some constant $\tau_6 > 0$ we have

$$
\left(\sqrt{g(y_1)} - \sqrt{g(y_2)}\right) \geq \tau_6\left(\sqrt{y_1} - \sqrt{y_2}\right),\ y_1 \geq y_2 \geq 0.
$$

vi) There are constants $\tau_7,\ \tau_8 > 0$ for which $g_1(y) := g(y)\,y^{-\tau_7}$ is monotonously increasing on $(0, +\infty)$, $g_2(y) := g(y)\,y^{-\tau_8}$ is monotonously decreasing on $(0, +\infty)$.

vii) (2.6) is satisfied for the function g given in (1.12).

We introduce the constant

$$
\alpha := \min\left(\tau_3\, D_0, D_1, D_2, D_3, \tau_3^2\, D_0, \min_i \operatorname*{ess\,inf}_{\Gamma} h_i, \tau_5 \operatorname*{ess\,inf}_{\Gamma} h_0\right)
$$

characterizing the speed of those kinetic processes (diffusion and surface reactions) which are important for the estimates in the following sections. We use the notation

$X := H^1(\Omega, \mathbb{R}^4)$, $Y := L^2(\Omega, \mathbb{R}^4)$, $Z := L^2(\Gamma, \mathbb{R}^4)$. Additionally let

$$V := \left\{ u \in L^2_{\text{loc}}(\mathbb{R}_+, X) \colon u \in L^\infty_{\text{loc}}\left(\mathbb{R}_+, L^4(\Omega, \mathbb{R}^4)\right) \right\},$$

$$W := \left\{ u \in L^2_{\text{loc}}(\mathbb{R}_+, X) \colon u' \in L^2_{\text{loc}}(\mathbb{R}_+, X^*) \right\}.$$

We define A, $R\colon X \longrightarrow X^*$ for u, $v \in X$ by

$$\begin{aligned}\langle A(u), v\rangle &:= \int_\Omega \left\{ D_0\, \varphi(u_0) \nabla u_0 \nabla v_0 + \sum_{i=1}^{3} D_i \nabla u_i \nabla v_i \right\} \mathrm{d}x \\ &\quad + \int_\Gamma \left\{ h_0(g(u_0) - u_3)(v_0 - v_3) + \sum_{i=1}^{3} h_i(u_i - \hat{u}_i) v_i \right\} \mathrm{d}\Gamma, \\ \langle R(u), v\rangle &:= -\int_\Omega \left\{ R_1(u)(v_1 + v_3 - v_0) + R_2(u)(v_2 + v_3) \right\} \mathrm{d}x\end{aligned}$$

where $\langle \cdot, \cdot \rangle$ denotes the dual pairing of X and X^*. We shall be concerned with finding a solution to

Problem (P):

$$u'(t) + A(u(t)) = R(u(t)) \quad \text{for a.e.}\, t \in \mathbb{R}_+,\ u(0) = U,\ u \in W \cap V,\ u \geq 0.$$

Here u' denotes the derivative of u with respect to time in the sense of X^*-valued distributions and $u \geq 0$ means that all components $u_i \geq 0$. For any $T \in \mathbb{R}_+$ we denote by S the finite time interval $[0, T]$ and define

$$V_S := \left\{ u \in L^2(S, X) \colon u \in L^\infty\left(S, L^4(\Omega, \mathbb{R}^4)\right) \right\},$$

$$W_S := \left\{ u \in L^2(S, X) \colon u' \in L^2(S, X^*) \right\}.$$

In the canonical way we extend the definition of the operators A, R to time functions from V_S. For any finite time interval S the reaction-diffusion system leads to

Problem ($\mathbf{P_S}$):

$$u' + A(u) = R(u),\ u(0) = U,\ u \in W_S \cap V_S,\ u \geq 0.$$

Now we introduce several symbols and collect some basic results which we shall use in our considerations. Let be $u \in \mathbb{R}^4$, $\delta \in \mathbb{R}$. By $u + \delta$, $\sqrt{u}$, u^p, $p \in \mathbb{R}$, $\ln u$, $|u|$, u^+ and u^- we denote the vector whose i–th component is $u_i + \delta$, $\sqrt{u_i}$, u_i^p, $\ln u_i$, $|u_i|$, $\sup(u_i, 0)$ and $\sup(-u_i, 0)$, respectively. If there is no danger of misunderstanding we shall write shortly L^p instead of $L^p(\Omega, \mathbb{R}^k)$, $k \in \mathbb{N}$, and H^1 instead of $H^1(\Omega)$. We exploit the Sobolev imbedding theorems as well as the following form of the Gagliardo-Nirenberg inequality (cf. [8]):
Let $\Omega \subset \mathbb{R}^2$, $u \in H^1(\Omega)$, then

$$\|u\|_{L^r} \leq c_0 \|u\|_{L^q}^{\theta} \|u\|_{H^1}^{1-\theta}, \text{ where } q < r,\ \theta = \frac{q}{r}. \tag{2.9}$$

Additionally, for estimates of traces we use the inequality:
Let $\Omega \subset \mathbb{R}^2$, $u \in H^1(\Omega)$, then

$$\|u\|^p_{L^p(\partial\Omega)} \le c\,\|u\|^{p-1}_{L^{2(p-1)}}\,\|u\|_{H^1}\,, \text{ where } p \ge 2. \tag{2.10}$$

A direct consequence of the Gagliardo-Nirenberg inequality is the following interpolation result:
Let $\Omega \subset \mathbb{R}^2$, $u \in L^\infty(\mathbb{R}_+, L^q(\Omega)) \cap L^2(\mathbb{R}_+, H^1(\Omega))$, $q \ge 1$, then $u \in L^p(\mathbb{R}_+, L^r(\Omega))$ with $p = \frac{2}{1-\theta}$, $r = \frac{q}{\theta}$, $\theta \in (0,1)$ and

$$\|u\|^p_{L^p(\mathbb{R}_+,L^r(\Omega))} \le c_0^p\,\|u\|^{p\theta}_{L^\infty(\mathbb{R}_+,L^q(\Omega))}\,\|u\|^2_{L^2(\mathbb{R}_+,H^1(\Omega))}\,. \tag{2.11}$$

In the sections concerning the upper and lower bounds of solutions to (P) we take advantage from the following lemma (cf. [10]):

Lemma 2.1. *Let $\tilde{k} > 0$, $p > 1$. Furthermore, let $\phi\colon [\tilde{k}, +\infty) \longrightarrow \mathbb{R}_+$ be a nonincreasing function such that, for $h \ge k \ge \tilde{k}$:*

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

Then $\phi(k) = 0$ if

$$k \ge \tilde{k} + 2^{-p/(p-1)}\,c_1\,\phi(\tilde{k})^{p-1}.$$

3. Estimates by the energy functional

It is easy to check that (2.5) implies the existence of exactly one solution u^* to the stationary problem corresponding to (P). This solution represents the thermodynamic equilibrium and it is given by

$$u_0^* = g^{-1}(\hat{u}_3),\ u_i^* = \hat{u}_i,\ i = 1,2,3. \tag{3.1}$$

Let

$$e(y,y^*) := \int_{y^*}^{y} \ln\frac{\eta}{y^*}\mathrm{d}\eta,\ e_g(y,y^*) := \int_{y^*}^{y} \ln\frac{g(\eta)}{g(y^*)}\mathrm{d}\eta,\ y \ge 0,\ y^* > 0.$$

Easily one obtains the estimates

$$\begin{gathered}\tau_7\, e(y,y^*) \le e_g(y,y^*) \le \tau_8\, e(y,y^*),\\ \left(\sqrt{y} - \sqrt{y^*}\right)^2 \le e(y,y^*) \le 2\,\left(\sqrt{y} - \sqrt{y^*}\right)^2 + \frac{2}{3\sqrt{y^*}}\left|\sqrt{y} - \sqrt{y^*}\right|^3,\\ e(y,y^*) \le \frac{1}{y^*}\left(y - y^*\right)^2.\end{gathered} \tag{3.2}$$

We define the density of the free energy $f\colon \mathbb{R}^4 \longrightarrow [0,+\infty]$,

$$f(u) := \begin{cases} e_g(u_0,u_0^*) + \sum_{i=1}^3 e(u_i,u_i^*) & \text{if } u \ge 0,\\ +\infty & \text{otherwise,}\end{cases}$$

as well as the free energy $F\colon Y \longrightarrow [0,+\infty]$,

$$F(u) := \int_\Omega f(u(x))\mathrm{d}x. \tag{3.3}$$

Since the function f has the properties of a positive and convex normal integrand the functional F will be proper, convex and lower semicontinuous (cf. [2]). It holds

