# LOCAL EXISTENCE RESULT OF THE SINGLE DOPANT DIFFUSION INCLUDING CLUSTER REACTIONS OF HIGH ORDER

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We consider the pair diffusion process which includes cluster reactions of high order. We are able to prove a local (in time) existence result in arbitrary space dimensions. The model includes a nonlinear system of reaction-drift-diffusion equations, a nonlinear system of ordinary differential equations in Banach spaces, and a nonlinear elliptic equation for the electrochemical potential. The local existence result is based on the fixed point theorem of Schauder.

#### 1. Introduction

During the doping process impurity atoms of higher or lower chemical valence as silicon are introduced into a silicon layer to influence its electrical properties. Such dopants penetrate under high temperatures, usually around 1000 °C, with the so-called *pair diffusion mechanism* into the (homogeneous) layer. A precise description of the process can be found in [2, 3, 4] and in the literature cited therein.

Usually, dopant atoms (A) occupy substitutional sites in the silicon crystal lattice, loosing (donors, such as Arsenic and Phosphorus) or gaining (acceptors, such as Boron) by this an electron. The dopants move by interacting with native *point defects* called interstitials (I) and vacancies (V). *Interstitials* are silicon atoms which are not placed on a lattice site and move through the crystal unconstrained, and *vacancies* are empty lattice sites. Both can form *mobile* pairs with dopant atoms (AI, AV), while the unpaired dopants are *immobile*. The formation and decay of such pairs as well as the recombination of defects cause a movement of the dopant atoms accumulate to immobile clusters (A<sub>cl</sub>) in the silicon lattice.

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These interactions can be modelled in terms of *chemical reactions* of arbitrary order. The resulting nonlinear model contains a set of reaction-drift-diffusion equations for the point defects and pairs, reaction equations for the immobile dopants and clusters as well as a Poisson equation for the electrochemical potential.

#### 2. The model

For  $i \in \{I, V, AI, AV, A, A_{cl}\}$  we consider the species  $X_i$  and denote their concentrations by  $C_i$ . We distinguish between mobile and immobile species defining

$$J := \{I, V, AI, AV\}, \qquad J' := \{A, A_{cl}\},$$
(2.1)

respectively. We denote by  $\mathbf{C} = (C_I, C_V, C_{AI}, C_{AV}, C_A, C_{A_{cl}})$  the corresponding concentration vector. Each of the  $X_i, i \in J \cup J'$ , is considered as the union of charged species  $X_i^{(j)}$ , with the charged states  $j \in S_i$ , where each  $S_i \subset \mathbb{Z}$ . Thus, if  $C_i^{(j)}$  denotes the concentration of  $X_i^{(j)}$ , the total concentrations  $C_i$  are defined as

$$C_i := \sum_{j \in S_i} C_i^{(j)} \quad \text{for } i \in J \cup J'.$$
(2.2)

The immobile species  $X_i$ ,  $i \in J'$ , usually obey one fixed charged state.

The chemical potential of the electrons is denoted by  $\psi$ . The charge density of the electrons *n* and holes *p* are assumed to obey the Boltzmann statistics, meaning that

$$n = n_i \exp\left(\frac{\psi}{U_T}\right), \qquad p = n_i \exp\left(-\frac{\psi}{U_T}\right).$$
 (2.3)

Moreover,

$$P_{i}(\psi) = \sum_{j \in S_{i}} K_{i}^{(j)} e^{-j\psi/U_{T}}$$
(2.4)

are reference concentrations with positive constants  $K_i^{(j)}$ . Set

$$a_i = \frac{C_i}{P_i(\psi)} \quad \text{for } i \in J \cup J', \tag{2.5}$$

which represents the electrochemical activity of the *i*th component.

We define  $Q_T := \Omega \times (0, T)$ , where  $\Omega \subset \mathbb{R}^n$ ,  $0 < T < \infty$  and  $3 \le n \in \mathbb{N}$ , with the lateral surface  $\Sigma_T := \partial \Omega \times (0, T)$ . We consider the following system of equations.

The *mobile* species for  $i \in J$  obey reaction-drift-diffusion equations

$$\frac{\partial C_i}{\partial t} + \operatorname{div} J_i = R_i ((C_k)_{k \in J \cup J'}, \psi) \quad \text{in } Q_T,$$

$$C_i(\cdot, 0) = C_i^0(\cdot) \quad \text{in } \Omega,$$

$$J_i \cdot \mathbf{n} = 0 \quad \text{on } \Sigma_T.$$
(2.6)

The *immobile* dopant concentration  $C_A$  obeys the reaction equation

$$\frac{\partial C_A}{\partial t} = R_A((C_k)_{k \in J \cup J'}, \psi) \quad \text{in } Q_T,$$

$$C_A(\cdot, 0) = C_A^0(\cdot) \quad \text{in } \Omega.$$
(2.7)

The *immobile* cluster concentration  $C_{A_{cl}}$  also obeys a reaction equation

$$\frac{\partial C_{A_{\rm cl}}}{\partial t} = R_{A_{\rm cl}} \left( \left( C_k \right)_{k \in J \cup J'}, \psi \right) \quad \text{in } Q_T,$$

$$C_{A_{\rm cl}}(\cdot, 0) = C^0_{A_{\rm cl}}(\cdot) \quad \text{in } \Omega.$$
(2.8)

The equation for the chemical potential of the electrons reads

$$-\frac{\epsilon}{e}\Delta\psi + 2n_i \sinh\left(\frac{\psi}{U_T}\right) = \sum_{i\in J\cup J'} Q_i(\psi)C_i \quad \text{in } Q_T,$$

$$\nabla\psi \cdot \mathbf{n} = 0 \quad \text{on } \Sigma_T,$$
(2.9)

where  $\epsilon, e$  are physical quantities. For  $i \in J$ , the drift-diffusion term is given by

$$J_i = -D_i(\psi) \left\{ \nabla C_i + Q_i(\psi) \nabla \left(\frac{\psi}{U_T}\right) C_i \right\},$$
(2.10)

with the diffusivity

$$D_{i}(\psi) = \sum_{j \in S_{i}} \frac{D_{i}^{(j)} K_{i}^{(j)} e^{-j\psi/U_{T}}}{P_{i}(\psi)},$$
(2.11)

where  $D_i^{(j)}$  are positive constants. Whereas,

$$Q_{i}(\psi) = \sum_{j \in S_{i}} \frac{j K_{i}^{(j)} e^{-j\psi/U_{T}}}{P_{i}(\psi)}$$
(2.12)

represents the total charge of the *i*th species for  $i \in J \cup J'$ .

Next, we put the reactions in concrete form. The source terms  $R_i(\mathbf{C}, \psi)$  result from the reactions occurring during the redistribution of the dopants. All

relevant reactions (including cluster formations of high order) occurring during the (single) dopant diffusion are due to (2.5) of the form

$$R_{A,I} := K_{A,I}(\psi) (a_A a_I - a_{AI}), \qquad R_{AV,I} := K_{AV,I}(\psi) (a_{AV} a_I - a_A), R_{A,V} := K_{A,V}(\psi) (a_A a_V - a_{AV}), \qquad R_{AI,V} := K_{AI,V}(\psi) (a_{AI} a_V - a_A), R_{I,V} := K_{I,V}(\psi) (a_I a_V - 1), \qquad R_{AI,AV} := K_{AI,AV}(\psi) (a_{AI} a_{AV} - a_A^2), (2.13)$$

as well as the cluster reaction

$$R_{A,AI,AV} := K_{A,AI,AV}(\psi) \left( a_A^l a_{AI}^m a_{AV}^n - a_{A_{\rm cl}} a_I^s a_V^r \right), \tag{2.14}$$

where  $l, m, n, s, r \in \mathbb{N}$ , cl := l + m + n (the size of the cluster) and for  $i, h, k \in J \cup J'$ , the reaction rate coefficients are

$$K_{i,h,k}(\psi) = \sum_{j \in S_{i,h,k}} K_{i,h,k}^{(j)} e^{-j\psi/U_T},$$
(2.15)

 $K_{i,h,k}^{(j)} > 0$  are constants and  $S_{i,h,k} \subset \mathbb{Z}$  are special sets of indices. Thus, the source terms  $R_i(\mathbb{C}, \psi)$  are for  $i \in J$  of the form

$$R_{I}(\mathbf{C}, \psi) = -R_{A,I} - R_{AV,I} - R_{I,V} + sR_{A,AI,AV},$$
  

$$R_{V}(\mathbf{C}, \psi) = -R_{A,V} - R_{AI,V} - R_{I,V} + rR_{A,AI,AV},$$
  

$$R_{AI}(\mathbf{C}, \psi) = R_{A,I} - R_{AI,V} - R_{AI,AV} - mR_{A,AI,AV},$$
  

$$R_{AV}(\mathbf{C}, \psi) = R_{A,V} - R_{AV,I} - R_{AI,AV} - nR_{A,AI,AV},$$
  
(2.16)

and for  $i \in J'$  we have

$$R_{A}(\mathbf{C}, \psi) = -R_{A,I} - R_{A,V} + R_{AI,V} + R_{AV,I} + 2R_{AI,AV} - lR_{A,AI,AV},$$
  

$$R_{A_{cl}}(\mathbf{C}, \psi) = R_{A,AI,AV}.$$
(2.17)

For the detailed description and physical meaning of the coefficients mentioned above, (see for instance [3].)

