



A moving-boundary problem for concrete carbonation: Global existence and uniqueness of weak solutions[☆]

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ABSTRACT

This paper deals with a one-dimensional coupled system of semi-linear parabolic equations with a kinetic condition on the moving boundary. The latter furnishes the driving force for the moving boundary. The main result is a global existence and uniqueness theorem of positive weak solutions. The system under consideration is modelled on the so-called carbonation of concrete – a prototypical chemical-corrosion process in a porous solid – concrete – which incorporates slow diffusive transport, interfacial exchange between wet and dry parts of the pores and, in particular, a fast reaction in thin layers, here idealized as a moving-boundary surface in the solid. We include simulation results showing that the model captures the qualitative behaviour of the carbonation process.

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1. Introduction

We study a two phase moving-boundary system with kinetic condition arising in the modeling of the concrete corrosion. The moving boundary represents in this framework the locus where a fast but non-instantaneous aggressive chemical reaction (called carbonation, see (1.1)) is localized. Due to the presence of the moving boundary and of the various production terms by dissolution, precipitation and mass transfer at the water/air interfaces in the pores, the system is strongly coupled, and hence, the derivation of *a priori* bounds of the solution becomes non-trivial.

The physical process can be summarized as follows: Carbon dioxide (CO₂), which is present under normal atmospheric conditions and also emitted as industrial output, attacks reinforced concrete structures by destroying their protection against corrosion. The loss of protection is basically induced by the transformation of dissolved calcium hydroxide (Ca(OH)₂) into calcite (CaCO₃). The loss of protection means in this context that once the calcium hydroxide is reacted away, the cement-based material can be easily attacked by sulfate or chloride ions [3,8,12,23], e.g. On this way the reinforcement becomes subject of corrosion, and hence, spalling or other unwanted effects can occur. The overall reaction–diffusion scenario is called *carbonation*. The core reaction can be described, in a first approximation [23,31,36], as



“aq” and “g” refer to species which are in an aqueous, and respectively, gaseous environment. The phenomenology of the process is apparently simple: Molecules of gaseous CO₂ from the atmosphere penetrate the concrete via the unsaturated

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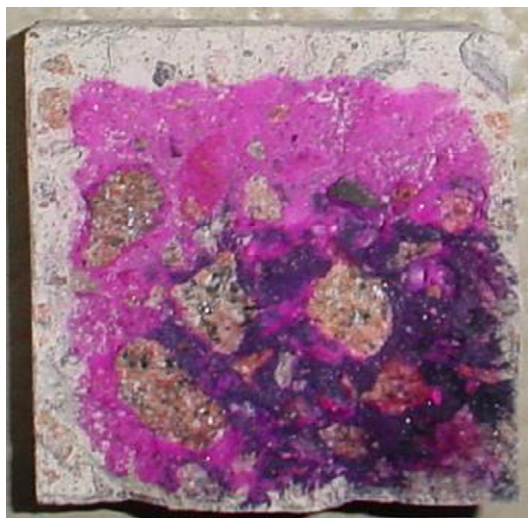


Fig. 1.1. Slice of partly carbonated concrete piece sprayed with phenolphthalein. Two distinct zones can be distinguished where the two reactants live. Courtesy of Prof. M. Setzer and Dr. U. Dahme, University of Essen-Duisburg, Germany.

porous matrix. After entering the air part of the pores, CO_2 is transported through the gaseous phase and is dissolved in the aqueous phase, where it is further transported towards the place where reaction (1.1) takes place. The second reactant, i.e. $\text{Ca}(\text{OH})_2$, is initially in the solid matrix. It arrives in the aqueous phase of the pores through a relatively strong dissolution process. Water and CaCO_3 are the reaction products. CaCO_3 precipitates instantaneously to the concrete fabrics and the water produced by (1.1) steadily distributes within the pores.

Due to the density change produced when transforming $\text{Ca}(\text{OH})_2$ into CaCO_3 , the impact of the carbonation process on concrete micro-structure is significant and possible repairs are often expensive. Therefore there is need of models capable to predict the depth of CO_2 penetration in concrete structures accurately. More details on this important durability issue can be found in [11,12,27] and references cited therein. Experiments show that the zone of reaction is narrowly confined to the interface between the unreacted solid and the product layer, i.e. the region where calcium carbonate precipitates to the solid matrix. In Fig. 1.1, such a macroscopic sharp reaction interface *separating* the carbonated region from the uncarbonated one is pointed out. Our aim is to understand the way this interface penetrates the material. A few relevant questions, which need to be addressed, are:

- Why is the moving-boundary modeling strategy applicable to carbonation?
- How can one define the interface position?
- How fast does the interface move into the material?