$\operatorname{dom} F = \{u \in Y : u \geq 0\}$. If $u \in \operatorname{dom} F$ then $F(u+\delta) \to F(u)$ for $\delta \downarrow 0$. If $u \in Y,\ u \geq \delta > 0$ then F is subdifferentiable and we have

$$\partial F(u)(x) = \nabla f(u(x)) \text{ for a.e. } x \in \Omega.$$

Moreover, for $u \in W_{[t_1,t_2]},\ u \geq \delta > 0$, the following differential formula

$$F(u(t_2)) - F(u(t_1)) = \int_{t_1}^{t_2} \left\langle u'(s), \nabla f\left(u(s)\right)\right\rangle \mathrm{d}s \tag{3.4}$$

is valid (cf. [1, 3]). Additionally, if u is a solution to (P) then equation (3.4) can be transformed to

$$F(u(t_2)) - F(u(t_1)) = -\int_{t_1}^{t_2} D(u(s))\, ds$$

where D denotes the dissipation rate:

$$D := D_{\text{diff}} + D_{\text{reac}} \colon \{u \in X : u \geq 0)\} \longrightarrow [0, +\infty],$$

$$D_{\text{diff}}(u) := 4 \int_\Omega \left\{ D_0\, \varphi(u_0)^2 \, |\nabla \sqrt{u_0}|^2 + \sum_{i=1}^{3} D_i \, |\nabla \sqrt{u_i}|^2 \right\} \mathrm{d}x,$$

$$D_{\text{reac}}(u) := \int_\Omega \left\{ \tilde{k}_1 (u_1\, u_3 - k_1\, g(u_0)) \ln \frac{u_1\, u_3}{k_1\, g(u_0)} + \tilde{k}_2 (u_2\, u_3 - k_2) \ln \frac{u_2\, u_3}{k_2} \right\} \mathrm{d}x$$

$$+ \int_\Gamma \left\{ h_0 \left(g(u_0) - u_3\right) \ln \frac{g(u_0)}{u_3} + \sum_{i=1}^{3} h_i \left(u_i - u_i^*\right) \ln \frac{u_i}{u_i^*} \right\} \mathrm{d}\Gamma.$$

Theorem 3.1. *If u is a solution to (P) then*

i) $F(u(t_2)) \leq F(u(t_1)) \quad$ *for* $\quad t_2 \geq t_1 \geq 0,$

ii) $\sup_{t \in \mathbb{R}_+} F(u(t)) \leq F(U),$

iii) $u \in L^\infty \left(\mathbb{R}_+, L^1 \left(\Omega, \mathbb{R}^4\right)\right),$

iv) $D(u) \in L^1(\mathbb{R}_+),$

v) $\nabla \sqrt{u_i} \in L^2 \left(\mathbb{R}_+, L^2 \left(\Omega, \mathbb{R}^2\right)\right),\ i = 0, \ldots, 3.$

Proof. In the following and later c denotes (possibly different) positive constants the values of which are not important. Let u be a solution to (P), assume that $0 \leq t_1 < t_2,\ \delta \leq 1$. We use the test function

$$v_\delta := \nabla f(u+\delta) \in L^2\left([0, t_2], X\right).$$

By (2.6) and Remark 2.1 we get

$$g(y+\delta) - g(y) \leq c\, \delta\, (1+y),$$
$$c + \ln \delta \leq \ln g(y+\delta) \leq \ln \tau_0 + \ln(y+\delta) + \ln(y+1+\delta) \leq c\,(1+y).$$

Additionally, we use

$$\nabla u_i \nabla (\ln u_i) = 4 |\nabla \sqrt{u_i}|^2,\ \ \nabla u_0 \nabla (\ln g(u_0)) \geq 4 \tau_3 |\nabla \sqrt{u_0}|^2$$

and (3.4). Therefore we have from (P)

$$
\begin{aligned}
&F(u(t_2)+\delta) - F(u(t_1)+\delta) \\
&\qquad + \int_{t_1}^{t_2} \Big\{ 4 \int_\Omega \Big[D_0\, \varphi(u_0)\, \varphi(u_0+\delta) \Big| \nabla \sqrt{u_0+\delta} \Big|^2 \\
&\qquad\qquad\qquad + \sum_{i=1}^{3} D_i \Big| \nabla \sqrt{u_i+\delta} \Big|^2 \Big] \mathrm{d}x + D_{\mathrm{reac}}(u+\delta) \Big\} \mathrm{d}s \\
&\qquad \le \int_0^{t_2} \Big\{ c\delta \Big(1 + |\ln\delta| + \sum_{i=0}^{3} \Big(\|u_i+1\|_{L^2}^2 + \|u_i+1\|_{L^2(\Gamma)}^2 \Big) \Big) \Big\} \mathrm{d}s \\
&\qquad \le \int_0^{t_2} c\delta \Big(1 + |\ln\delta| + \sum_{i=0}^{3} \|u_i+1\|_{H^1}^2 \Big) \mathrm{d}s \\
&\qquad \le t_2 c\delta (1+|\ln\delta|) + c\delta \sum_{i=0}^{3} \|u_i+1\|_{L^2([0,t_2],H^1)}^2 .
\end{aligned}
$$

Since $u \in L^2_{\mathrm{loc}}(\mathbb{R}^+, X)$, the norms on the right hand side are finite. Letting $\delta \downarrow 0$ we get by Fatou's Lemma

$$
F(u(t_2)) + \int_{t_1}^{t_2} D(u(s))\,\mathrm{d}s \le F(u(t_1)).
$$

This proves i). By setting $t_1 = 0$, $t_2 = t$ for $t \in \mathbb{R}_+$ we get ii) and iv). By the definition of $D(u)$ and (2.6), v) follows. The inequality

$$
\|u\|_{L^1(\Omega)} \le F(u) + c
$$

yields assertion iii). $\square$

Lemma 3.1. *For every $R > 0$ there exists a $c_R > 0$ such that*

$$
\begin{aligned}
F(u) \le c_R \Big\{ &\sum_{i=0}^{3} \|\nabla \sqrt{u_i}\|_{L^2}^2 \\
&+ \int_\Gamma \Big[(g(u_0) - u_3) \ln \frac{g(u_0)}{u_3} + \sum_{i=1}^{3} (u_i - u_i^*) \ln \frac{u_i}{u_i^*} \Big] \mathrm{d}\Gamma \Big\}
\end{aligned}
$$

for $u \in M_R := \{u \in X : \sqrt{u} \in X,\ F(u) \le R\}$.

Proof. Let be $u \in M_R$, $w := \sqrt{u} - \sqrt{u^*}$. From (3.2) we conclude that

$$
c\, \|w\|_Y^2 \le F(u) \le c\, \Big(\|w\|_Y^2 + \|w\|_{L^3(\Omega,\mathbb{R}^4)}^3 \Big) . \tag{3.5}
$$

The Gagliardo-Nirenberg inequality (2.9) yields

$$
\|w\|_{L^3(\Omega,\mathbb{R}^4)}^3 \le c_0\, \|w\|_X\, \|w\|_Y^2 \le c_0\, \|w\|_X^2\, \|w\|_Y
$$

such that

$$
F(u) \le c\, \Big(1 + \sqrt{F(u)} \Big)\, \|w\|_X^2 \le \tilde{c}_R\, \|w\|_X^2 .
$$

Because of the well known estimate

$$
\|w\|_X^2 \le c\, \left(\sum_{i=0}^{3} \|\nabla w_i\|_{L^2}^2 + \|w\|_Z^2 \right) \tag{3.6}
$$

we get

$$F(u) \leq c \left(\sum_{i=0}^{3} \|\nabla w_i\|_{L^2}^2 + \|w\|_Z^2 \right). \tag{3.7}$$

On the other hand, we have

$$\begin{aligned}
&\int_\Gamma \left[(g(u_0) - u_3) \ln \frac{g(u_0)}{u_3} + \sum_{i=1}^{3} (u_i - u_i^*) \ln \frac{u_i}{u_i^*} \right] \mathrm{d}\Gamma \\
&\geq c \int_\Gamma \left[\left| \sqrt{g(u_0)} - \sqrt{u_3} \right|^2 + \sum_{i=1}^{3} \left| \sqrt{u_i} - \sqrt{u_i^*} \right|^2 \right] \mathrm{d}\Gamma \\
&\geq c \int_\Gamma \left[\left| \sqrt{g(u_0)} - \sqrt{g(u_0^*)} \right|^2 + \sum_{i=1}^{3} \left| \sqrt{u_i} - \sqrt{u_i^*} \right|^2 \right] \mathrm{d}\Gamma \\
&\geq c \, \|w\|_Z^2 .
\end{aligned}$$

Together with (3.7) the assertion follows. □

As a consequence of Lemma 3.1 we get

$$F(u) \leq \frac{c_R}{\alpha} D(u) \quad \forall \, u \in M_R, \; R > 0.$$

Inequalities of this type have been proved in [6] for a large class of reaction-diffusion equations. These results could be used to verify the assertion of Lemma 3.1, too. Here we were able to give a short proof in a more direct way. The assertion of Lemma 3.1 will be the essential tool to show that the free energy $F(u(t))$ of a solution to (P) decays exponentially as time tends to infinity without using global bounds for this solution. Later such global bounds will be obtained starting from energetic estimates derived here.