Moreover, we set the constants  $\epsilon$ , e,  $U_T$ ,  $2n_i$  equal to one for the analytical investigations.

#### 3. Problem (P)

Now we summarize the basic properties of the coefficients appearing in the equations. The notation of the function spaces corresponds to that in [5, 6]. If we consider some function space *Y*, we denote by  $Y_+$  the cone of its nonnegative elements. Operations on vectors have to be understood componentwise. Throughout the paper,  $\Lambda > 0$  denotes a generic constant, which we supply with indices if the occasion arises.

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As can easily be seen, the coefficients appearing in the equations for  $i \in J \cup J'$ and  $k \in J$  have the following properties

$$D_{k}, Q_{i}, P_{i} \in C^{2}(\mathbb{R}), \qquad 0 < \Lambda_{1} \leq D_{k}(\psi) \leq \Lambda_{2},$$
  

$$\left|D_{k}^{(l)}(\psi)\right|, \left|Q_{i}^{(l)}(\psi)\right| \leq \Lambda_{3} \quad \text{with } Q_{i}'(\psi) < 0,$$
  

$$P_{i}(\psi) = P_{i}(0) \exp\left(-\int_{0}^{\psi} Q_{i}(s) ds\right), \quad P_{i}(0) > 0,$$
(3.1)

for all  $\psi \in \mathbb{R}$  and derivatives (l = 0, 1, 2) of required order two.

Furthermore,

$$0 < K_{i,h,k}(\psi) \in C^2(\mathbb{R}), \tag{3.2}$$

for  $i, h, k \in J \cup J'$  and where

$$P_{i}(\psi), K_{i,h,k}(\psi) \leq \Lambda_{4} \exp(\Lambda_{5}|\psi|).$$
(3.3)

The source terms (2.16) and (2.17) obey the growth conditions

$$R_{i}(\mathbf{C},\psi) \leq \lambda_{1}(\psi) \left(\sum_{k \in J \cup J'} \left(C_{k}\right)^{l+m+n} + 1\right) \quad \text{for } i \in J,$$
(3.4)

$$R_A(\mathbf{C},\psi) \le -\lambda_2(\psi) (C_A)^l + \lambda_3(\psi) \left(\sum_{k\in J} (C_k)^{l+m+n} + 1\right), \qquad (3.5)$$

$$R_{A_{\rm cl}}(\mathbf{C},\psi) \le -\lambda_4(\psi)C_{A_{\rm cl}} + \lambda_5(\psi)\left(\sum_{k\in J} \left(C_k\right)^{l+m+n} + 1\right),\tag{3.6}$$

respectively, where  $\lambda_r \in C(\mathbb{R})$  for r = 1, ..., 5,  $\lambda_r(\psi) > 0$  for all  $\psi \in \mathbb{R}$ , and under the assumption of *nonnegative* concentrations  $\mathbf{C} = (C_k)_{k \in J \cup J'}$ .

For  $i \in J \cup J'$ , the source terms satisfy the property

$$R_i(\mathbf{C}, \psi) \ge 0, \tag{3.7}$$

for all  $\psi \in \mathbb{R}$ ,  $\mathbf{C} \in \mathbb{R}^6_+$  and if  $C_i = 0$ .

Finally, we assume

$$\Omega \subset \mathbb{R}^{n} \text{ is bounded,} \quad n \geq 3,$$
  

$$\partial \Omega \in C^{1,1},$$
  

$$C_{i}^{0} \geq 0 \quad \text{in } \Omega \text{ for } i \in J \cup J',$$
  

$$C_{i}^{0} \in W_{p}^{2-2/p}(\Omega) \quad \text{for } i \in J,$$
  

$$C_{i}^{0} \in C(\bar{\Omega}) \quad \text{for } i \in J'.$$
  
(3.8)

Since in our case, |J| = 4 and |J'| = 2 are the numbers of mobile and immobile species, respectively, the formulation of the problem reads.

Definition 3.1. Let  $p \in (n+2, \infty)$ . We denote the system of (2.6), (2.7), (2.8), and (2.9) by (**P**), and call the vector  $((C_i)_{i \in J}, (C_i)_{i \in J'}, \psi)$  a solution of (**P**) if

$$((C_i)_{i \in J}, (C_i)_{i \in J'}, \psi) \\ \in [W_p^{2,1}(Q_{T_f})]^4 \times [C^1([0, T_f]; C(\bar{\Omega}))]^2 \times W_p^1(0, T_f; W_p^2(\Omega))$$
(3.9)

and satisfies (**P**) for some  $T_f \in (0, \infty)$ .

### 4. Ordinary differential equations

In this section, we consider the system of ordinary differential equations in Banach spaces (2.7) and (2.8). For given functions  $(C_k)_{k \in J}$  and  $\psi$ , with the properties

$$C_k \ge 0, \quad C_k, \psi \in C([0, T]; C(\overline{\Omega})), \tag{4.1}$$

we state an existence result, which we need in the next section.

In accordance with the results and notation used in [7], we extend (2.7) and (2.8) to the whole interval  $[0, \infty)$  and write them in the form

$$\dot{u} = \alpha_1 + \alpha_2 w - \alpha_3 u - \alpha_4 u^2 - \alpha_5 u^l \quad \text{in } [0, \infty), \ u(0) = u_0, \dot{w} = \beta_1 u^l - \beta_2 w \quad \text{in } [0, \infty), \ w(0) = w_0,$$
(4.2)

where  $l \in \mathbb{N}$ , and we make the functions  $C_k, \psi \in C([0, T]; C(\overline{\Omega})), k \in J$ , continuous by

$$\tilde{C}_k(t,\cdot) := \begin{cases} C_k(t,\cdot), & \text{if } t \in [0,T]; \\ C_k(T,\cdot), & \text{if } t \in (T,\infty), \end{cases}$$

$$(4.3)$$

(the same with  $\psi$ ) those functions, which are contained in the coefficients  $\alpha_i$ ( $i \in I_A := \{1, ..., 5\}$ ) and  $\beta_j$  ( $j \in I_B := \{1, 2\}$ ) due to (2.17). With (3.1) and (3.2) we conclude that

$$\alpha_i, \beta_j \in C([0,\infty); C(\bar{\Omega})), \quad \text{with } \alpha_i(t,x), \beta_j(t,x) \ge 0 \text{ in } [0,\infty) \times \bar{\Omega}.$$
(4.4)

Moreover, from (2.17) we conclude that

$$\alpha_5(t,x) = l\beta_1(t,x), \quad \alpha_2(t,x) = l\beta_2(t,x) \quad \text{in } [0,\infty) \times \bar{\Omega}. \tag{4.5}$$

We have  $C_+(\bar{\Omega}) \subset C(\bar{\Omega})$  is closed and convex. Let

$$f := (f_1, f_2) : [0, \infty) \times [C_+(\bar{\Omega})]^2 \longrightarrow [C(\bar{\Omega})]^2, \tag{4.6}$$

where

$$f_{1}(t, (u, w)) := f_{1}(t, (u, w))(x)$$

$$= \alpha_{1}(t, x) + \alpha_{2}(t, x)w(x) - \alpha_{3}(t, x)u(x)$$

$$- \alpha_{4}(t, x)u^{2}(x) - \alpha_{5}(t, x)u^{l}(x),$$

$$f_{2}(t, (u, w)) := f_{2}(t, (u, w))(x) = \beta_{1}(t, x)u^{l}(x) - \beta_{2}(t, x)w(x),$$
(4.7)

which is continuous and maps bounded sets into bounded sets.