The reader can find in [25,27,29] some of our answers. In this paper, we focus on the unidimensional motion of the interface. Therefore, transport and reaction near corners or around macroscopic fissures, which are typically occurring in porous media (see [9,10], e.g.), cannot be described here. Despite this geometrical restriction, the problem is much more general than we state it in the context of carbonation. A wealth of other reaction–diffusion scenarios arising in geochemistry ([30], e.g.), polymer industry ([1,37], e.g.) or life sciences ([15], e.g.) may be tackled by conceptually close moving-boundary modeling strategies.

The paper is organized as follows. In Section 2 we describe the moving-boundary PDE–ODE system that we propose to model the penetration of the carbonation interface in concrete. In Section 3, we introduce some notation and function spaces in order to prepare a functional framework where the problem can be tackled. This is also the place where we present our weak formulation and state the main result – a global existence–uniqueness theorem of positive weak solutions. The bulk of the proofs is given in Section 4. In Section 5 we illustrate numerically a simple carbonation scenario following the strategy Section 2. We conclude the paper with Section 6, where we shortly evaluate the moving-boundary model from both analysis and modeling points of view.

The results of this paper have been announced in [29]. They constitute a part of the results from the PhD thesis [27] of the first author.

2. Moving-sharp interface carbonation model

We consider the carbonation penetration in a wall made of concrete whose chemistry, humidity level, and micro-structure are well known [36]. Let the positive x -axis be directed normally to the reaction interface, say $\Gamma(t)$, pointing into the uncarbonated part. The basic geometry is sketched in Fig. 2.1. At initial time $t = 0$, we assume that the origin

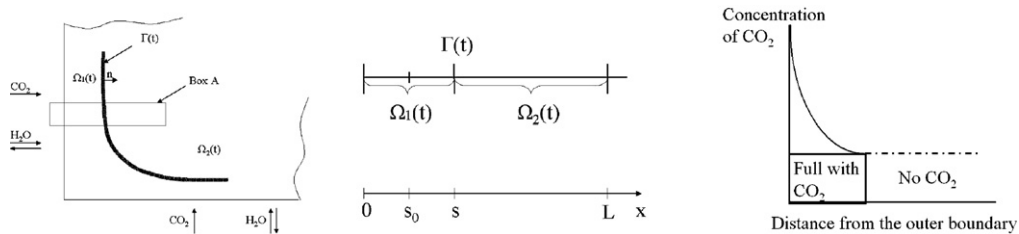


Fig. 2.1. Left: Basic geometry for the moving sharp-interface model. The box A is the region which our model refers to. Center: Schematic 1D geometry. The reactants are spatially segregated at any time t . Right: Definition of the interface position.

located at $x = 0$ is behind the reaction interface $\Gamma(t)$. Assuming that the reactants, whose mass concentration only depends on the real variables x and t , are separated but available for reaction, we expect that the reaction interface moves as $x = s(t)$ for $t \in S_T :=]0, T[$ such that $s(0) = s_0$. Here $T \in]0, +\infty]$, $s_0 \in]0, L[$, and $L \in]0, +\infty[$ are given, see Fig. 2.1 (center). Note that the case $s_0 = 0$ is excluded for two reasons: First, it describes a different process, namely the surface initialization of carbonation coupled with carbonation in the interior, which leads to different models [14]. Secondly, it complicates the mathematical analysis. Among others one would have to take care of the degeneracies induced by the Landau transformation (3.1). We refer to [16,17] to somehow related subjects involving conditions like $s_0 = 0$. Here, we assume $s_0 > 0$; the situation $s_0 = 0$ (the appearance of the carbonated phase) will be addressed elsewhere. We denote the mass concentration of the reactants and products as follows: $\bar{u}_1 := [\text{CO}_2(\text{aq})]$, $\bar{u}_2 := [\text{CO}_2(\text{g})]$, $\bar{u}_4 := [\text{CaCO}_3(\text{aq})]$ and $\bar{u}_5 := [\text{H}_2\text{O}]$ are the chemical species present in the region $\Omega_1(t) := [0, s(t)[$; $\bar{u}_3 := [\text{Ca}(\text{OH})_2(\text{aq})]$ and $\bar{u}_6 := [\text{H}_2\text{O}]$ are species present in $\Omega_2(t) :=]s(t), L]$. For ease of notation, we use the set of indices $\mathcal{I} := \mathcal{I}_1 \cup \{4\} \cup \mathcal{I}_2$, where $\mathcal{I}_1 := \{1, 2, 5\}$ points out the active concentrations in $\Omega_1(t)$ and $\mathcal{I}_2 := \{3, 6\}$ refers to the active concentrations living in $\Omega_2(t)$. Specifically, we take into account that $\text{CaCO}_3(\text{aq})$ is not transported in $\Omega := \Omega_1(t) \cup \Gamma(t) \cup \Omega_2(t)$, therefore the only partly dissipative character of the model. Then, we are led to discuss the *moving-boundary problem* of determining the concentrations $\bar{u}_i(x, t)$, $i \in \mathcal{I}$ and the interface position $s(t)$ which satisfy for all $t \in S_T$ the equations