Theorem 3.2. *If u is a solution to (P) then*

$$\begin{aligned}
&i) && F(u(t)) \leq e^{-\lambda t} F(U) \quad \forall \, t \geq 0, \; \textit{for some } \lambda > 0, \\
&ii) && \|u(t) - u^*\|_{L^1(\Omega, \mathbb{R}^4)} \leq c \, e^{-\lambda t/2} \quad \forall \, t \geq 0, \\
&iii) && u - u^* \in L^1 \left(\mathbb{R}_+, L^1 \left(\Omega, \mathbb{R}^4 \right) \right).
\end{aligned}$$

Proof. i) Let $\lambda := \frac{\alpha}{c_R}$ with c_R from Lemma 3.1, where $R = F(U)$. We use the test function $e^{\lambda t} v_\delta$, where v_δ is defined in the proof of Theorem 3.1, and a differential formula similar to (3.4) for $w \in W_{[0,t]}$, $w \geq \delta > 0$,

$$e^{\lambda t} F(w(t)) - F(w(0)) = \int_0^t \left\{ \lambda e^{\lambda s} F(w) + e^{\lambda s} \langle w'(s), \nabla f(w(s)) \rangle \right\} \mathrm{d}s.$$

Using the estimates for the reaction and boundary terms given in Theorem 3.1 we obtain

$$
\begin{aligned}
&e^{\lambda t}F(u(t)+\delta)-F(U+\delta)\\
&\quad\le\int_0^t e^{\lambda s}\Bigg[\lambda F(u+\delta)-\alpha\Bigg(\sum_{i=0}^{3}\Big\|\nabla\sqrt{u_i+\delta}\Big\|_{L^2}^2\\
&\qquad\qquad+\int_\Gamma\Big\{\sum_{i=1}^{3}(u_i+\delta-u_i^*)\ln\frac{u_i+\delta}{u_i^*}\\
&\qquad\qquad\qquad+(g(u_0+\delta)-u_3-\delta)\ln\frac{g(u_0+\delta)}{u_3+\delta}\Big\}\mathrm{d}\Gamma\Bigg)\\
&\qquad\qquad+c\,\delta\Big(1+|\ln\delta|+\sum_{i=0}^{3}\Big(\|u_i+1\|_{L^2}^2+\|u_i+1\|_{L^2(\Gamma)}^2\Big)\Big)\Bigg]\mathrm{d}s.
\end{aligned}
$$

By Lemma 3.1 it follows

$$
\begin{aligned}
&e^{\lambda t}F(u(t)+\delta)-F(U+\delta)\\
&\qquad\le\int_0^t e^{\lambda s}c\,\delta\Big(1+|\ln\delta|+\sum_{i=0}^{3}\|u_i+1\|_{H^1}^2\Big)\mathrm{d}s\\
&\qquad\le e^{\lambda t}c\,\delta\Big[t(1+|\ln\delta|)+\sum_{i=0}^{3}\|u_i+1\|_{L^2([0,t],H^1)}^2\Big].
\end{aligned}
$$

Like in the proof of Theorem 3.1, $\|u+1\|_{L^2([0,t],X)}$ is finite for every $t\in\mathbb{R}_+$. Letting $\delta\downarrow 0$ we get

$$
e^{\lambda t}F(u(t))\le F(U)\quad\forall\,t\in\mathbb{R}_+.
$$

ii) By the inequality

$$
|y-y^*|\le\left|\sqrt{y}-\sqrt{y^*}\right|^2+2\sqrt{y^*}\left|\sqrt{y}-\sqrt{y^*}\right|
$$

and by i) we obtain

$$
\begin{aligned}
\|u(t)-u^*\|_{L^1(\Omega,\mathbb{R}^4)}&\le\left\|\sqrt{u}-\sqrt{u^*}\right\|_Y^2+c\left\|\sqrt{u}-\sqrt{u^*}\right\|_Y\\
&\le c\left(F(U)e^{-\lambda t}+\sqrt{F(U)}e^{-\lambda t/2}\right)\\
&\le c\,e^{-\lambda t/2}.
\end{aligned}
$$

From this assertions ii) and iii) follow. □

4. Further a-priori estimates

To prove further a-priori estimates for solutions to (P) we pass over to the variable $w:=u-u^*$. Only in this variable one can hope to get $L^2(\mathbb{R}_+,L^2)$-estimates for powers of this variable.

Theorem 4.1. *If u is a solution to (P) then*

$$
\forall n\in\mathbb{N}:\ |w|^n\in L^\infty(\mathbb{R}_+,Y)\cap L^2(\mathbb{R}_+,X).
$$

For the proof of the theorem we use the following lemma:

Lemma 4.1. *Let $m \geq 4,\ r := \frac{m}{4}$. If u is a solution to (P) and*

$$|w|^{l/8} \in L^\infty(\mathbb{R}_+, Y) \cap L^2(\mathbb{R}_+, Y),\ m \geq l \geq 4,\ l \in \mathbb{N},$$

then the solution u to (P) has the regularity property

$$|w_i|^{\frac{r+1}{2}},\ |w_3|^{\frac{m+1}{8}} \in L^\infty\left(\mathbb{R}_+, L^2(\Omega)\right) \cap L^2\left(\mathbb{R}_+, H^1(\Omega)\right),\ i = 0, 1, 2.$$

Proof of Theorem 4.1. We use the notation of Lemma 4.1. By Theorem 3.1 and 3.2 the assumptions of Lemma 4.1 for $r = 1$ are satisfied. We explain that the application of Lemma 4.1 for r reproduces the corresponding assumptions for $r + \frac{1}{4}$. For the component $|w_3|$ there is nothing to show. From $|w_i| \in L^\infty(\mathbb{R}_+, L^{r+1}(\Omega))$ we have $|w_i| \in L^\infty\left(\mathbb{R}_+, L^{r+\frac{1}{4}}(\Omega)\right)$, easily one obtains from $|w_i|^{\frac{m}{8}},\ |w_i|^{\frac{m+4}{8}} \in L^2(\mathbb{R}_+, L^2(\Omega))$ that $|w_i|^{\frac{m+1}{8}} \in L^2(\mathbb{R}_+, L^2(\Omega))$, $i = 0, 1, 2$. The repeated application of this lemma gives the regularity stated in Theorem 4.1. □

Proof of Lemma 4.1. Let $v := |w|$. We use formally the test function

$$\left(v_0^r \operatorname{sgn}(w_0),\ v_1^r \operatorname{sgn}(w_1),\ v_2^r \operatorname{sgn}(w_2),\ v_3^{\frac{m-3}{4}} \operatorname{sgn}(w_3)\right).$$

As mentioned in Section 1 these different powers of the components of w in the test function are necessary to handle the second order reaction terms on the boundary. More precisely the following estimates are obtained by test functions of this kind where v_i are replaced by $v_i^K := \min\{v_i, K\}$, $i = 0, 1, 2, 3,\ K > 0$. It is possible to get estimates which are independent of K. Letting $K \longrightarrow \infty$ we shall obtain the inequalities derived now.

$$\begin{aligned}
&\sum_{i=0}^{2}\left[\tfrac{1}{r+1}\|v_i(t)\|_{L^{r+1}}^{r+1} + \alpha\int_0^t\left\{\tfrac{m}{(r+1)^2}\left\|\nabla v_i^{\frac{r+1}{2}}\right\|_{L^2}^2 + \|v_i\|_{L^{r+1}(\Gamma)}^{r+1}\right\}\mathrm{d}s\right] \\
&+ \tfrac{4}{m+1}\|v_3(t)\|_{L^{\frac{m+1}{4}}}^{\frac{m+1}{4}} + \alpha\int_0^t\left\{\tfrac{16(m-3)}{(m+1)^2}\left\|\nabla v_3^{\frac{m+1}{8}}\right\|_{L^2}^2 + \|v_3\|_{L^{\frac{m+1}{4}}(\Gamma)}^{\frac{m+1}{4}}\right\}\mathrm{d}s \\
&\leq c\int_0^t\left\{\int_\Omega\left\{[v_1 v_3 + v_1 + v_3]\, v_0^r + \left[v_3 + v_0 + v_0^2\right] v_1^r + v_3 v_2^r\right.\right. \\
&\qquad\qquad \left. + \left[v_0 + v_0^2 + v_1 + v_2\right] v_3^{\frac{m-3}{4}}\right\}\mathrm{d}x \\
&\qquad \left. + \int_\Gamma\left\{v_3 v_0^r + \left[v_0^2 + v_0\right]\ v_3^{\frac{m-3}{4}}\right\}\mathrm{d}\Gamma\right\}\mathrm{d}s + c(r).
\end{aligned} \tag{4.1}$$