LEMMA 4.1. Let (4.4) and (4.5) be satisfied. Then system (4.2) has a unique, nonnegative solution

$$(u,w) \in \left[C^1([0,\infty); C(\bar{\Omega}))\right]^2, \tag{4.8}$$

which satisfies the estimate

$$\|u(t)\|_{C(\bar{\Omega})} + \|w(t)\|_{C(\bar{\Omega})} \le \|u_0\|_{C(\bar{\Omega})} + \|w_0\|_{C(\bar{\Omega})} + \hat{\Lambda}_0(t),$$
(4.9)

where  $\hat{\Lambda}_0 \in C_+([0,\infty))$ , which depends on the coefficients  $\alpha_i$ ,  $\beta_j$  and the initial data.

Proof. We proceed in several steps.

(I) We have to ensure that

$$(u, w) + hf(t, (u, w)) \in [C_+(\bar{\Omega})]^2 \text{ for } h > 0$$
 (4.10)

and for all  $t \in [0, \infty)$  and  $(u, w) \in [C_+(\bar{\Omega})]^2$ . Since  $\alpha_1, \alpha_2 w \ge 0$  we get

$$u(x) + hf_1(t, (u, w))(x) \geq u(x) - hu(x)(\alpha_3(t, x) + \alpha_4(t, x)u(x) + \alpha_5(t, x)u^{l-1}(x)) \geq 0,$$
(4.11)

if

$$h < \left( \left\| \alpha_{3}(t) \right\|_{C(\bar{\Omega})} + \left\| \alpha_{4}(t) \right\|_{C(\bar{\Omega})} \|u\|_{C(\bar{\Omega})} + \left\| \alpha_{5}(t) \right\|_{C(\bar{\Omega})} \left\| u^{l-1} \right\|_{C(\bar{\Omega})} \right)^{-1}.$$
(4.12)

Similarly, we deduce that

$$w(x) + hf_2(t, (u, w))(x) \ge w(x) + h(\beta_1(t, x)u^l(x) - \beta_2(t, x)w(x)) \ge w(x)(1 - h\beta_2(t, x)) \ge 0,$$
(4.13)

if

$$h < \left( \left\| \beta_2(t) \right\|_{C(\bar{\Omega})} \right)^{-1}.$$
 (4.14)

(II) Next, we prove the unique existence of a local solution. Let a, R > 0,  $t_0 \in [0, \infty), t \in [t_0, t_0 + a]$  and let  $u_{t_0}, w_{t_0} \in [C_+(\bar{\Omega})]^2$  be the corresponding initial data with

$$\left\| \left( u_{t_0}, w_{t_0} \right) - (u, w) \right\|_{C([t_0, t_0 + a]; C(\bar{\Omega}))}, \left\| \left( u_{t_0}, w_{t_0} \right) - \left( \bar{u}, \bar{w} \right) \right\|_{C([t_0, t_0 + a]; C(\bar{\Omega}))} \le R.$$
(4.15)

We get a local Lipschitz condition, that is,

$$\begin{split} \left\| f_{1}(t,(u,w)) - f_{1}(t,(\bar{u},\bar{w})) \right\|_{C(\bar{\Omega})} + \left\| f_{2}(t,(u,w)) - f_{2}(t,(\bar{u},\bar{w})) \right\|_{C(\bar{\Omega})} \\ &\leq \left\| \alpha_{2} \right\|_{C([t_{0},t_{0}+a];C(\bar{\Omega}))} \left\| w - \bar{w} \right\|_{C(\bar{\Omega})} + \left\| \alpha_{3} \right\|_{C([t_{0},t_{0}+a];C(\bar{\Omega}))} \left\| u - \bar{u} \right\|_{C(\bar{\Omega})} \\ &+ \tilde{R} \left\| \alpha_{4} \right\|_{C([t_{0},t_{0}+a];C(\bar{\Omega}))} \left\| u - \bar{u} \right\|_{C(\bar{\Omega})} + \hat{R}(\left\| \alpha_{5} \right\|_{C([t_{0},t_{0}+a];C(\bar{\Omega}))} \left\| u - \bar{u} \right\|_{C(\bar{\Omega})} \\ &+ \left\| \beta_{1} \right\|_{C([t_{0},t_{0}+a];C(\bar{\Omega}))} \left\| u - \bar{u} \right\|_{C(\bar{\Omega})} + \left\| \beta_{2} \right\|_{C([t_{0},t_{0}+a];C(\bar{\Omega}))} \left\| w - \bar{w} \right\|_{C(\bar{\Omega})} \\ &\leq \Lambda \left( \left\| u - \bar{u} \right\|_{C(\bar{\Omega})} + \left\| w - \bar{w} \right\|_{C(\bar{\Omega})} \right), \end{split}$$

$$(4.16)$$

where we set  $||u + \bar{u}||_{C(\bar{\Omega})} \leq \tilde{R}$  and  $\sum_{j=0}^{l-1} ||u^{l-1-j}\bar{u}^j||_{C(\bar{\Omega})} \leq \hat{R}$ . From [7, Theorem 3.1, page 216], we conclude the existence of a local,

From [7, Theorem 3.1, page 216], we conclude the existence of a local, nonnegative solution to the right of (4.2) from the point  $(t_0, (u_{t_0}, w_{t_0}))$ .

(III) Finally, we derive a priori estimates in order to extend the solution to the maximal right-open interval, which is in our case  $[0, \infty)$  as we will see. Now let (u, w) be a solution of (4.2) in some interval  $J \subset [0, \infty)$ . Thus, for  $t \in J$  we have

$$u(t) + w(t) = u_0 + w_0 + \int_0^t f_1(s, (u(s), w(s))) + f_2(s, (u(s), w(s))) ds.$$
(4.17)

Let  $x \in \overline{\Omega}$ , then from (4.3), step (I), and (4.5), it follows that

$$w(t,x) \leq u(t)(x) + w(t)(x)$$
  

$$\leq u_{0}(x) + w_{0}(x) + \int_{0}^{t} (\alpha_{1}(s,x) + w(s,x)(l-1)\beta_{2}(s,x) + u^{l}(s,x)(1-l)\beta_{1}(s,x))ds$$
  

$$\leq ||u_{0}||_{C(\bar{\Omega})} + ||w_{0}||_{C(\bar{\Omega})} + \int_{0}^{t} (\alpha_{1}(s,x) + w(s,x)(l-1)\beta_{2}(s,x))ds$$
  

$$\leq ||u_{0}||_{C(\bar{\Omega})} + ||w_{0}||_{C(\bar{\Omega})} + t ||\alpha_{1}||_{C([0,T];C(\bar{\Omega}))} + (l-1)||\beta_{2}||_{C([0,T];C(\bar{\Omega}))} \int_{0}^{t} w(s,x)ds.$$
(4.18)

Gronwall's lemma yields

$$\|w(t)\|_{C(\bar{\Omega})} \leq \left(\|u_0\|_{C(\bar{\Omega})} + \|w_0\|_{C(\bar{\Omega})} + t\|\alpha_1\|_{C([0,T];C(\bar{\Omega}))}\right) e^{t(l-1)\|\beta_2\|_{C([0,T];C(\bar{\Omega}))}}$$
  
=:  $\hat{\Lambda}(t)$  (4.19)

for all  $t \in J$ . From this we immediately get

$$\|u(t)\|_{C(\bar{\Omega})} \le \|u_0\|_{C(\bar{\Omega})} + t(\|\alpha_1\|_{C([0,T];C(\bar{\Omega}))} + \|\alpha_2\|_{C([0,T];C(\bar{\Omega}))}\hat{\Lambda}(t)),$$
(4.20)

which we summarize as

$$\|u(t)\|_{C(\bar{\Omega})} + \|w(t)\|_{C(\bar{\Omega})} \le \|u_0\|_{C(\bar{\Omega})} + \|w_0\|_{C(\bar{\Omega})} + \hat{\Lambda}_0(t) \quad \forall t \in J.$$
(4.21)

Since  $\hat{\Lambda}_0 \in C_+([0,\infty))$ , we conclude, with [7, Proposition 1.1, page 200], the existence of a global solution, that is, the solution exists for any  $t \in [0,\infty)$ .