$$\begin{cases} (\phi\phi_w\bar{u}_i)_{,t} + (-D_i v_{i2}\phi\phi_w\bar{u}_{i,x})_x = f_{i,\text{Henry}}, & x \in \Omega_1(t), \quad i \in \{1, 2\}, \\ (\phi\phi_w\bar{u}_3)_{,t} + (-D_3\phi\phi_w\bar{u}_{3,x})_x = f_{\text{Diss}}, & x \in \Omega_2(t), \\ (\phi\phi_w\bar{u}_4)_{,t} = f_{\text{Prec}} + f_{\text{Reac}\Gamma}, & x = s(t) \in \Gamma(t), \\ (\phi\bar{u}_5)_{,t} + (-D_5\phi\bar{u}_{5,x})_x = 0, & x \in \Omega_1(t), \\ (\phi\bar{u}_6)_{,t} + (-D_6\phi\bar{u}_{6,x})_x = 0, & x \in \Omega_2(t). \end{cases} \quad (2.1)$$

The initial and boundary conditions are $\phi\phi_w v_{i2}\bar{u}_i(x, 0) = \hat{u}_{i0}(x)$, $i \in \mathcal{I}$, $x \in \Omega(0)$, $\phi\phi_w v_{i2}\bar{u}_i(0, t) = \lambda_i(t)$, $i \in \mathcal{I}_1$, $\bar{u}_{i,x}(L, t) = 0$, $i \in \mathcal{I}_2$, where $t \in S_T$. Specific to our problem, we impose the following interface conditions

$$\begin{cases} [j_1 \cdot n]_{\Gamma(t)} = -\eta_{\Gamma}(s(t), t) + s'(t)[\phi\phi_w\bar{u}_1]_{\Gamma(t)}, \\ [j_i \cdot n]_{\Gamma(t)} = \eta_{\Gamma}(s(t), t)\delta_{5i} + s'(t)[\phi\phi_w v_{i2}\bar{u}_i]_{\Gamma(t)}, \quad i \in \{2, 5, 6\}, \\ [j_3 \cdot n]_{\Gamma(t)} = -\eta_{\Gamma}(s(t), t) + s'(t)[\phi\phi_w\bar{u}_3]_{\Gamma(t)}, \end{cases} \quad (2.2)$$

$$\phi\phi_w\bar{u}_5(s(t), t) = \phi\phi_w\bar{u}_6(s(t), t), \quad (2.3)$$

$$s'(t) = \alpha \frac{\eta_{\Gamma}(s(t), t)}{\phi\phi_w\bar{u}_3(s(t), t)} =: \psi_{\Gamma}(s(t), t), \quad s(0) = s_0, \quad (2.4)$$

where $v_{12} = v_{32} := 1$, $v_{22} := \frac{\phi_a}{\phi_w}$, $v_{52} = v_{62} := \frac{1}{\phi_w}$, $v_{i\ell} := 1$ ($i \in \mathcal{I}$, $\ell \in \mathcal{I} - \{2\}$), δ_{ij} ($i, j \in \mathcal{I}$) is Kronecker's symbol, $j_i := -D_i v_{i\ell}\phi\phi_w\bar{u}_i$ ($i, \ell \in \mathcal{I}_1 \cup \mathcal{I}_2$) are the corresponding effective diffusive fluxes and $\alpha > 0$. Here D_i , L and s_0 are strictly positive constants, λ_i are prescribed in agreement with the environmental conditions to which Ω – a part of a concrete sample (cf. Fig. 2.1 (center)) – is exposed, see [12,34]. An argument for the boundary conditions (2.2) is based on the so-called *pillbox lemma* (see [22]). The initial conditions $\hat{u}_{i0} > 0$ are determined by the chemistry of the cement. The hardened mixture of aggregate, cement and water (i.e. the concrete) imposes ranges for the porosity $\phi > 0$ and also for the water and air fractions, $\phi_w > 0$ and $\phi_a > 0$. Since the active concentrations are small, the constant-porosity assumption [7,36] is valid. The productions terms $f_{i,\text{Henry}}$, f_{Diss} , f_{Prec} and $f_{\text{Reac}\Gamma}$ are sources or sinks by Henry-like interfacial transfer mechanisms, dissolution, precipitation, and carbonation reactions. Typical examples are:

$$\begin{cases} f_{i,\text{Henry}} := (-1)^i P_i(\phi\phi_w\bar{u}_1 - Q_i\phi\phi_a\bar{u}_2) \quad (P_i > 0, Q_i > 0), \quad i \in \{1, 2\}, \\ f_{\text{Diss}} := -S_{3,\text{diss}}(\phi\phi_w\bar{u}_3 - u_{3,\text{eq}}), \quad S_{3,\text{diss}} > 0, \quad f_{\text{Prec}} := 0, \quad f_{\text{Reac}\Gamma} := \eta_{\Gamma}. \end{cases} \quad (2.5)$$

In (2.5), $\eta_{\Gamma}(s(t), t)$ denotes the carbonation reaction rate. It is defined in the following fashion: Let $\bar{u} = (\bar{u}_1, \dots, \bar{u}_6)^t$ be the vector of concentrations and M_{Λ} the set of parameters $\Lambda := (\Lambda_1, \dots, \Lambda_m)^t$ chosen to describe the reaction rate. For our purposes, it suffices to assume that M_{Λ} is a non-empty compact subset of $\mathbb{R}_+^m$. We introduce the function

$$\eta_{\Gamma} : \mathbb{R}^6 \times M_{\Lambda} \rightarrow \mathbb{R}_+ \quad \text{by} \quad \eta_{\Gamma}(\bar{u}(x, t), \Lambda) := k\phi\phi_w\bar{u}_1^p(x, t)\bar{u}_3^q(x, t), \quad x = s(t). \quad (2.6)$$

In (2.6), $m := 3$ and $\Lambda := \{p, q, k\phi\phi_w\} \in \mathbb{R}_+^3$. We define the reaction rate $\eta_\Gamma(s(t), t)$ and the term $\psi_\Gamma(s(t), t)$ in (2.4) by

$$\eta_\Gamma(s(t), t) := \eta_\Gamma(\bar{u}(s(t), t), \Lambda), \quad \psi_\Gamma(s(t), t) := \psi_\Gamma(\bar{u}(s(t), t), \Lambda), \quad (2.7)$$

where η_Γ is given by the classical power-law ansatz (2.6); see [19]. In the engineering literature, there is a whole variety of reaction rates used in the context of carbonation [14,31,33]; (2.6), with $p > 0$ and $q > 0$, seems to be the ansatz most widely used. Note that some mass-balance equations act in $\Omega_1(t)$, while other act in $\Omega_2(t)$ or at $\Gamma(t)$. All of the three space regions are varying in time and they are *a priori* unknown.

The system (2.1)–(2.7) forms the *sharp-interface carbonation model*. We abbreviate it as (P_Γ) . The model consists of a coupled semi-linear system of parabolic equations that has a moving *a priori* unknown internal boundary $\Gamma(t)$, where the carbonation reaction is assumed to take place. The coupling between the equations and the non-linearities comes from the influence of the chemical reaction on the transport part and also from the dependence of the moving regions $\Omega_1(t)$ and $\Omega_2(t)$ on $s(t)$.

2.1. Remarks around (2.2) and (2.4)

The interface conditions require further explanation. The term $\eta_\Gamma(s(t), t) \approx \frac{1}{\alpha} s'(t)$ denotes the number of grams per volume and time that is transported by diffusion to the interface $\Gamma(t)$. In (2.2), $\pm \phi\phi_w \bar{u}(s(t), t) s'(t)$ accounts for the mass flux induced by the motion of $\Gamma(t)$ in order to preserve the conservation of mass. The conditions (2.2) express jumps in the gradients of concentrations across $\Gamma(t)$. They are typical interface relations for a surface-reaction mechanism, i.e. the classical Rankine–Hugoniot jump relations, cf. [6, Section 1.2.E], e.g. The law (2.4), which we call *kinetic* or *non-equilibrium* condition, governs the dynamics of the reaction interface. (2.4) is exact for the 1D case and has been derived via *first principles* in [27]. We rely on (2.4) to determine the position of the interface once the reactants concentration at $\Gamma(t)$ is known. Kinetic laws show in many situations a regularizing effect by ensuring the global (in time) existence of the solutions. Nevertheless, if they are posed inappropriately, then they can induce a blow up in concentration (see [21,28], e.g.) or in the speed $s'(t)$ of the interface, and hence, all regularizing effects are lost. Further examples of moving-boundary problems with kinetic conditions are treated, for instance, in [15,37,39].