$\|\nabla u_i\|_{L^2}^2 + \|u_i\|_{L^2(\Gamma)}^2$ is a norm equivalent to the usual H^1-norm. The several boundary and volume integrals are treated with (2.10), the Gagliardo-Nirenberg inequality (2.9) and Young's inequality in a suitable way. Additionally the assumed $L^\infty(\mathbb{R}_+, L^2)$–regularity of lower powers of v is used. Here we demonstrate the method by one of the boundary terms:

$$\begin{aligned}
\int_\Gamma v_0^2\, v_3^{\frac{m-3}{4}}\,\mathrm{d}\Gamma &\le \left\|v_0^2\right\|_{L^{\frac{m+1}{4}}(\Gamma)} \left\|v_3^{\frac{m-3}{4}}\right\|_{L^{\frac{m+1}{m-3}}(\Gamma)} = \left\|v_0^{\frac{r+1}{2}}\right\|^{\frac{4}{r+1}}_{L^{\frac{m+1}{r+1}}(\Gamma)} \left\|v_3^{\frac{m+1}{8}}\right\|^{\frac{2(m-3)}{m+1}}_{L^2(\Gamma)} \\
&\le c \left\|v_0^{\frac{r+1}{2}}\right\|^{\frac{4(\beta-1)}{(r+1)\beta}}_{L^{2(\beta-1)}} \left\|v_0^{\frac{r+1}{2}}\right\|^{\frac{4}{(r+1)\beta}}_{H^1} \left\|v_3^{\frac{m+1}{8}}\right\|^{\frac{2(m-3)}{m+1}}_{L^2(\Gamma)} \\
&\le c \left\|v_0^{\frac{r+1}{2}}\right\|^{\frac{4}{(r+1)\beta}(1+(\beta-1)(1-\theta))}_{H^1} \left\|v_3^{\frac{m+1}{8}}\right\|^{\frac{m-3}{m+1}}_{L^2} \left\|v_3^{\frac{m+1}{8}}\right\|^{\frac{m-3}{m+1}}_{H^1},
\end{aligned}$$

where $\beta := \frac{m+1}{r+1}$, $\theta := \frac{r}{(\beta-1)(r+1)}$. Because the exponent of the H^1-norm of $v_0^{\frac{r+1}{2}}$ is smaller than two, we obtain from the Young inequality with $p' := \frac{(m+1)(r+1)}{4r^2-r-1}$

$$\begin{aligned}
\int_\Gamma v_0^2\, v_3^{\frac{m-3}{4}}\,\mathrm{d}\Gamma &\le \varepsilon \left\|v_0^{\frac{r+1}{2}}\right\|^2_{H^1} + c \left\|v_3^{\frac{m+1}{8}}\right\|^{\frac{(m-3)\,p'}{m+1}}_{L^2} \left\|v_3^{\frac{m+1}{8}}\right\|^{\frac{(m-3)p'}{m+1}}_{H^1} \\
&\le \varepsilon \left\|v_0^{\frac{r+1}{2}}\right\|^2_{H^1} + c \left\|v_3^{\frac{m+1}{8}}\right\|^{\frac{(m-3)\,p' m}{(m+1)^2}}_{L^{\frac{2m}{m+1}}} \left\|v_3^{\frac{m+1}{8}}\right\|^{\frac{(m+2)(m-3)p'}{(m+1)^2}}_{H^1} \\
&\le \varepsilon \left\|v_0^{\frac{r+1}{2}}\right\|^2_{H^1} + c \left\|v_3\right\|^{\frac{(m-3)\,r\,p'}{2(m+1)}}_{L^r} \left\|v_3^{\frac{m+1}{8}}\right\|^{\frac{(m+2)(m-3)p'}{(m+1)^2}}_{H^1}.
\end{aligned}$$

The exponent of the H^1-norm of $v_3^{\frac{m+1}{8}}$ is smaller than two, too. We use Young's inequality again. With $q' := (m+1)(4r^2-r-1)(8r^3-6r^2+2)^{-1}$, $v_3 \in L^\infty(\mathbb{R}_+, L^r)$ and the inequality $(m-3)(m+1)^{-1}\,p'\,q' \ge 2$ we conclude

$$\begin{aligned}
\int_\Gamma v_0^2\, v_3^{\frac{m-3}{4}}\,\mathrm{d}\Gamma &\le \varepsilon \left(\left\|v_0^{\frac{r+1}{2}}\right\|^2_{H^1} + \left\|v_3^{\frac{m+1}{8}}\right\|^2_{H^1} \right) + c \left\|v_3\right\|^{\frac{(m-3)\,r\,p'\,q'}{2(m+1)}}_{L^r} \\
&\le \varepsilon \left(\left\|v_0^{\frac{r+1}{2}}\right\|^2_{H^1} + \left\|v_3^{\frac{m+1}{8}}\right\|^2_{H^1} \right) + c \left\|v_3\right\|^r_{L^r} \\
&\le \varepsilon \left(\left\|v_0^{\frac{r+1}{2}}\right\|^2_{H^1} + \left\|v_3^{\frac{m+1}{8}}\right\|^2_{H^1} \right) + c \left\|v_3^{\frac{r}{2}}\right\|^2_{L^2}.
\end{aligned}$$

Similar to this estimate the other terms can be treated. This leads to

$$\begin{aligned}
&\sum_{i=0}^{2} \left[\|v_i(t)\|^{r+1}_{L^{r+1}} + (1+\varepsilon) \int_0^t \left\|v_i^{\frac{r+1}{2}}\right\|^2_{H^1} \mathrm{d}s \right] + \|v_3(t)\|^{\frac{m+1}{4}}_{L^{\frac{m+1}{4}}} + (1+\varepsilon) \int_0^t \left\|v_3^{\frac{m+1}{8}}\right\|^2_{H^1} \mathrm{d}s \\
&\le \varepsilon \int_0^t \left[\sum_{i=0}^{2} \left\|v_i^{\frac{r+1}{2}}\right\|^2_{H^1} + \left\|v_3^{\frac{m+1}{8}}\right\|^2_{H^1} \right] \mathrm{d}s + c(r) \Big[1 + \int_0^t \sum_{i=0}^{3} \left\|v_i^{\frac{r}{2}}\right\|^2_{L^2} \mathrm{d}s \Big] \\
&\quad + \int_0^t f(v_3) \sum_{i=0}^{2} \left\|v_i^{\frac{r+1}{2}}\right\|^2_{L^2} \mathrm{d}s
\end{aligned}$$

where the last term with some $f(v_3) \in L^1(\mathbb{R}_+)$ only occurs if $r \le \frac{5}{4}$. Thus we can apply Gronwall's Lemma. Because of $v_i \in L^r(\mathbb{R}_+, L^r(\Omega))$ we get

$$\sum_{i=0}^{2}\left[\|v_i(t)\|_{L^{r+1}}^{r+1} + \int_0^t \left\|v_i^{\frac{r+1}{2}}\right\|_{H^1}^2 \mathrm{d}s\right] + \|v_3(t)\|_{L^{\frac{m+1}{4}}}^{\frac{m+1}{4}} + \int_0^t \left\|v_3^{\frac{m+1}{8}}\right\|_{H^1}^2 \mathrm{d}s \le c(r) \quad \forall\, t \in \mathbb{R}_+.$$

Thus $v_i^{\frac{r+1}{2}}, v_3^{\frac{m+1}{8}} \in L^\infty(\mathbb{R}_+, L^2(\Omega)) \cap L^2(\mathbb{R}_+, H^1(\Omega))$, $i = 0,1,2$. $\square$

Theorem 4.2. *If u is a solution to (P) then $u \in L^\infty(\mathbb{R}_+, L^\infty(\Omega, \mathbb{R}^4))$.*

Proof. i) Let u be a solution to (P), $w := u - u^*$. Because of Theorem 4.1, imbedding and trace theorems and (2.11) it is easy to check that there exists an element $b \in L^4\left(\mathbb{R}_+, (W^{1,5/4}(\Omega))^*\right)$ such that for all $v \in L^{4/3}\left(\mathbb{R}_+, W^{1,5/4}(\Omega)\right)$

$$\int_0^\infty \sum_{j=0}^{3}\left[\int_\Omega (w_j^2 + |w_j|)v\,\mathrm{d}x + \int_\Gamma (w_j^2 + |w_j|)v\,\mathrm{d}\Gamma\right]\mathrm{d}s = \langle b, v\rangle .$$

ii) Let $k \ge \max\{1, \|U\|_{L^\infty(\Omega,\mathbb{R}^4)}\}$. We use the test function $v := (u - u^* - k)^+$ and denote by m_{jk} the Lebesgue measure of the set $\{x \in \Omega : u_j - u_j^* > k\}$. Then

$$\begin{aligned}
\sum_{i=0}^{3}\Big[\|v_i(t)\|_{L^2}^2 &+ 2\hat{c}\int_0^t \|v_i\|_{H^1}^2 \mathrm{d}s\Big] \\
&\le c\int_0^t \sum_{i=0}^{3} \|b\|_{(W^{1,5/4})^*}\|v_i\|_{W^{1,5/4}}\,\mathrm{d}s \\
&\le c\int_0^t \sum_{i=0}^{3} \|b\|_{(W^{1,5/4})^*}\|v_i\|_{H^1}\, m_{ik}^{3/10}\mathrm{d}s \\
&\le \int_0^t \sum_{i=0}^{3}\left(\hat{c}\,\|v_i\|_{H^1}^2 + c\,\|b\|_{(W^{1,5/4})^*}^2\, m_{ik}^{3/5}\right)\mathrm{d}s.
\end{aligned}$$