For later use, we state a compactness result concerning equation (4.2). Let  $n+2 and <math>\alpha_i, \beta_j \in C([0,T]; C_+(\bar{\Omega})) \cap L^1(0,T; W^1_p(\Omega))$  for  $i \in I_A$ ,  $j \in I_B$ . Let

$$r := \left| I_A \right| + \left| I_B \right|, \tag{4.22}$$

then we define the operator

$$L: \left[C\left([0,T]; C_{+}(\bar{\Omega})\right) \cap L^{1}(0,T; W^{1}_{p}(\Omega))\right]^{r} \longrightarrow \left[C\left([0,T]; C_{+}(\bar{\Omega})\right)\right]^{2},$$
(4.23)

by

$$L((\alpha_i)_{i\in I_A}, (\beta_j)_{j\in I_B}) = (u, w),$$
(4.24)

where (u, w) is a solution of (4.2) in [0, T].

We use Ascoli's theorem (see [7]) to state the following result.

LEMMA 4.2. The mapping stated in (4.23) is compact.

*Proof.* Let  $\{((\alpha_i^n)_{i \in I_A}, (\beta_j^n)_{j \in I_B})\}_{n \in \mathbb{N}} \subset [C([0, T]; C_+(\bar{\Omega})) \cap L^1(0, T; W_p^1(\Omega))]^r$  be a sequence, satisfying

$$\| ((\alpha_{i}^{n})_{i \in I_{A}}, (\beta_{j}^{n})_{j \in I_{B}}) \|_{[C([0,T];C_{+}(\bar{\Omega}))]^{r}} + \| ((\alpha_{i}^{n})_{i \in I_{A}}, (\beta_{j}^{n})_{j \in I_{B}}) \|_{[L^{1}(0,T;W^{1}_{p}(\Omega))]^{r}} \leq \bar{\Lambda},$$

$$(4.25)$$

with a constant  $\bar{\Lambda} > 0$ .

We consider the sequence  $\{(u_n, w_n)\}_{n \in \mathbb{N}} \subset [C([0, T]; C_+(\bar{\Omega}))]^2$ , defined by  $(u_n, w_n) = L((\alpha_i^n)_{i \in I_A}, (\beta_j^n)_{j \in I_B}).$ 

We again proceed in several steps.

(I) We have to show that  $\{u_n, w_n\}_{n \in \mathbb{N}}$  is equicontinuous in the time variable. Let

$$f_{1}^{n}(t,(u,w))(x) = \alpha_{1}^{n}(t,x) + \alpha_{2}^{n}(t,x)w(x) - \alpha_{3}^{n}(t,x)u(x) - \alpha_{4}^{n}(t,x)u^{2}(x) - \alpha_{5}^{n}(t,x)u^{l}(x),$$
(4.26)  
$$f_{2}^{n}(t,(u,w))(x) = \beta_{1}^{n}(t,x)u^{l}(x) - \beta_{2}^{n}(t,x)w(x).$$

For s < t we have the estimate,

$$\begin{aligned} \left\| u_{n}(t) - u_{n}(s) \right\|_{C(\bar{\Omega})} + \left\| w_{n}(t) - w_{n}(s) \right\|_{C(\bar{\Omega})} \\ &\leq \int_{s}^{t} \left\| f_{1}^{n} \left( \tau, \left( u_{n}(\tau), w_{n}(\tau) \right) \right) \right\|_{C(\bar{\Omega})} d\tau + \int_{s}^{t} \left\| f_{2}^{n} \left( \tau, \left( u_{n}(\tau), w_{n}(\tau) \right) \right) \right\|_{C(\bar{\Omega})} d\tau \\ &\leq (t-s)\tilde{\Lambda}, \end{aligned}$$

$$(4.27)$$

where the constant  $\tilde{\Lambda} > 0$  is independent of *n*. This proves the equicontinuity.

(II) Finally, we have to verify that, for any  $t \in [0, T]$ , the set  $\{u_n(t), w_n(t)\}_{n \in \mathbb{N}} \subset [C(\overline{\Omega})]^2$  is relatively compact. We apply the theorem of Arcelá-Ascoli.

(1) From (4.9) we get the estimate

$$|u_n(t)(x)| + |w_n(t)(x)| \le ||u_n(t)||_{C(\bar{\Omega})} + ||w_n(t)||_{C(\bar{\Omega})} \le \hat{\Lambda}_0(T)$$
(4.28)

for all  $x \in \overline{\Omega}$ , which is independent of  $n \in \mathbb{N}$ .

(2) It remains to prove the equicontinuity in  $\overline{\Omega}$ . Let  $x \neq y \in \overline{\Omega}$ . A short calculation and the application of Gronwall's lemma yield

$$\begin{aligned} |u_{n}(t)(x) - u_{n}(t)(y)| + |w_{n}(t)(x) - w_{n}(t)(y)| \\ \leq \exp(\Lambda_{1}T)\Lambda_{2}(|u_{0}(x) - u_{0}(y)| + |w_{0}(x) - w_{0}(y)| \\ + \int_{0}^{T} \sum_{i \in I_{A}} |\alpha_{i}^{n}(s, x) - \alpha_{i}^{n}(s, y)| ds \\ + \int_{0}^{T} \sum_{j \in I_{B}} |\beta_{j}^{n}(s, x) - \beta_{j}^{n}(s, y)| ds) \end{aligned}$$
(4.29)

for all  $t \in [0, T]$  and some constants  $\Lambda_1, \Lambda_2$  which are composed of the quantities  $\overline{\Lambda}, \widehat{\Lambda}$  introduced in the present derivation.

Since each component of  $(\alpha_i^n)_{i \in I_A}, (\beta_j^n)_{j \in I_B}$  belongs to  $L^1(0, T; W_p^1(\Omega))$ , it results, from the embedding theorems, (see [5]) that it also belongs to  $L^1(0, T;$ 

 $C^{\lambda}(\bar{\Omega})$ ) with  $0 < \lambda \leq 1 - n/p$ . Thus, we get

$$\int_{0}^{T} \frac{\left|\alpha_{1}^{n}(s,x) - \alpha_{1}^{n}(s,y)\right|}{\|x - y\|^{\lambda}} ds \|x - y\|^{\lambda}$$

$$\leq \int_{0}^{T} \left\|\alpha_{1}^{n}(s)\right\|_{C^{\lambda}(\bar{\Omega})} ds \|x - y\|^{\lambda} \leq T\Lambda \|x - y\|^{\lambda},$$
(4.30)

and similarly with the other coefficients. In summary, we conclude that

$$\begin{aligned} \left| u_{n}(t)(x) - u_{n}(t)(y) \right| + \left| w_{n}(t)(x) - w_{n}(t)(y) \right| \\ &\leq \Lambda \left( \left| u_{0}(x) - u_{0}(y) \right| + \left| w_{0}(x) - w_{0}(y) \right| + \|x - y\|^{\lambda} \right), \end{aligned}$$
(4.31)

which yields, combined with the continuity of the initial data, the desired equicontinuity and completes the proof of compactness.  $\Box$ 

#### 5. Poisson equation

Next, we collect results concerning the elliptic equation (2.9). We sketch the results and refer the reader for a detailed analysis to [1, 8, 9, 10]. The following results regarding the Poisson equation are valid in any space dimension.

Let  $n and <math>\mathbf{C} \in [L^p_+(\Omega)]^6$ . Then we are able to show (with the help of Leray-Schauder's fixed point theorem, see [1]) that there exists a unique solution

$$\psi \in W_p^2(\Omega) \tag{5.1}$$

of (2.9). Moreover, there exists a constant  $\Lambda_p > 0$  such that

$$\|\psi\|_{W^2_p(\Omega)} \le \Lambda_p \sum_{i \in J \cup J'} \|C_i\|_{L^p(\Omega)},\tag{5.2}$$

and the stability estimate

$$\left\|\psi - \tilde{\psi}\right\|_{W_{p}^{2}(\Omega)} \leq \Lambda_{p} \sum_{i \in J \cup J'} \left\|C_{i} - \tilde{C}_{i}\right\|_{L^{p}(\Omega)}$$

$$(5.3)$$

for all  $\mathbf{C}, \tilde{\mathbf{C}} \in [L^p_+(\Omega)]^6$  and the corresponding  $\psi, \tilde{\psi}$  satisfying the Poisson equation. Estimate (5.3) is also true, if only one of the concentrations is nonnegative. We will use this fact in (6.53).