The present setting is only applicable when the reaction rate is very rapid and the diffusion of the gaseous CO_2 is sufficiently slow, or in other terms, when the characteristic time of the carbonation reaction is much smaller than the characteristic time of the diffusion of the fastest species. The quotient of the characteristic times may cause the concentrations of the active chemical species and their gradient to have a jump at $\Gamma(t)$. The magnitude of the jump typically depends on the concentration itself. Notice that when dealing with reaction–diffusion scenarios one typically imposes the continuity of concentrations across interfaces. A special feature brought in by (2.1)–(2.7) is that concentration fields are not obliged to be continuous everywhere. They may have finite jumps at $\Gamma(t)$. At the macroscopic level it is not *a priori* clear what actually happens with the reactants at $\Gamma(t)$. For our case, complete reaction at $\Gamma(t)$ would immediately imply the case of *infinitely fast* chemical reaction in which the reactants practically vanish at $\Gamma(t)$ (see [13], e.g.). We refer the reader to [32,35] for reaction–diffusion scenarios where discontinuities in concentrations arise at moving boundaries.

3. Main results

3.1. Preliminaries

For each $i \in \mathcal{I}_1 \cup \mathcal{I}_2$, we denote $H_i := L^2(a, b)$ and set $[a, b] := [0, 1]$ for $i \in \mathcal{I}_1$ and $[a, b] := [1, 2]$ for $i \in \mathcal{I}_2$. Moreover, $\mathbb{H} := \prod_{i \in \mathcal{I}_1 \cup \mathcal{I}_2} H_i$, $V_i := \{u \in H^1(a, b) : u_i(a) = 0\}$, $i \in \mathcal{I}_1$, $V_i := H^1(a, b)$, $i \in \mathcal{I}_2$, $V_w := \{(u_5, u_6) \in V_5 \times V_6 : u_5(1) = u_6(1)\}$. In addition, $|\cdot| := \|\cdot\|_{L^2(a, b)}$ and $\|\cdot\| := \|\cdot\|_{H^1(a, b)}$. Note that $\|u_3\|_{V_3} = |u_y|_{H_3} + |u_3(1)|$ and $|(u_5, u_6)|_{V_w} = |u_{5,y}|_{H_5} + |u_{6,y}|_{H_6}$. Furthermore,

$$\mathbb{V} = \left\{ (u_1, u_2, u_3, u_5, u_6) \in \prod_{i \in \mathcal{I}_1 \cup \mathcal{I}_2} V_i : u_5(1) = u_6(1) \right\}.$$

If $(X_i : i \in \mathcal{I})$ is a sequence of given sets X_i , then $X^{|\mathcal{I}_1 \cup \mathcal{I}_2|}$ denotes the product $\prod_{i \in \mathcal{I}_1 \cup \mathcal{I}_2} X_i := X_1 \times X_2 \times X_3 \times X_5 \times X_6$. The set $W_2^1(S; \mathbb{V}, \mathbb{H}) := \{u \in L^2(S, \mathbb{V}) : u' \in L^2(S, \mathbb{V}^*)\}$ forms a Banach space with the norm $\|u\|_{W_2^1} = \|u\|_{L^2(S, \mathbb{V})} + \|u'\|_{L^2(S, \mathbb{V}^*)}$. Details on the Sobolev and L^p -spaces, which appear in the paper but are not listed here, can be found in [40], e.g.

Note that sometimes $u(1)$ and $u_{,y}(1)$ replace $u(1, t)$ and $u_{,y}(1, t)$, respectively.

We reformulate the system (2.1)–(2.7): Let $\hat{u}_i := \phi\phi_w \bar{u}_i$, $i \in \{1, 3, 4\}$, $\hat{u}_2 := \phi\phi_a \bar{u}_2$, $\hat{u}_i := \phi \bar{u}_i$, $i \in \{5, 6\}$, and write down (P_Γ) on fixed domains. As result of this procedure, we obtain the transformed model (3.3)–(3.14).