Thus we obtain the inequality

$$\begin{aligned}
\sum_{i=0}^{3}\Big[\|v_i(t)\|_{L^2}^2 &+ \hat{c}\int_0^t \|v_i\|_{H^1}^2 \mathrm{d}s\Big] \\
&\le c\sum_{i=0}^{3}\|b\|_{L^4\left(\mathbb{R}_+,(W^{1,5/4})^*\right)}^2 \left\|m_{ik}^{3/5}\right\|_{L^2(\mathbb{R}_+)} \\
&\le c\sum_{i=0}^{3}\|b\|_{L^4\left(\mathbb{R}_+,(W^{1,5/4})^*\right)}^2 \|m_{ik}\|_{L^{6/5}(\mathbb{R}_+)}^{3/5} \\
&\le c\sum_{i=0}^{3}\|m_{ik}\|_{L^{6/5}(\mathbb{R}_+)}^{3/5}.
\end{aligned} \tag{4.2}$$

Since $k \ge 1$ and

$|u_i - u_i^*| \in L^\infty\left(\mathbb{R}_+, L^2(\Omega)\right) \cap L^2\left(\mathbb{R}_+, H^1(\Omega)\right) \subset L^\infty\left(\mathbb{R}_+, L^{4/3}(\Omega)\right) \cap L^2\left(\mathbb{R}_+, H^1(\Omega)\right)$

we have from (2.11)

$$\int_0^\infty m_{ik}^{6/5}\mathrm{d}s \le \int_0^\infty \left(\int_\Omega |u_i - u_i^*|^3 \mathrm{d}x\right)^{6/5}\mathrm{d}s = \|u_i - u_i^*\|_{L^{18/5}(\mathbb{R}_+,L^3)}^{18/5} < c.$$

iii) Let us define

$$\phi(k) := \left(\int_0^\infty \sum_{i=0}^{3} m_{ik}^{6/5} \mathrm{d}s \right)^{5/22} .$$

Then we obtain for $h > k$ by the Gagliardo-Nirenberg inequality (2.9) and (4.2) the following estimate:

$$\begin{aligned}
(h-k)\phi(h) &= \left(\int_0^\infty \sum_{i=0}^{3} \left[(h-k)^{11/3} m_{ih} \right]^{6/5} \mathrm{d}s \right)^{5/22} \\
&\le \left(\int_0^\infty \sum_{i=0}^{3} \|v_i\|_{L^{11/3}}^{22/5} \mathrm{d}s \right)^{5/22} \\
&\le \left(c \int_0^\infty \sum_{i=0}^{3} \|v_i\|_{L^2}^{12/5} \|v_i\|_{H^1}^{2} \mathrm{d}s \right)^{5/22} \\
&\le c \left(\sum_{i=0}^{3} \|v_i\|_{L^\infty(\mathbb{R}_+, L^2)}^{12/5} \|v_i\|_{L^2(\mathbb{R}_+, H^1)}^{2} \right)^{5/22} \\
&\le c \left(\sum_{i=0}^{3} \|m_{ik}\|_{L^{6/5}(\mathbb{R}_+)}^{3/5} \right)^{(5/22)\cdot(11/5)} \\
&= c \left(\sum_{i=0}^{3} \int_0^\infty m_{ik}^{6/5} \mathrm{d}s \right)^{(5/22)\cdot(11/10)} \qquad \le c\phi(k)^{11/10}.
\end{aligned}$$

By Lemma 2.1 we conclude that there is a $\tilde{k}$ such that $\phi(k) = 0$ for all $k \ge \tilde{k}$. Therefore by the definition of ϕ it follows $u - u^* \in L^\infty(\mathbb{R}_+, L^\infty(\Omega, \mathbb{R}^4))$, thus $u \in L^\infty(\mathbb{R}_+, L^\infty(\Omega, \mathbb{R}^4))$. $\square$

Remark 4.1. Theorem 4.2 implies that $u|_\Gamma \in L^\infty(\mathbb{R}_+, L^\infty(\Gamma, \mathbb{R}^4))$.

5. Existence

Our aim is to show that there is a solution to (P). By the following reason it is sufficient to prove that (P_S) is solvable for all $T \in \mathbb{R}_+$. Let u_{T_0} be a solution to $(P_{[0,T_0]})$, then $u_{T_0} \in L^\infty([0,T_0], L^\infty(\Omega, \mathbb{R}^4))$. Thus there exists a $\theta_1 \le T_0$, θ_1 near to T_0 such that $u_{T_0}(\theta_1) \in L^\infty(\Omega, \mathbb{R}^4)$. Because the problem is autonomous we now can solve $(P_{[\theta_1, 2T_0]})$ with initial value $u_{T_0}(\theta_1)$ by u_{2T_0}. For

$$\tilde{u}_{2T_0}(t) := \begin{cases} u_{T_0}(t) & \text{if } t \in [0, \theta_1] \\ u_{2T_0}(t) & \text{if } t \in [\theta_1, 2T_0] \end{cases}$$

it is easy to check that $\tilde{u}_{2T_0} \in W_{[0,2T_0]} \cap V_{[0,2T_0]}$. Continuing this procedure we construct a solution to (P) by

$$u(t) := u_{kT_0}(t) \quad \text{if } t \in [\theta_{k-1}, \theta_k], \ \theta_0 = 0.$$

Thus it remains to show that for every $T \in \mathbb{R}_+$ there is a solution to (P_S). Let $T \in \mathbb{R}_+$ be arbitrarily fixed, $M > 1$ and

$$\rho(u) := \left(\max\left\{ 1, \sum_{i=0}^{3} |u_i|^2 / M^2 \right\} \right)^{-1}.$$

We denote by $\langle\langle\cdot,\cdot\rangle\rangle$ the dual pairing of $L^2(S,X)$ and $L^2(S,X^*)$. We define the regularized operators $A_M,\ B_M,\ R_M\colon L^2(S,X)\longrightarrow L^2(S,X^*)$ by

$$\langle\langle A_M(u),v\rangle\rangle := \int_0^T\int_\Omega \left\{ D_0\,\varphi(u_0^+)\nabla u_0\nabla v_0 + \sum_{i=1}^3 D_i\nabla u_i\nabla v_i\right\}\,\mathrm{d}x\,\mathrm{d}t,$$

$$\langle\langle B_M(u),v\rangle\rangle := \int_0^T\int_\Gamma \rho(u)\left\{ h_0(g(u_0^+)-u_3^+)(v_0-v_3) + \sum_{i=1}^3 h_i(u_i^+-\hat{u}_i)v_i\right\}\,\mathrm{d}\Gamma\,\mathrm{d}t,$$

$$\langle\langle R_M(u),v\rangle\rangle := -\int_0^T\int_\Omega \rho(u)\left\{ R_1(u^+)(v_1+v_3-v_0) + R_2(u^+)(v_2+v_3)\right\}\,\mathrm{d}x\,\mathrm{d}t$$

and consider the corresponding

Problem ($\mathbf{P_M}$):

$$u' + A_M(u) + B_M(u) = R_M(u),\ u(0)=U,\ u\in W_S.$$

Lemma 5.1. *If u is a solution to (P_M) then $u\geq 0$ and*

$$\|u\|_{L^\infty(S,L^\infty(\Omega,\mathbb{R}^4))},\ \|u|_\Gamma\|_{L^\infty(S,L^\infty(\Gamma,\mathbb{R}^4))}\leq c$$

where c is independent of M.

Proof. i) Since $-u^-\in L^2(S,X)$ it follows from (P_M) that

$$\sum_{i=0}^3\left(\frac{1}{2}\left\|u_i^-(t)\right\|_{L^2}^2 + \alpha\int_0^t\left\|\nabla u_i^-\right\|_{L^2}^2\mathrm{d}s\right)\leq 0.$$

Hence $u_i^-=0,\ i=0,1,2,3$.
ii) Applying the procedure of the proof of Theorem 3.1 to (P_M) we get

$$\|u\|_{L^\infty(S,L^1(\Omega,\mathbb{R}^4))}\leq c,\ \|\nabla\sqrt{u_i}\|_{L^2(S,L^2(\Omega,\mathbb{R}^2))}\leq c,\ i=0,\dots,3,$$

independently of M. Therefore, because S is a finite time interval,

$$u-u^*\in L^1\left(S,L^1\left(\Omega,\mathbb{R}^4\right)\right)\cap L^\infty\left(S,L^1\left(\Omega,\mathbb{R}^4\right)\right),\ \sqrt{u}-\sqrt{u^*}\in L^2(S,X).$$

Theorem 4.1 is true also for the solutions to (P_M). A result corresponding to that of Lemma 4.1 is obtained by a similar proof. Instead of using estimate (4.1) we have to conclude now in the following way: The factor in front of the $L^{r+1}(\Gamma)$– and $L^{\frac{m+1}{4}}(\Gamma)$–norms on the left-hand side now is not bounded from below. Therefore we omit these terms (they are positive), and the $L^2(\Omega)$-parts of the H^1-norms of powers of $|u-u^*|$ on the right-hand side are treated by Gronwall's Lemma. The gradient terms are again compensated by those on the left-hand side. With the notation of Lemma 4.1 we get

$$\|v_3\|_{L^\infty\left(S,L^{\frac{m+1}{4}}(\Omega)\right)}\leq c,\ \left\|\nabla v_3^{\frac{m+1}{8}}\right\|_{L^2(S,L^2(\Omega,\mathbb{R}^2))}\leq c,$$

independently of M. Thus, because S is a finite intervall,

$$\left\|v_3^{\frac{m+1}{8}}\right\|_{L^2(S,H^1(\Omega))}\leq c,$$

independently of M. Analogously we obtain the corresponding estimates for v_i, $i = 0, 1, 2$. Similar changes have to take place in the proof of Theorem 4.2, which yields the asserted $L^\infty(S, L^\infty)$-estimate, independently of M. $\square$