If  $C_i \in C([0, T]; L^p(\Omega))$  for  $i \in J \cup J'$ , then we immediately get that

$$\psi \in C\left([0,T]; W_p^2(\Omega)\right),\tag{5.4}$$

and that there exists a constant  $\Lambda_p > 0$  such that

$$\|\psi\|_{C([0,T];W_p^2(\Omega))} \le \Lambda_p \sum_{i \in J \cup J'} \|C_i\|_{C([0,T];L^p(\Omega))}.$$
(5.5)

If in addition,  $C_i \in W_p^1(0, T; L^p(\Omega)) \cap C([0, T]; C(\overline{\Omega}))$  for  $i \in J \cup J'$ , we are able to show that

$$\psi \in W_p^1(0,T; W_p^2(\Omega)), \tag{5.6}$$

and that there exists another constant  $\Lambda_p > 0$  satisfying

$$\|\psi\|_{W_{p}^{1}(0,T;W_{p}^{2}(\Omega))} \leq \Lambda_{p} \sum_{i \in J \cup J'} \|C_{i}\|_{W_{p}^{1}(0,T;L^{p}(\Omega))}.$$
(5.7)

Thus, we have summarized all results concerning  $\psi$ , which we need for further investigations.

#### 6. Existence and uniqueness

Using the fixed point theorem of Schauder, we prove the existence of a strong solution according to Definition 3.1. We are able to formulate the following main result.

THEOREM 6.1. Under the assumptions (3.1), (3.2), (3.3), (3.4), (3.5), (3.6), (3.7), and (3.8), there exists an instant of time  $T_f > 0$ , such that the system of (2.6), (2.7), (2.8), and (2.9) has a unique solution. The solution satisfies  $\mathbb{C} \ge 0$ .

The proof of this theorem consists of several steps, which we present in the next subsections. We start with a modification of our problem.

Definition 6.2. If we replace in (**P**) the source terms by  $R_i((C_k^+)_{k \in J}, (C_k)_{k \in J'}, \psi)$ and the right-hand side in the Poisson equation by  $\sum_{i \in J} Q_i(\psi)C_i^+ + \sum_{i \in J'} Q_i(\psi)C_i$ , where

$$C_i^{+} := \begin{cases} C_i, & \text{if } C_i \ge 0; \\ 0, & \text{if } C_i < 0, \end{cases}$$
(6.1)

we denote the modified system by  $(\mathbf{P}^+)$ .

In the next subsection, we will show that, for any solution of  $(\mathbf{P}^+)$ , the concentrations are nonnegative. Then we will prove the existence of a strong solution of problem  $(\mathbf{P}^+)$  with the help of Schauder's fixed point theorem in Sobolev spaces and use regularity results to get the desired smoothness. This (nonnegative) solution obviously solves  $(\mathbf{P})$ , too. Finally, we have to show that there exists no other solution of  $(\mathbf{P})$ , which concludes the proof of Theorem 6.1.

### **6.1. Problem** (**P**<sup>+</sup>)

LEMMA 6.3. Let  $p \in (1, \infty)$  and  $((C_i)_{i \in J \cup J'}, \psi) \in [W_p^{2,1}(Q_{T_f})]^4 \times [C^1([0, T_f]; C(\bar{\Omega}))]^2 \times W_p^1(0, T_f; W_p^2(\Omega))$  be a solution of  $(\mathbf{P}^+)$ , then  $C_i \ge 0$  for  $i \in J$ .

*Proof.* For  $i \in J$ , we test the equation

$$\frac{\partial C_i}{\partial t} + \operatorname{div} J_i = R_i \left( \left( C_k^+ \right)_{k \in J'}, \left( C_k \right)_{k \in J'}, \psi \right), \tag{6.2}$$

with  $C_i^- := C_i^+ - C_i$ , where  $J_i$  is defined in (2.10). We get with appropriate constants the estimate

$$\begin{split} &\int_{\Omega} \left(C_{i}^{-}(t)\right)^{2} dx + \int_{0}^{t} \int_{\Omega} \left(\Lambda_{1} \left(\nabla C_{i}^{-}\right)^{2} + R_{i} \left(\left(C_{k}^{+}\right)_{k \in J}, \left(C_{k}\right)_{k \in J'}, \psi\right) C_{i}^{-}\right) dx \, ds \\ &\leq \Lambda \left(\frac{\varepsilon}{2} \int_{0}^{t} \int_{\Omega} \left(\nabla C_{i}^{-}\right)^{2} dx \, ds + \Lambda_{\varepsilon} \int_{0}^{t} \int_{\Omega} \left(\nabla \psi\right)^{2} \left(C_{i}^{-}\right)^{2} dx \, ds\right) \\ &\leq \Lambda \left(\frac{\varepsilon}{2} \int_{0}^{t} \int_{\Omega} \left(\nabla C_{i}^{-}\right)^{2} dx \, ds + \Lambda_{\varepsilon} \int_{0}^{t} \left\|\nabla \psi\right\|_{C(\bar{\Omega})}^{2} \left\|C_{i}^{-}\right\|_{L^{2}(\Omega)}^{2} ds\right), \end{split}$$
(6.3)

where we used Young's inequality and properties (3.1) and (3.2). Since  $C_i^+ C_i^- = 0$ , we are able to apply property (3.7) to omit the reaction rates. We choose  $\varepsilon > 0$  such that  $\Lambda \varepsilon / 2 = \Lambda_1$ , then we get

$$\|C_{i}^{-}(t)\|_{L^{2}(\Omega)}^{2} \leq \Lambda \int_{0}^{t} \|\nabla\psi\|_{C(\bar{\Omega})}^{2} \|C_{i}^{-}\|_{L^{2}(\Omega)}^{2} ds.$$
(6.4)

We have  $\nabla \psi \in L^2(0,T; C(\overline{\Omega}))$  and  $C_i^- \in C([0,T]; L^2(\Omega))$ , so we can use Gronwall's lemma, saying that

$$\|C_i^{-}(t)\|_{L^2(\Omega)}^2 = 0 \quad \forall t \in [0, T].$$
(6.5)

**6.2. Fixed point iteration for**  $(\mathbf{P}^+)$ . Now we prove the existence of a local solution of  $(\mathbf{P}^+)$  in Sobolev spaces by means of the fixed point theorem of Schauder. Let

$$p \in (n+2,\infty). \tag{6.6}$$

Set

$$\frac{\Lambda_0}{2} := \sum_{i \in J} \|C_i^0\|_{W_p^{2-2/p}(\Omega)} + \sum_{i \in J'} \|C_i^0\|_{C(\bar{\Omega})} + 1,$$

$$K_0 := \sum_{i \in J} K_i,$$

$$G_0 := k(1 + K_0)\Lambda_0,$$
(6.7)

where the constants  $K_i$ , k > 0 depend on known quantities only and will be specified below.

We define the set

$$X_{T} := \left\{ (\mathscr{C}, \phi) \in \left[ W_{p}^{2,1}(Q_{T}) \right]^{4} \times C([0,T]; W_{p}^{1}(\Omega)) : \\ \left\| \left( \mathscr{C}_{i} \right)_{i \in J} \right\|_{W_{p}^{2,1}(Q_{T})} \leq K_{0} \Lambda_{0}, \|\phi\|_{C([0,T]; W_{p}^{1}(\Omega))} \leq G_{0} \right\}$$

$$(6.8)$$

for some  $T \in (0, \infty)$ .