Let $t \in S_T$ be arbitrarily fixed. In our setting, the fixed-domain transformations [24] read:

$$(x, t) \in [0, s(t)] \times \bar{S}_T \longmapsto (y, t) \in [a, b] \times \bar{S}_T, \quad y = \frac{x}{s(t)} \quad \text{for } i \in \mathcal{I}_1, \quad (3.1)$$

$$(x, t) \in [s(t), L] \times \bar{S}_T \longmapsto (y, t) \in [a, b] \times \bar{S}_T, \quad y = a + \frac{x - s(t)}{L - s(t)} \quad \text{for } i \in \mathcal{I}_2. \quad (3.2)$$

We introduce the notation $u_i(y, t) := \hat{u}_i(x, t) - \lambda_i(t)$ for all $y \in [a, b]$ and $t \in S_T$. The model equations become

$$(u_i + \lambda_i)_{,t} - \frac{1}{s^2(t)} (D_i u_{i,y})_{,y} = f_i(u + \lambda) + y \frac{s'(t)}{s(t)} u_{i,y}, \quad i \in \mathcal{I}_1, \quad (3.3)$$

$$(u_i + \lambda_i)_{,t} - \frac{1}{(L - s(t))^2} (D_i u_{i,y})_{,y} = f_i(u + \lambda) + (2 - y) \frac{s'(t)}{L - s(t)} u_{i,y}, \quad i \in \mathcal{I}_2, \quad (3.4)$$

where u is the vector of concentrations $(u_1, u_2, u_3, u_5, u_6)^t$ and λ represents the boundary data $(\lambda_1, \lambda_2, \lambda_3, \lambda_5, \lambda_6)^t$. We make use of λ_3 and λ_6 only for notational simplicity ($\lambda_3 := \lambda_6 := 0$). The vectors of concentrations u_0 and λ are assumed to be compatible, i.e.

$$u_{0i}(0) = \lambda_i(0), \quad \text{and hence} \quad \hat{u}_i(0) = 0 \quad \text{for } i \in \mathcal{I}_1. \quad (3.5)$$

The transformed initial, boundary and interface conditions are

$$u_i(y, 0) = u_{i0}(y), \quad i \in \mathcal{I}_1 \cup \mathcal{I}_2, \quad u_i(a, t) = 0, \quad i \in \mathcal{I}_1, \quad u_{i,y}(b, t) = 0, \quad i \in \mathcal{I}_2, \quad (3.6)$$

$$\frac{-D_1}{s(t)} u_{1,y}(1) = \eta_\Gamma(1, t) + s'(t)(u_1(1) + \lambda_1), \quad (3.7)$$

$$\frac{-D_2}{s(t)} u_{2,y}(1) = s'(t)(u_2(1) + \lambda_2), \quad (3.8)$$

$$\frac{-D_3}{L - s(t)} u_{3,y}(1) = -\eta_\Gamma(1, t) + s'(t)(u_3(1) + \lambda_3), \quad (3.9)$$

$$\frac{-D_5}{s(t)} u_{5,y}(1) + \frac{D_6}{L - s(t)} u_{6,y}(1) = -\eta_\Gamma(1, t), \quad u_5(1) = u_6(1), \quad (3.10)$$

where $\eta_\Gamma(1, t)$ denotes the reaction rate that acts in the y - t plane. This is defined by

$$\eta_\Gamma(1, t) := \eta_\Gamma(\bar{u}(ys(t), t) + \lambda(t), \Lambda), \quad y \in [0, 1], \quad (3.11)$$

for given $\Lambda \in M_\Lambda$ and η_Γ as in (2.6). $\psi_\Gamma(1, t)$ is defined analogously. We also mention that $u_{i0}(y) = \hat{u}_{i0}(x) - \lambda_i(0)$, where $x = ys_0$, $y \in [0, 1]$ for $i \in \mathcal{I}_1$, and $x = s_0 + (y - 1)(L - s_0)$, $y \in [1, 2]$ for $i \in \mathcal{I}_2$. Finally, two ordinary differential equations

$$s'(t) = \psi_\Gamma(1, t) \quad \text{and} \quad v'_4(t) = f_4(v_4(t)) \quad \text{a.e. } t \in S_T, \quad (3.12)$$

where

$$v_4(t) := \hat{u}_4(x, t) \quad [\text{with } \hat{u}_4 := \phi \phi_w \bar{u}_4] \quad \text{for } x = s(t) \text{ and } t \in S_T, \quad (3.13)$$