To prove the existence of a solution to (P_M) we use a fixed point principle. Let $w \in W_S$ be arbitrarily fixed. We define the operator $A_w\colon L^2(S,X) \longrightarrow L^2(S,X^*)$ by

$$\langle\langle A_w(u), v\rangle\rangle := \int_0^T \int_\Omega \left\{ D_0\, \varphi(w_0^+)\nabla u_0 \nabla v_0 + \sum_{i=1}^3 D_i \nabla u_i \nabla v_i \right\} \mathrm{d}x\, \mathrm{d}t.$$

Then A_w is a monotone, radially continuous operator, $A_w + \lambda I$ is coercive. Because of $R_M(w) - B_M(w) \in L^2(S, X^*)$ it follows from standard results on evolution equations (see e.g. [4]) that there is exactly one solution to

Problem ($\mathbf{P_w}$):

$$u' + A_w(u) = R_M(w) - B_M(w),\ u(0) = U,\ u \in W_S.$$

By $Q\colon W_S \longrightarrow W_S$ we denote the mapping assigning to w the solution u to (P_w), $u = Q(w)$.

Lemma 5.2. *The mapping $Q\colon W_S \longrightarrow W_S$ is completely continuous.*

Proof. Let $\{w_n\} \subset W_S$ be bounded. Then, by standard compactness results (see e.g. Lions [13, Chap.1]) $\{w_n\}$ is precompact in $L^2(S,Y)$ and $L^2(S,Z)$, and without any loss of generality we may assume that $w_n \to w$ in $L^2(S,Y)$ and $L^2(S,Z)$. Let $u_n = Q(w_n)$, $u = Q(w)$. By means of the test function $u_n - u$ we obtain

$$\begin{aligned}\frac{1}{2}\|(u_n-u)(t)\|_Y^2 + \int_0^t \int_\Omega \Big\{ D_0 \Big[\varphi(w_{n0}^+)\nabla u_{n0} - \varphi(w_0^+)\nabla u_0\Big]\nabla(u_{n0}-u_0) \\ + \sum_{i=1}^3 D_i\ |\nabla(u_{ni}-u_i)|^2 \Big\}\mathrm{d}x\mathrm{d}s \\ \le \int_0^t \langle R_M(w_n) - R_M(w) - B_M(w_n) + B_M(w), u_n - u\rangle \mathrm{d}s.\end{aligned}$$

The functions $\kappa_l\colon \mathbb{R}^4 \to \mathbb{R},\ l = 1, \ldots, 4$, defined by

$$\kappa_1(y) := \rho(y),\ \kappa_2(y) := \rho(y)\, g(y_0),\ \kappa_3(y) := \rho(y)\, y_i,\ \kappa_4(y) := \rho(y)\, y_i\, y_j$$

are Lipschitz continuous. Because of

$$\begin{aligned}&\Big(\varphi(w_{n0}^+)\nabla u_{n0} - \varphi(w_0^+)\nabla u_0\Big)\ \nabla(u_{n0}-u_0) \\ &\qquad = \varphi(w_{n0}^+)|\nabla(u_{n0}-u_0)|^2 + \Big(\varphi(w_{n0}^+) - \varphi(w_0^+)\Big)\ \nabla u_0 \nabla(u_{n0}-u_0)\end{aligned}$$

we arrive at

$$
\begin{aligned}
&\frac{1}{2}\left\|(u_n-u)(t)\right\|_Y^2+\alpha\int_0^t\sum_{i=0}^3\left\|\nabla(u_{ni}-u_i)\right\|_{L^2}^2\,\mathrm{d}s\\
&\leq\int_0^t\bigg\{\int_\Omega D_0\left|\varphi(w_{n0}^+)-\varphi(w_0^+)\right||\nabla u_0||\nabla(u_{n0}-u_0)|\mathrm{d}x\\
&\qquad+c(M)\int_\Omega\sum_{i,j=0}^3|w_{nj}-w_j|\,|u_{ni}-u_i|\,\mathrm{d}x\\
&\qquad+c(M)\int_\Gamma\sum_{i,j=0}^3|w_{nj}-w_j|\,|u_{ni}-u_i|\,\mathrm{d}\Gamma\bigg\}\mathrm{d}s\\
&\leq c(M)\left\|u_n-u\right\|_{L^2(S,X)}\bigg[\bigg(\int_0^t\int_\Omega\left|\varphi(w_{n0}^+)-\varphi(w_0^+)\right|^2|\nabla u_0|^2\mathrm{d}x\,\mathrm{d}s\bigg)^{\frac{1}{2}}\\
&\qquad\qquad+\left\|w_n-w\right\|_{L^2(S,Y)}+\left\|w_n-w\right\|_{L^2(S,Z)}\bigg].
\end{aligned}
$$

From properties of superposition operators we conclude that

$$\int_0^t\int_\Omega\left|\varphi(w_{n0}^+)-\varphi(w_0^+)\right|^2|\nabla u_0|^2\mathrm{d}x\mathrm{d}s\;\to 0\text{ for }n\to\infty.$$

Therefore we get $u_n\to u$ in $L^2(S,X)$. Additionally we have

$$
\begin{aligned}
&\|u_n'-u'\|_{L^2(S,X^*)}\\
&=\|R_M(w_n)-R_M(w)-B_M(w_n)+B_M(w)-A_{w_n}(u_n)+A_w(u)\|_{L^2(S,X^*)}\\
&\leq\sup_{\|v\|_{L^2(S,X)}\leq 1}\bigg\{c\left\|v\right\|_{L^2(S,X)}\bigg[\left\|u_n-u\right\|_{L^2(S,X)}+\left\|w_n-w\right\|_{L^2(S,Y)}+\left\|w_n-w\right\|_{L^2(S,Z)}\\
&\qquad\qquad+\bigg(\int_0^T\int_\Omega\left|\varphi(w_{n0}^+)-\varphi(w_0^+)\right|^2|\nabla u_0|^2\mathrm{d}x\mathrm{d}s\bigg)^{\frac{1}{2}}\bigg]\bigg\}\\
&\to 0\text{ for }n\to\infty.
\end{aligned}
$$

Thus, $u_n\to u$ in W_S. By similar arguments the continuity of Q can be shown. Therefore Q is completely continuous. □

Lemma 5.3. *There exists a fixed point of Q.*

Proof. Let $u=Q(w)$. By means of the test function u we have by the Gagliardo-Nirenberg inequality (2.9)

$$
\begin{aligned}
\|u(t)\|_Y^2\;+\;&2\alpha\int_0^t\sum_{i=0}^3\|\nabla u_i\|_{L^2}^2\,\mathrm{d}s\\
\leq\;&c+\int_0^t c(M)\bigg(\sum_{i=0}^3\Big[\|u_i\|_{L^2}^2+\|u_i\|_{L^2(\Gamma)}^2\Big]+1\bigg)\mathrm{d}s\\
\leq\;&c+\int_0^t\bigg\{\alpha\sum_{i=0}^3\|\nabla u_i\|_{L^2}^2+c(M)\bigg(\sum_{i=0}^3\|u_i\|_{L^2}^2+1\bigg)\bigg\}\mathrm{d}s.
\end{aligned}
$$

Gronwall's Lemma implies

$$\|u(t)\|_Y^2 + \alpha \int_0^t \sum_{i=0}^{3} \|\nabla u_i\|_{L^2}^2 \, \mathrm{d}s \leq c(M,T) \; \forall \, t \in S.$$

Consequently,

$$\|u\|_{L^2(S,X)} \leq \hat{c}(M,T).$$

Additionally we have by the definition of R_M, B_M and $A_M(u)$ and the boundedness of u in $L^2(S,X)$

$$\|u'\|_{L^2(S,X^*)} \leq \|R_M(w)\|_{L^2(S,X^*)} + \|B_M(w)\|_{L^2(S,X^*)} + \|A_w(u)\|_{L^2(S,X^*)} \leq \check{c}(M,T).$$

Therefore Q maps W_S into the (bounded) ball

$$\Big\{ u \in W_S : \|u\|_{W_S} \leq \hat{c}(M,T) + \check{c}(M,T) \Big\}.$$

Because of Lemma 5.2 the assertion follows from Schauder's Fixed Point Theorem. $\square$

Lemma 5.4. *The problem (P_M) is solvable.*

Proof. The assertion of Lemma 5.4 follows immediately by Lemma 5.3. $\square$

Lemma 5.5. *For each fixed $T < \infty$ there exists a solution to (P_S).*

Proof. Let M be chosen greater than the $L^\infty(S, L^\infty(\Omega, \mathbb{R}^4))$–bounds obtained in Lemma 5.1. Then by means of Lemma 5.4 and Lemma 5.1 we get a solution u to (P_M) with $u \geq 0$, $\|u\|_{L^\infty(S,L^\infty(\Omega,\mathbb{R}^4))} \leq M$, and consequently $u \in V_S$. Therefore, u is also a solution to problem (P_S) . $\square$