We consider the vector-valued mapping

$$Z: X_T \longrightarrow \left[ W_p^{2,1}(Q_T) \right]^4 \times C\left( [0,T]; W_p^1(\Omega) \right), \tag{6.9}$$

by

$$Z((\mathscr{C}_k)_{k\in J}, \phi) = ((C_k)_{k\in J}, \psi), \qquad (6.10)$$

where  $C_i$ ,  $i \in J$ , is the solution of

$$\frac{\partial C_i}{\partial t} - \operatorname{div} \left\{ D_i(\psi) \left[ \nabla C_i + Q_i(\psi) \nabla \psi C_i \right] \right\} = R_i \left( \left( \mathscr{C}_k^+ \right)_{k \in J}, \left( C_k \right)_{k \in J'}, \psi \right) \quad \text{in } Q_T,$$
$$\nabla C_i \cdot \mathbf{n} = 0 \quad \text{on } \Gamma_T,$$
$$C_i(\cdot, 0) = C_i^0 \quad \text{in } \Omega,$$
(6.11)

and  $\psi$  is the solution of

$$-\Delta \psi + \sinh(\psi) = \sum_{i \in J} Q_i(\psi) \mathscr{C}_i^+ + \sum_{i \in J'} Q_i(\psi) C_i \quad \text{in } Q_T,$$
  
$$\nabla \psi \cdot \mathbf{n} = 0 \quad \text{on } \Gamma_T.$$
(6.12)

Therefore,  $C_i$ ,  $i \in J'$ , is the nonnegative solution of the ordinary differential equation in the Banach spaces,

$$\frac{\partial C_i}{\partial t} = R_i \left( \left( {}^{\mathcal{C}}_k^+ \right)_{k \in J}, \left( C_k \right)_{k \in J'}, \phi \right) \quad \text{in } Q_T,$$

$$C_i(\cdot, 0) = C_i^0 \quad \text{in } \Omega.$$
(6.13)

Now we check the properties of the mapping required in the fixed point theorem in the following steps (I), (II), and (III).

(Ia) The mapping Z is well defined, since system (6.11), (6.12) has a unique solution

$$\left(\left(C_{i}\right)_{i\in J},\psi\right)\in\left[W_{p}^{2,1}\left(Q_{T}\right)\right]^{4}\times W_{p}^{1}\left(0,T;W_{p}^{2}(\Omega)\right).$$
(6.14)

In order to see the solvability of (6.11), (6.12), we first note that, for  $i \in J$  each  $\mathscr{C}_i \in W_p^{2,1}(Q_T)$  (cf. (6.6)) also belongs due to the embedding theorems to the space  $C([0, T]; C(\overline{\Omega}))$  and so do the *cuts*. The function  $\phi \in C([0, T]; W_p^1(\Omega))$  is also continuous in both variables. Having this in mind, we can say that for given

 $((\mathscr{C}_i)_{k \in J}, \phi) \in [C([0, T]; C(\overline{\Omega}))]^5$ , the nonlinear system (6.13) has according to Lemma 4.1 a unique solution, that is,

$$C_A, C_{A_{\rm cl}} \in C^1([0, T]; C(\bar{\Omega})),$$
 (6.15)

which satisfies  $C_A$ ,  $C_{A_{cl}} \ge 0$ .

From (6.15) and embedding theorems, it follows that the coefficients as well as the right-hand side of (6.11) are continuous, and thus they also belong to the space  $L^p(Q_T)$  for any  $p \ge 1$ , especially for  $p \in (n+2, \infty)$ . In addition, the right-hand side of (6.12) belongs to the space  $W_p^1(0, T; L^p(\Omega))$ . So with (3.8), the parabolic theory (see [5]) and the result (5.6) concerning the elliptic equation yield (6.14).

(Ib) For later use, we state an estimate. We get, by testing (6.13) with  $(\partial/\partial t)(C_i^1 - C_i^2)|(\partial/\partial t)(C_i^1 - C_i^2)|^{p-2}$ ,  $i \in J'$ , combined with the linear theory of ordinary differential equations in Banach spaces, and from the linear elliptic theory applied to (6.12) that there exists a constant  $\Lambda > 0$ , such that the stability estimate

$$\sum_{i \in J'} \|C_i^1 - C_i^2\|_{W_p^1(0,T;L^p(\Omega))} + \|\psi_1 - \psi_2\|_{L^p(0,T;W_p^2(\Omega))}$$

$$\leq \Lambda \left( \sum_{i \in J} \|\mathcal{C}_i^{1+} - \mathcal{C}_i^{2+}\|_{L^p(0,T;L^p(\Omega))} + \|\phi_1 - \phi_2\|_{L^p(0,T;L^p(\Omega))} \right)$$
(6.16)

holds for all  $\phi_1, \phi_2, \mathscr{C}_i^{1+}, \mathscr{C}_i^{2+} \in L^p(0, T; L^p(\Omega))$  and the corresponding solutions  $C_i^1, C_i^2$  of (6.13) as well as  $\psi_1, \psi_2$  of (6.12).

(II) We show, that there exists an instant of time  $T_f \in (0, \infty)$ , such that  $Z(X_{T_f}) \subseteq X_{T_f}$ .

At first, we state the constants  $K_i$ , k > 0 defined in (6.7). In order to discuss  $K_i > 0$ , we write (6.11) for  $i \in J$  in the form

$$\frac{\partial C_i}{\partial t} - D_i(\psi) \Delta C_i = F_i, \qquad (6.17)$$

where

$$F_{i} = R_{i} \left( \left( \mathscr{C}_{k}^{+} \right)_{k \in J}, \left( C_{k} \right)_{k \in J'}, \psi \right) + \operatorname{div} \left\{ D_{i}(\psi) Q_{i}(\psi) \nabla \psi C_{i} \right\} + D'(\psi) \nabla \psi \cdot \nabla C_{i}.$$
(6.18)

Let  $T_0 \in (0, \infty)$  and set  $K_i \equiv K_i(T_0)$ . Then the parabolic theory yields the estimate

$$\|C_i\|_{W_p^{2,1}(Q_T)} \le \frac{K_i}{2} \big( \|C_i^0\|_{W_p^{2-2/p}(\Omega)} + \|F_i\|_{L^p(0,T;L^p(\Omega))} \big), \tag{6.19}$$

which is true for all  $T \in (0, T_0]$ , and where  $K_i > 0$  remains bounded for any

finite  $T_0 > 0$  (see [5]). For (6.12) we get according to (4.9) and (5.5) the estimate

$$\|\psi\|_{C([0,T];W_{p}^{2}(\Omega))} \leq k\left(\sum_{i \in J} \left\|\mathscr{C}_{i}^{+}\right\|_{C([0,T];L^{p}(\Omega))} + \sum_{i \in J'} \left\|C_{i}\right\|_{C([0,T];L^{p}(\Omega))}\right),$$
(6.20)

with a constant k > 0.

We start to estimate inequality (6.20). We get with (4.9)

$$\|\psi\|_{C([0,T];W_{p}^{2}(\Omega))} \leq k \left( \sum_{i \in J} \|\mathscr{C}_{i}^{+}\|_{C([0,T];L^{p}(\Omega))} + \sum_{i \in J'} \|C_{i}\|_{C([0,T];L^{p}(\Omega))} \right)$$
$$\leq k \left( \Lambda_{0}K_{0} + \frac{\Lambda_{0}}{2} + \Lambda_{\Omega}\hat{\Lambda}_{0}(T) \right),$$
(6.21)

where  $\hat{\Lambda}_0(T) > 0$  depends only on quantities defined in (6.8), with  $\hat{\Lambda}_0(T) \to 0$ for  $T \to 0$ . We choose  $T_1 \in (0, T]$  such that

$$\Lambda_{\Omega}\hat{\Lambda}_{0}(T_{1}) \leq \frac{\Lambda_{0}}{2}, \tag{6.22}$$

then we conclude that

$$\|\psi\|_{C([0,T_1];W_p^1(\Omega))} \le \|\psi\|_{C([0,T_1];W_p^2(\Omega))} \le G_0,$$
(6.23)

where  $G_0$  is defined in (6.7).

Moreover, the local solution  $\psi \in W_p^1(0, T_1; W_p^2(\Omega))$  satisfies estimate (5.7) with  $\mathscr{C}_i^+$  instead of  $C_i$  for  $i \in J$  therein. Next, we get with (6.19) the estimates

$$\begin{aligned} \|C_{i}\|_{W_{p}^{2,1}(Q_{T})} &\leq \frac{K_{i}}{2} \left( \|C_{i}^{0}\|_{W_{p}^{2-2/p}(\Omega)} + \|R_{i}((\mathscr{C}_{k}^{+})_{k\in J}, (C_{k})_{k\in J'}, \psi)\|_{L^{p}(0,T;L^{p}(\Omega))} \\ &+ \|\operatorname{div} \{D_{i}(\psi)Q_{i}(\psi)\nabla\psi C_{i}\}\|_{L^{p}(0,T;L^{p}(\Omega))} \\ &+ \|D'(\psi)\nabla\psi \cdot \nabla C_{i}\|_{L^{p}(0,T;L^{p}(\Omega))} \right) \\ &\leq \frac{K_{0}}{2} \left( \frac{\Lambda_{0}}{2} + \|R_{i}((\mathscr{C}_{k}^{+})_{k\in J}, (C_{k})_{k\in J'}, \psi)\|_{L^{p}(0,T;L^{p}(\Omega))} \\ &+ \|\operatorname{div} \{D_{i}(\psi)Q_{i}(\psi)\nabla\psi C_{i}\}\|_{L^{p}(0,T;L^{p}(\Omega))} \\ &+ \|D'(\psi)\nabla\psi \cdot \nabla C_{i}\|_{L^{p}(0,T;L^{p}(\Omega))} \right) \end{aligned}$$

$$(6.24)$$

for  $i \in J$ , and where the constants  $K_0$ ,  $\Lambda_0$  are defined in (6.7).