complete the model formulation. Furthermore, we take

$$s(0) = s_0, \quad v_4(0) = \hat{u}_{40}. \quad (3.14)$$

Let $\varphi := (\varphi_1, \varphi_2, \varphi_3, \varphi_5, \varphi_6)^t \in \mathbb{V}$ be an arbitrary test function and take $t \in S_T$. To write down the weak formulation of (3.3)–(3.14) in a compact form, we introduce the notation:

$$\begin{cases} a(s, u, \varphi) := \frac{1}{s} \sum_{i \in \mathcal{I}_1} (D_i u_{i,y}, \varphi_{i,y}) + \frac{1}{L - s} \sum_{i \in \mathcal{I}_2} (D_i u_{i,y}, \varphi_{i,y}), \\ b_f(u, s, \varphi) := s \sum_{i \in \mathcal{I}_1} (f_i(u), \varphi_i) + (L - s) \sum_{i \in \mathcal{I}_2} (f_i(u), \varphi_i), \\ e(s', u, \varphi) := \sum_{i \in \mathcal{I}_1 \cup \mathcal{I}_2} g_i(s, s', u(1)) \varphi_i(1), \\ h(s', u, \varphi) := s' \sum_{i \in \mathcal{I}_1} (y u_{i,y}, \varphi_i) + s' \sum_{i \in \mathcal{I}_2} ((2 - y) u_{i,y}, \varphi_i), \end{cases} \quad (3.15)$$

for any $u, \varphi \in \mathbb{V}$ and $s \in W^{1,2}(S_T)$. The term $a(\cdot)$ incorporates the diffusive part of the model, $b_f(\cdot)$ comprises volume productions, $e(\cdot)$ sums up reaction terms acting on $\Gamma(t)$ and $h(\cdot)$ is a non-local term due to fixing of the domain. For our application, the interface terms g_i ($i \in \mathcal{I}_1 \cup \mathcal{I}_2$) are given by

$$\begin{cases} g_1(s, s', u) := \eta_\Gamma(1, t) + s'(t)u_1(1), & g_2(s, s', u) := s'(t)u_2(1), \\ g_3(s, s', u) := \eta_\Gamma(1, t) - s'(t)u_3(1), & g_5(s, s', u) := \eta_\Gamma(1, t), \\ g_6(s, s', u) := 0, \end{cases} \quad (3.16)$$

whereas the volume terms f_i ($i \in \mathcal{I}$) are defined as

$$\begin{cases} f_1(u) := P_1(Q_1 u_2 - u_1), & f_4(\hat{u}) := \eta_{\Gamma}(s(t), t), \\ f_2(u) := -P_2(Q_2 u_2 - u_1), & f_5(u) := 0, \\ f_3(u) := S_{3,\text{diss}}(u_{3,\text{eq}} - u_3), & f_6(u) := 0. \end{cases} \quad (3.17)$$

We assume that the initial and boundary data as well as the model parameters satisfy the restrictions:

$$\lambda_5 \in W^{1,\infty}(S_T), \quad \lambda \in W^{1,2}(S_T)^{|\mathcal{I}_1 \cup \mathcal{I}_2|}, \quad \lambda(t) \geq 0 \quad \text{a.e. } t \in \bar{S}_T, \quad (3.18)$$

$$u_{3,\text{eq}} \in L^\infty(S_T), \quad u_{3,\text{eq}}(t) \geq 0 \quad \text{a.e. } t \in \bar{S}_T, \quad (3.19)$$

$$u_0 \in L^\infty(a, b)^{|\mathcal{I}_1 \cup \mathcal{I}_2|}, \quad u_0(y) + \lambda(0) \geq 0 \quad \text{a.e. } y \in [a, b], \quad (3.20)$$

$$\hat{u}_{40} \in L^\infty(0, s_0), \quad \hat{u}_4(x, 0) > 0 \quad \text{a.e. } x \in [0, s_0], \quad (3.21)$$

$$s_0 > 0, \quad L_0 < L < +\infty, \quad s_0 < L_0, \quad (3.22)$$

$$\min\{S_{3,\text{diss}}, P_1, Q_1, P_2, Q_2, D_\ell(\ell \in \mathcal{I}_1 \cup \mathcal{I}_2)\} > 0. \quad (3.23)$$