Because S was arbitary, we have proved

Theorem 5.1. *There exists a solution to (P).*

6. Additional regularity properties

In this section we use regularity results for parabolic equations with mixed boundary conditions by Gröger, Rehberg (see [7]). An investigation of the proofs given in [7] shows that these regularity results are applicable also in case of pure Neumann boundary conditions. Let $S := [0,T]$ be any finite time interval. Supposing (2.7) we transform problem (P_S) to one which can be handled by methods of [7]. Let u be a solution of (P_S), $\bar{u} := u - U$. Then we have $\bar{u}(0) = 0$, $\bar{u}' = u'$. Let p be near 2, $p > 2$ and q with

$$\frac{1}{p} + \frac{1}{q} < \frac{1}{2}. \tag{6.1}$$

We consider the operators

$$\widetilde{R}\colon L^2(S,X) \times W^{1,p}(\Omega,\mathbb{R}^4) \longrightarrow L^2(S,X^*),\ \widetilde{A}\colon L^2(S,X) \longrightarrow L^2(S,X^*)$$

defined by

$$
\begin{aligned}
-\langle\langle \widetilde{R}(u,U),v\rangle\rangle &:= -\langle\langle R(u),v\rangle\rangle \\
&\quad + \int_0^T\int_\Omega \left\{ D_0\,\varphi(u_0)\nabla U_0\nabla v_0 + \sum_{i=1}^3 D_i\nabla U_i\nabla v_i \right\}\,\mathrm{d}x\,\mathrm{d}t \\
&\quad + \int_0^T\int_\Gamma \left\{ h_0(g(u_0)-u_3)(v_0-v_3) + \sum_{i=1}^3 h_i(u_i-\hat{u}_i)v_i \right\}\,\mathrm{d}\Gamma\,\mathrm{d}t. \\
\langle\langle \widetilde{A}(\bar{u}),v\rangle\rangle &:= \int_0^T\int_\Omega \left\{ D_0\,\widetilde{\varphi}(\bar{u}_0)\nabla\bar{u}_0\nabla v_0 + \sum_{i=1}^3 D_i\nabla\bar{u}_i\nabla v_i \right\}\,\mathrm{d}x\,\mathrm{d}t
\end{aligned}
$$

where $\widetilde{\varphi}(\bar{u}_0) := \varphi(\bar{u}_0+U_0)$. Because of (P_S) $\bar{u}$ is a solution to

$$
\bar{u}' + \widetilde{A}(\bar{u}) = \widetilde{R}(u,U), \qquad \bar{u}(0)=0, \qquad \bar{u}\in W_S. \tag{6.2}
$$

From the preceding a-priori estimates (see Theorem 4.2) and (2.6) and by (2.7) it follows that

$$
\widetilde{R}(u,U) \in L^q\left(S, W^{1,p'}(\Omega,\mathbb{R}^4)^*\right)
$$

where $\frac{1}{p}+\frac{1}{p'}=1$ and p, q satisfy (6.1). According to the regularity result of [7] we get for the solution $\bar{u}$ to (6.2) and therefore for the solution u to (P_S)

Theorem 6.1. *If we additionally assume (2.7), then there exists a $p_0>2$ such that for every $q\in[1,\infty)$ and every $p\in[2,p_0]$ solutions u to (P_S) have the regularity property*

$$
u \in L^q\left(S, W^{1,p}(\Omega,\mathbb{R}^4)\right) \cap W^{1,q}\left(S, W^{1,p'}(\Omega,\mathbb{R}^4)^*\right).
$$

7. Uniqueness

Theorem 7.1. *Under the additional hypothesis (2.7) there exists a unique solution to problem (P).*

Proof. It sufficies to prove uniqueness on every finite time interval S. Let u and $\tilde{u}$ be solutions of (P) and $\bar{u} := u-\tilde{u}$. Then $\bar{u}\in L^2(S,X)$ and

$$
\begin{aligned}
&\frac{1}{2}\,\|\bar{u}(t)\|_Y^2 + \alpha\int_0^t \sum_{i=0}^3 \left(\|\nabla\bar{u}_i\|_{L^2}^2 + \|\bar{u}_i\|_{L^2(\Gamma)}^2\right)\mathrm{d}s \\
&\qquad \le \int_0^t \Big\{ \langle R(u)-R(\tilde{u}),\bar{u}\rangle + \int_\Omega D_0\,|\varphi(u_0)-\varphi(\tilde{u}_0)||\nabla\tilde{u}_0||\nabla\bar{u}_0|\mathrm{d}x \\
&\qquad + \int_\Gamma h_0\left(|g(u_0)-g(\tilde{u}_0)||\bar{u}_3| + |\bar{u}_3||\bar{u}_0|\right)\mathrm{d}\Gamma\Big\}\mathrm{d}s \quad \forall\, t\in S.
\end{aligned}
$$

Because of the L^∞-estimates, local Lipschitz continuity of φ and the Lipschitz continuity of ψ we get by (3.6), the Hölder, Gagliardo-Nirenberg and Young inequalities for p, q given in Theorem 6.1

$$
\begin{aligned}
&\frac{1}{2}\,\|\bar{u}(t)\|_Y^2\\
&\quad\le \int_0^t \Big\{-\hat{c}\,\|\bar{u}\|_X^2 + c\sum_{i=0}^{3}\Big(\|\bar{u}_i\|_{L^2(\Gamma)}^2 + \|\bar{u}_i\|_{L^2}^2\Big) + c\,\|\bar{u}_0\|_{L^q}\,\|\nabla\tilde{u}_0\|_{L^p}\,\|\nabla\bar{u}_0\|_{L_2}\Big\}\,\mathrm{d}s\\
&\quad\le \int_0^t \Big\{-\frac{\hat{c}}{2}\,\|\bar{u}\|_X^2 + c\,\|\bar{u}\|_Y^2 + c\,\|\bar{u}_0\|_{H^1}^{2-\frac{2}{q}}\,\|\nabla\tilde{u}_0\|_{L^p}\,\|\bar{u}_0\|_{L^2}^{\frac{2}{q}}\Big\}\,\mathrm{d}s\\
&\quad\le c\int_0^t \Big\{\|\bar{u}\|_Y^2 + \|\nabla\tilde{u}_0\|_{L^p}^q\,\|\bar{u}\|_Y^2\Big\}\,\mathrm{d}s \quad \forall\, t\in S.
\end{aligned}
$$

Theorem 6.1 implies that $\|\nabla\tilde{u}_0\|_{L^q(S,L^p)} \le c$, thus Gronwall's Lemma completes the proof. □

8. Additional remarks

Theorem 8.1. *If u is a solution to (P) then*

$$\|u(t)-u^*\|_{L^p(\Omega,\mathbb{R}^4)} \le c\,e^{-\lambda_p t} \quad \forall\, t\ge 0,\ \textit{where } p\in[1,+\infty),\ c,\ \lambda_p>0.$$

Proof. Let be $p\in[1,+\infty)$. Since

$$u_i \in L^\infty(\mathbb{R}_+, L^\infty(\Omega)) \cap C\left(\mathbb{R}_+, L^2(\Omega)\right)$$

the function u_i is a continuous mapping from $\mathbb{R}_+$ into $L^\infty(\Omega)$ equipped with the weak* topology and

$$\|u_i(t)-u_i^*\|_{L^\infty} \le \|u_i-u_i^*\|_{L^\infty(\mathbb{R}_+,L^\infty(\Omega))} \quad \forall\, t\in\mathbb{R}_+,\ i=0,\dots,3. \tag{8.1}$$

By means of (8.1) and Theorem 3.2 we obtain

$$
\begin{aligned}
\|u_i(t)-u_i^*\|_{L^p}^p &\le \|u_i(t)-u_i^*\|_{L^1}\,\|u_i-u_i^*\|_{L^\infty(\mathbb{R}_+,L^\infty(\Omega))}^{p-1}\\
&\le c^p\,e^{-\lambda t/2} \qquad \forall\, t\in\mathbb{R}_+,\ i=0,\dots,3. \quad \square
\end{aligned}
$$

Theorem 8.2. *Let (2.8) be satisfied. If u is a solution to (P) then*

$$\ln u \in L^\infty\left(\mathbb{R}_+, L^\infty\left(\Omega,\mathbb{R}^4\right)\right).$$

Proof. Because of Theorem 4.2 it remains to show that u is globally bounded from below. It is sufficient to prove that for every finite time interval S the solution u is bounded from below by a positive constant not depending on S. By (2.8) there is a positive constant $c_0<1$ such that $U_i\ge c_0,\ i=0,1,2,3$. Let $T\in\mathbb{R}_+$ be arbitrarily fixed, $\tilde{k}:=\max\{1,-\ln c_0\},\ k\ge\tilde{k},\ \delta>0$. We introduce

$$m_{3k} := \operatorname{mes}\Big\{x\in\Omega : \ln u_3 < -k\Big\}.$$

We use the test function

$$\Big(0,0,0,-\frac{v}{u_3+\delta}\Big),\ v := \Big(\ln(u_3+\delta)+k\Big)^-.$$

Thereby we take into account that

$$u \in L^\infty\left(\mathbb{R}_+, L^\infty(\Omega, \mathbb{R}^4)\right), \; u|_\Gamma \in L^\infty\left(\mathbb{R}_+, L^\infty(\Gamma, \mathbb{R}^4)\right)$$

and

$$-\int_0^t u_3' \frac{v}{u_3+\delta} \mathrm{d}s = \frac{1}{2} v(t)^2, \quad \nabla u_3 \nabla\left(\frac{-v}{u_3+\delta}\right) \geq |\nabla v|^2, \quad \frac{v}{u_3+\delta} \geq v^2.$$