We estimate the first  $L^p$ -norm in (6.24). Using the growth conditions (3.4), we see that there exists a constant  $\Lambda_1 > 0$ , just depending on known quantities defined in (6.8), such that

$$\begin{split} \|R_{i}((\mathscr{C}_{k}^{+})_{k\in J}, (C_{k})_{k\in J'}, \psi)\|_{L^{p}(0,T;L^{p}(\Omega))} \\ &\leq T^{1/p}\Lambda_{\Omega}\|\lambda_{i}(\psi)\|_{C([0,T];C(\bar{\Omega}))} \\ &\times \left(\sum_{k\in J}\|(\mathscr{C}_{k}^{+})^{s}\|_{C([0,T];C(\bar{\Omega}))} + \sum_{k\in J'}\|(C_{k})^{s}\|_{C([0,T];C(\bar{\Omega}))} + 1\right) \\ &\leq T^{1/p}\Lambda_{1}, \end{split}$$

$$(6.25)$$

where s := l + m + n and  $\lambda_i \in C(\mathbb{R})$ ,  $i \in J$ . We consider the second  $L^p$ -norm in (6.24), which is

$$\operatorname{div}\left\{D_{i}(\psi)Q_{i}(\psi)\nabla\psi C_{i}\right\} = \left(D_{i}'(\psi)Q_{i}(\psi) + D_{i}(\psi)Q_{i}'(\psi)\right)\left(\nabla\psi\right)^{2}C_{i} + D_{i}(\psi)Q_{i}(\psi)\Delta\psi C_{i} + D_{i}(\psi)Q_{i}(\psi)\nabla\psi\cdot\nabla C_{i}.$$
(6.26)

We use (3.1) to get the estimate

$$\begin{split} \|D_{i}(\psi)Q_{i}(\psi)\nabla\psi\cdot\nabla C_{i}\|_{L^{p}(0,T;L^{p}(\Omega))} \\ &\leq T^{1/p}\Lambda\|\nabla\psi\|_{C([0,T];L^{p}(\Omega))}\|\nabla C_{i}\|_{C([0,T];C(\bar{\Omega}))} \\ &\leq T^{1/p}\Lambda\|\nabla\psi\|_{C([0,T];L^{p}(\Omega))}\|C_{i}\|_{W^{2,1}_{p}(Q_{T})}, \end{split}$$
(6.27)

where the last inequality is true for n+2 , (see [5]) an*explanation*of our special choice of <math>p. The other terms in (6.26) and the last  $L^p$ -norm in (6.24) may be estimated similarly. Again we can say that there exists a constant  $\Lambda_2 > 0$ , just depending on known quantities, such that

$$\| \operatorname{div} \{ D_{i}(\psi) Q_{i}(\psi) \nabla \psi C_{i} \} \|_{L^{p}(0,T;L^{p}(\Omega))} + \| D'(\psi) \nabla \psi \cdot \nabla C_{i} \|_{L^{p}(0,T;L^{p}(\Omega))}$$
  
$$\leq T^{1/p} \Lambda_{2} \| C_{i} \|_{W^{2,1}_{p}(Q_{T})}.$$
(6.28)

Thus, in summary,

$$\left(1 - T^{1/p} \frac{K_0 \Lambda_2}{2}\right) \|C_i\|_{W_p^{2,1}(Q_T)} \le \frac{K_0}{2} \left(\frac{\Lambda_0}{2} + T^{1/p} \Lambda_1\right).$$
(6.29)

We choose  $T_f \in (0, T_1]$ , such that

$$0 < T_f^{1/p} \le \min\left\{\frac{1}{K_0\Lambda_2}, \frac{\Lambda_0}{2\Lambda_1}\right\},\tag{6.30}$$

then

$$\|C_i\|_{W_p^{2,1}(Q_{T_f})} \le K_0 \Lambda_0 \quad \text{for } i \in J,$$
 (6.31)

and so  $Z: X_{T_f} \to X_{T_f}$ .

(III) Compactness and continuity of the mapping.

We proceed with the following lemma.

LEMMA 6.4. The mapping

$$Z: X_{T_f} \longrightarrow X_{T_f} \tag{6.32}$$

is compact and continuous.

Proof. At first, we note that the embedding

$$W_p^1(0, T_f; W_p^2(\Omega)) \subset C\left(\left[0, T_f\right]; W_p^1(\Omega)\right)$$
(6.33)

is compact. Thus, from (6.14), the mapping is compact in the second variable. Now let  $\{(\mathscr{C}_i^m)_{i \in J}, \phi_m\}_{m \in \mathbb{N}} \subset X_{T_f}$ .

(1) From the compact embedding of  $W_p^{2,1}(Q_{T_f})$  into the space

$$Y := L^p \left( 0, T_f; W_p^1(\Omega) \right) \tag{6.34}$$

there exists a subsequence  $\mathscr{C}_i^n \to \mathscr{C}_i$  in Y for  $n \to \infty$ . This is also true for the *cuts*, that is,

$$\mathscr{C}_i^{n+} \longrightarrow \mathscr{C}_i^+ \quad \text{in } Y \text{ for } n \longrightarrow \infty.$$
 (6.35)

(2) If we apply Lemma 4.2 to the system (6.13) we conclude that there exists a subsequence

$$C_i^n \longrightarrow C_i \quad \text{in } C([0, T_f]; C(\overline{\Omega})) \text{ for } n \longrightarrow \infty, \ i \in J'.$$
 (6.36)

(3) From (6.33), (6.35), and (6.36) we get the convergence of a subsequence

$$\psi_n \longrightarrow \psi \quad \text{in } C([0, T_f]; W_p^1(\Omega)) \text{ for } n \longrightarrow \infty.$$
 (6.37)

Let  $C_i^n, C_i, i \in J$ , be the solutions of (6.11). We set

$$\bar{\mathscr{C}}_{i}^{n} := \mathscr{C}_{i}^{n+} - \mathscr{C}_{i}^{+}, \quad \text{for } i \in J, 
\bar{C}_{i}^{n} := C_{i}^{n} - C_{i}, \quad \text{for } i \in J \cup J', 
\bar{\psi}^{n} := \psi_{n} - \psi.$$
(6.38)

In  $Q_{T_f}$ , we consider the system for  $\bar{C}_i^n$ ,  $i \in J$ , which is

$$\frac{\partial \bar{C}_i^n}{\partial t} - \operatorname{div}\left\{B_1 \nabla \bar{C}_i^n\right\} + B_2 \nabla \bar{C}_i^n + B_3 \bar{C}_i^n = \bar{F}_i^n, \tag{6.39}$$

where

$$\bar{F}_{i}^{n} = A_{1} (D_{i}(\psi_{n}) - D_{i}(\psi)) + A_{2} (D_{i}'(\psi_{n}) - D_{i}'(\psi)) 
+ A_{3} (Q_{i}(\psi_{n}) - Q_{i}(\psi)) + A_{4} (Q_{i}'(\psi_{n}) - Q_{i}'(\psi)) + A_{5} \nabla \bar{\psi}^{n} 
+ A_{6} \Delta \bar{\psi}^{n} + R_{i} ((\mathscr{C}_{k}^{n+})_{k \in I}, (C_{k}^{n})_{k \in I'}, \psi_{n}) - R_{i} ((\mathscr{C}_{k}^{+})_{k \in I}, (C_{k})_{k \in I'}, \psi), 
(6.40)$$

and with the boundary conditions  $\nabla \bar{C}_i^n \cdot \mathbf{n} = 0$  on  $\Sigma_T$ , and zero initial conditions.

We do not discuss the coefficients *A*, *B* (supplied with indices) appearing in the linear equations in detail, but we mention that they belong at least to the space  $C([0, T_f]; L^p(\Omega))$ , which will be discussed in a moment.