Thus we obtain

$$\begin{aligned}
\frac{1}{2}\|v(t)\|_{L^2}^2 \quad &+ \quad \hat{c}\int_0^t \|v\|_{H^1}^2 \,\mathrm{d}s \\
&\leq \quad \int_0^t \left\{\int_\Omega (\tilde{k}_1\, u_1 + \tilde{k}_2\, u_2)\, v \,\mathrm{d}x + \int_\Gamma (h_0 + h_3)\, v \,\mathrm{d}\Gamma\right\} \mathrm{d}s \\
&\leq \quad c\int_0^t \|v\|_{W^{1,1}(\Omega)} \,\mathrm{d}s \\
&\leq \quad c\int_0^t \|v\|_{H^1}\, m_{3k}^{1/2} \,\mathrm{d}s \\
&\leq \quad \int_0^t \left\{\frac{\hat{c}}{2}\|v\|_{H^1}^2 + c\, m_{3k}\right\} \mathrm{d}s.
\end{aligned}$$

Therefore we get

$$\|v(t)\|_{L^2}^2 + \int_0^t \|v\|_{H^1}^2 \,\mathrm{d}s \leq c\int_0^T m_{3k} \,\mathrm{d}s.$$

Letting $\delta \downarrow 0$ we obtain (cf. the definition of v)

$$\begin{aligned}
\left\|(\ln u_3 + k)^-(t)\right\|_{L^2}^2 &+ \int_0^t \left\|(\ln u_3 + k)^-\right\|_{H^1}^2 \,\mathrm{d}s \\
&\leq c\int_0^T m_{3k} \,\mathrm{d}s \quad \forall\, t \in [0,T],
\end{aligned} \tag{8.2}$$

independently of T. For $k \geq \tilde{k}$ we define $\phi(k)$ by

$$\phi(k) := \left(\int_0^T m_{3k} \mathrm{d}s\right)^{1/4}.$$

Taking advantage of (2.9) and (8.2) we obtain the following estimate:

$$\begin{aligned}
(h-k)\phi(h) &= \left(\int_0^T (h-k)^4 m_{3h} \,\mathrm{d}s\right)^{1/4} \\
&\leq \left(\int_0^T \left\|(\ln u_3 + k)^-\right\|_{L^4}^4 \mathrm{d}s\right)^{1/4} \\
&\leq c\left(\int_0^T \left\|(\ln u_3 + k)^-\right\|_{H^1}^2 \left\|(\ln u_3 + k)^-\right\|_{L^2}^2 \mathrm{d}s\right)^{1/4} \\
&\leq c\left(\left\|(\ln u_3 + k)^-\right\|_{L^\infty(S,L^2)}^2 \left\|(\ln u_3 + k)^-\right\|_{L^2(S,H^1)}^2\right)^{1/4} \\
&\leq c\left(\int_0^T m_{3k} \mathrm{d}s\right)^{1/2} = c_3\, \phi(k)^2.
\end{aligned}$$

The constant $c_3 > 0$ is independent on T. By Lemma 2.1 we get

$$\phi(k) = 0 \quad \text{if } k \geq k_0 := \tilde{k} + \frac{1}{4} c_3 \, \phi(\tilde{k}).$$

Therefore we obtain the estimate $u_3 \geq e^{-k_0}$. Since k_0 is independent of T, e^{-k_0} is a global lower bound of u_3. The same procedure can be used to get the lower bounds of u_1 and u_2. The knowledge of the global lower bound for u_3, which is also a lower bound for u_3 on Γ, allows us to treat the equation for u_0 by the same technique. □

If one is interested in results concerning any finite time interval S, assumption (2.5) is not necessary. By means of somewhat changed proofs the following results for solutions to (P_S) are available.

Theorem 8.3. *Let S be any bounded time interval and suppose that* (2.4)*,* (2.6)*,* (2.7) *and* (2.8) *hold. Then there exists exactly one solution u to (P_S) and*

$$\|\ln u\|_{L^\infty(S, L^\infty(\Omega, \mathbb{R}^4))} \leq c_S$$

where in general c_S depends on the length of the time interval S.

Proof. Modifying the proof of Theorem 3.1 we now use (formally) the test function

$$\left(\ln g(u_0), \ln \frac{u_1}{k_1}, \ln \frac{u_2}{k_2}, \ln u_3\right).$$

Expressions coming from the time derivative terms are estimated by

$$y \ln y - \beta \, y \geq \ \frac{1}{2}|y| - c.$$

In the boundary terms we exploit

$$(u_i - \hat{u}_i) \ln \frac{u_i}{c} \geq -c_1, \ \ i = 1, 2, 3, \ \ c = \text{const}.$$

We obtain

$$\|u_i\|_{L^\infty(S, L^1)}, \ \ \|\nabla \ \sqrt{u_i}\|_{L^2(S, L^2)} \leq \ c, \ \ i = 0, \ldots, 3,$$

and thus, because S is finite, $\|\sqrt{u}\|_{L^2(S,X)} \leq c(S)$. Now we apply the methods of the proofs of Theorem 4.1 and Lemma 4.1 to u instead of $|u - u^*|$. From the $L^\infty(S, L^2)$–bound of powers of u_i and the $L^2(S, L^2)$–bound of the gradient of powers of u_i we obtain the $L^2(S, H^1)$–bound for this power of u_i, depending on the length of the time interval. Upper and lower bounds, regularity results corresponding to Theorem 6.1, existence and uniqueness for the solution to (P_S) follow by the same methods as those used before. In all the above estimates where we took advantage of the boundary integrals now Gronwall's Lemma helps to obtain the desired estimates. □

REFERENCES

1. H. Brézis, *Opérateurs maximaux monotones et semi-groups de contractions dans les espaces de Hilbert*, North-Holland Math. Studies, no. 5, North–Holland, Amsterdam, 1973.
2. I. Ekeland and R. Temam, *Convex analysis and variational problems*, Studies in Math. and its Appl., vol. 1, North–Holland, Amsterdam, 1976.
3. H. Gajewski and K. Gröger, *Semiconductor equations for variable mobilities based on Boltzmann statistics or Fermi–Dirac statistics*, Math. Nachr. **140** (1989), 7–36.
4. H. Gajewski, K. Gröger, and K. Zacharias, *Nichtlineare Operatorgleichungen und Operatordifferentialgleichungen*, Akademie–Verlag, Berlin, 1974.
5. U. Gösele, W. Frank, and A. Seeger, *Mechanism and kinetics of the diffusion of gold in silicon*, Appl. Phys. **23** (1980), 361–368.
6. K. Gröger, *Free energy estimates and asymptotic behaviour of reaction–diffusion processes*, to appear.
7. K. Gröger and J. Rehberg, *On the regularity of solutions to parabolic equations in case of mixed boundary conditions*, to appear.
8. D. Henry, *Geometric theory of semilinear parabolic equations*, Lect. Notes in Math., no. 840, Springer, Berlin–Heidelberg–New York, 1981.
9. R. Hünlich, U. Krause, R. Model, A. Pomp, I. Schmelzer, H. Stephan, N. Strecker, and S. Unger, *Der 2D-Technologiesimulator DIOS*, Nutzerhandbuch, Karl-Weierstraß-Institut für Mathematik, Berlin, 1991.
10. D. Kinderlehrer and G. Stampacchia, *An introduction to variational inequalities and their applications*, Academic Press, New York, 1980.
11. M. R. Kump and R. W. Dutton, *The efficient simulation of coupled point defect and impurity diffusion*, IEEE Trans. CAD **7** (1988), 191–204.
12. M. E. Law and R. W. Dutton, *Verification of analytic point defect models using SUPREM–IV*, IEEE Trans. CAD **7** (1988), 181–190.
13. J. L. Lions, *Quelques méthodes de résolution des problèmes aux limites non linéaires*, Dunod Gauthier–Villars, Paris, 1969.
14. D. Mathiot and J. C. Pfister, *Dopant diffusion in silicon: A consistent view involving nonequilibrium defects*, J. Appl. Phys. **55** (1984), 3518–3530.
15. B. J. Mulvaney and W. B. Richardson, *Model for defect–impurity pair diffusion in silicon*, Appl. Phys. Lett. **51** (1987), 1439–1441.
16. B. J. Mulvaney, W. B. Richardson, and T. L. Crandle, *PEPPER – A process simulator for VLSI*, IEEE Trans. CAD **8** (1989), 336–349.
17. M. Orlowski, *Unified model for impurity diffusion in silicon*, Appl. Phys. Lett. **53** (1988), 1323–1325.