The parabolic theory (see [5]) yields

$$\sum_{i \in J} \left\| \bar{C}_{i}^{n} \right\|_{W_{p}^{2,1}(Q_{T_{f}})} \leq \Lambda \sum_{i \in J} \left\| \bar{F}_{i}^{n} \right\|_{L^{p}(0,T_{f};L^{p}(\Omega))}.$$
(6.41)

In order to show the convergence of the left-hand side, we have to estimate the right-hand side of (6.41) with the help of (5.3) as well as (6.35) and (6.36).

For this, we use the mean value theorem to get

$$Q_i(\psi_n) - Q_i(\psi) = \int_0^1 Q'_i(\tilde{\psi}(s)) ds \bar{\psi}^n, \qquad (6.42)$$

(the same with the other coefficients which depend on  $\psi$ ), where  $\tilde{\psi}(s) = s\psi_n + (1-s)\psi$ . Representatively, we estimate the term  $A_3(Q_i(\psi_n) - Q_i(\psi))$ , where a short calculation gives

$$A_3 = D'_i(\psi)C_i(\nabla\psi)^2 + D_i(\psi)\nabla C_i \cdot \nabla\psi + D_i(\psi)C_i\Delta\psi.$$
(6.43)

Therefore,  $\Delta \psi \in C([0, T_f]; L^p(\Omega))$ , whereas the other functions are continuous due to embedding results, so we get  $A_3 \in C([0, T_f]; L^p(\Omega))$ . Thus,

$$\begin{split} \left\| A_{3} \int_{0}^{1} \mathcal{Q}_{i}^{\prime} (\tilde{\psi}(s)) ds \bar{\psi}^{n} \right\|_{L^{p}(0,T_{f};L^{p}(\Omega))} \\ &\leq \Lambda \Big( \left\| \bar{\psi}^{n} \right\|_{L^{p}(0,T_{f};L^{p}(\Omega))} + \left\| \Delta \psi \bar{\psi}^{n} \right\|_{L^{p}(0,T_{f};L^{p}(\Omega))} \Big) \\ &\leq \Lambda \Big( 1 + \left\| \Delta \psi \right\|_{C([0,T_{f}];L^{p}(\Omega))} \left\| \bar{\psi}^{n} \right\|_{L^{p}(0,T_{f};C(\bar{\Omega}))} \Big) \\ &\leq \Lambda \Big\| \bar{\psi}^{n} \Big\|_{L^{p}(0,T_{f};W_{p}^{2}(\Omega))} \\ &\leq \Lambda \Big( \sum_{i \in J} \left\| \bar{\mathcal{C}}_{i}^{n} \right\|_{L^{p}(0,T_{f};L^{p}(\Omega))} + \sum_{i \in J^{\prime}} \left\| \bar{\mathcal{C}}_{i}^{n} \right\|_{L^{p}(0,T_{f};L^{p}(\Omega))} \Big). \end{split}$$
(6.44)

The other terms in (6.41) may be estimated similarly. Thus, we are able to show that there exists a constant  $\Lambda > 0$  satisfying

$$\sum_{i \in J} \|\bar{F}_{i}^{n}\|_{L^{p}(0,T_{f};L^{p}(\Omega))} \leq \Lambda \left( \sum_{i \in J} \|\bar{\mathcal{C}}_{i}^{n}\|_{L^{p}(0,T_{f};L^{p}(\Omega))} + \sum_{i \in J'} \|\bar{C}_{i}^{n}\|_{L^{p}(0,T_{f};L^{p}(\Omega))} \right),$$
(6.45)

which implies convergence in the left-hand side of (6.41). This and (6.33) prove the compactness of the mapping Z.

The *continuity* can be obtained by similar arguments. More precisely, we take a sequence  $\{(\mathcal{C}_i^n)_{i \in J}, \phi_n\}_{n \in \mathbb{N}} \subset X_{T_f}$ . From this we get that

$$\mathscr{C}_i^{n+} \longrightarrow \mathscr{C}_i^+ \quad \text{in } L^p(0, T_f; W_p^1(\Omega)) \cap W_p^1(0, T_f; L^p(\Omega)),$$
 (6.46)

as well as

$$\phi_n \longrightarrow \phi \quad \text{in } C([0, T_f]; W_p^1(\Omega))$$

$$(6.47)$$

for  $n \to \infty$ .

We consider the differences in (6.11), (6.12), and (6.13), use inequalities (5.3) and (6.16) to get the continuity of the mapping Z.

From steps (I), (II), and (III), we conclude the existence of a local, nonnegative solution of problem  $(\mathbf{P}^+)$ .

**6.3.** Uniqueness and problem (P). The solution of  $(\mathbf{P}^+)$  obviously solves problem (P), too. In order to show that the (nonnegative) solution, which we denote by  $C_i^1, \psi^1, i \in J \cup J'$ , is the only one, we assume the existence of another, not necessarily, nonnegative solution  $C_i^2, \psi^2, i \in J \cup J'$ .

We again consider the system for the respective differences  $\bar{C}_i := C_i^1 - C_i^2$ ,  $i \in J \cup J'$ , which is for  $i \in J$  exactly the same as (6.39) if we replace the cuts  $(\mathscr{C}_k^{n+})_{k\in J}$  and  $(\mathscr{C}_k^+)_{k\in J}$  in the right-hand side  $\bar{F}_i$  by the solution vectors  $(C_k^1)_{k\in J}$ and  $(C_k^2)_{k\in J}$ , respectively. We test the *i*th equation with  $\bar{C}_i$  and if we set

$$\|\cdot\|_{V^{1,0}(Q_t)}^2 := \sup_{0 \le \tau \le t} \|\cdot\|_{L^2(\Omega)}^2 + \|\cdot\|_{L^2(0,t;H^1(\Omega))}^2, \tag{6.48}$$

we get, with the same methods presented in the previous sections, the inequality

$$\begin{split} \|\bar{C}_{i}\|_{V^{1,0}(Q_{t})}^{2} &\leq \Lambda \bigg(\Lambda_{\varepsilon} \sum_{k \in J \cup J'} \int_{0}^{t} \|g(s)\|_{L^{\infty}(\Omega)}^{2} \|\bar{C}_{k}(s)\|_{L^{2}(\Omega)}^{2} ds \\ &+ \frac{\varepsilon}{2} \sum_{k \in J} \|\bar{C}_{k}\|_{V^{1,0}(Q_{t})}^{2} + \|\bar{\psi}\|_{L^{2}(0,t;H^{1}(\Omega))} \bigg) \quad \text{for } i \in J, \end{split}$$

$$(6.49)$$

with some  $g \in L^2(0, t; L^{\infty}(\Omega))$  and  $\varepsilon > 0$  arbitrarily.

Similarly, we deduce that

$$\begin{aligned} \|\bar{C}_{i}(t)\|_{L^{2}(\Omega)}^{2} \\ \leq \Lambda \bigg(\sum_{k \in J \cup J'} \int_{0}^{t} \|g(s)\|_{L^{\infty}(\Omega)}^{2} \|\bar{C}_{k}(s)\|_{L^{2}(\Omega)}^{2} ds + \|\bar{\psi}\|_{L^{2}(0,t;H^{1}(\Omega))} \bigg) \quad \text{for } i \in J'. \end{aligned}$$

$$\tag{6.50}$$

Summation over  $i \in J \cup J'$ , the choice of a suitable  $\varepsilon > 0$  and the application of the stability estimate (5.3) yield

$$\sum_{i \in J \cup J'} \left\| \bar{C}_i(t) \right\|_{L^2(\Omega)}^2 \le \Lambda \sum_{i \in J \cup J'} \int_0^t \left( 1 + \|g\|_{L^\infty(\Omega)}^2 \right) \left\| \bar{C}_i \right\|_{L^2(\Omega)}^2 ds \quad \forall t \in [0, T_f].$$
(6.51)

So, we conclude with Gronwall's lemma

$$\sum_{i \in J \cup J'} \|\bar{C}_i(t)\|_{L^2(\Omega)}^2 = 0,$$
(6.52)

and this in turn yields with (5.3) that

$$\left\|\psi_1(t) - \psi_2(t)\right\|_{H^1(\Omega)} = 0.$$
(6.53)

This proves the unique solvability of (**P**), which is Theorem 6.1.  $\Box$ 

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