We denote

$$m_0 := \min\{s_0, L - L_0\}, \quad M_0 := \max\{L_0, L - s_0\}. \quad (3.24)$$

Set

$$\mathcal{K} := \prod_{i \in \mathcal{I}_1 \cup \mathcal{I}_2} [0, k_i], \quad (3.25)$$

and, for fixed $\Lambda \in M_\Lambda$, we take

$$M_{\eta_{\Gamma}} := \max_{\bar{u} \in \mathcal{K}} \{\eta_{\Gamma}(\bar{u}, \Lambda)\}. \quad (3.26)$$

In (3.25) we set

$$\begin{cases} k_i := \max\{u_{i0}(y) + \lambda_i(t), \lambda_i(t) : y \in [a, b], t \in \bar{S}_T\}, & i = 1, 2, 3, 6, \\ k_4 := \max\{\hat{u}_{40}(x) + M_{\eta_{\Gamma}} T : x \in [0, s(t)], t \in \bar{S}_T\}, \\ k_5 := \max\{u_{50}(y) + \lambda_5(t), \lambda_6(t), \kappa : y \in [a, b], t \in \bar{S}_T\}, \\ k_6 := k_5, \end{cases} \quad (3.27)$$

where

$$M_{\eta_{\Gamma}} - k_5 s_0 \leq 0. \quad (3.28)$$

Definition 3.1 (Local Weak Solution). We call the triple (u, v_4, s) a local weak solution to problem (3.3)–(3.14) if there is a $\delta \in]0, T]$ with $S_\delta :=]0, \delta[$ such that

$$s_0 < s(\delta) \leq L_0, \quad (3.29)$$

$$v_4 \in W^{1,4}(S_\delta), \quad s \in W^{1,4}(S_\delta), \quad (3.30)$$

$$u \in W_2^1(S_\delta; \mathbb{V}, \mathbb{H}) \cap [\bar{S}_\delta \mapsto L^\infty(a, b)]^{|\mathcal{I}_1 \cup \mathcal{I}_2|}. \quad (3.31)$$

For all $\varphi \in \mathbb{V}$ and a.e. $t \in S_\delta$ we have

$$\begin{cases} s \sum_{i \in \mathcal{I}_1} (u_{i,t}(t), \varphi_i) + (L - s) \sum_{i \in \mathcal{I}_2} (u_{i,t}(t), \varphi_i) + a(s, u, \varphi) + e(s', u + \lambda, \varphi) \\ \quad = b_f(u + \lambda, s, \varphi) + h(s', u, y, \varphi) - s \sum_{i \in \mathcal{I}_1} (\lambda_{i,t}(t), \varphi_i) - (L - s) \sum_{i \in \mathcal{I}_2} (\lambda_{i,t}(t), \varphi_i), \\ s'(t) = \eta_{\Gamma}(1, t), \quad v_4'(t) = f_4(v_4(t)) \quad \text{a.e. } t \in S_\delta, \\ u(0) = u_0 \in \mathbb{H}, \quad s(0) = s_0, \quad v_4(0) = \hat{u}_{40}. \end{cases} \quad (3.32)$$

3.2. Hypotheses on the model parameters

The only assumptions that are needed are the following:

- (A) Fix $\Lambda \in M_\Lambda$. Let $\eta_\Gamma(\bar{u}, \Lambda) > 0$, if $\bar{u}_1 > 0$ and $\bar{u}_3 > 0$, and $\eta_\Gamma(\bar{u}, \Lambda) = 0$, otherwise. For any fixed $\bar{u}_1 \in \mathbb{R}$, η_Γ is bounded.
- (B) The reaction rate $\eta_\Gamma : \mathbb{R}^6 \times M_\Lambda \rightarrow \mathbb{R}_+$ is locally Lipschitz. This restricts the choice of p and q in (2.6).
- (C1) $1 > k_3 \geq \max_{\bar{S}_T} \{|u_{3,eq}(t)| : t \in \bar{S}_T\}$; $D_5 - M_{\eta_\Gamma} L^2 > 0$.
- (C2) $Q_1 k_2 \leq k_1$; $k_1 \leq Q_2 k_2$.

(A)–(C) can be interpreted in the following way: (A) means that the reaction takes place if both $\text{CO}_2(\text{aq})$ and $\text{Ca}(\text{OH})_2(\text{aq})$ are present. The last part of (A) prevents the unreacted region to vanish completely. (B) is mainly needed from mathematical reasons (it simply helps proving the local existence of weak solutions). On the other hand, (B) represents a quite natural assumption if one finally wants a PDE model whose solution depends continuously on data and parameters. (C1) is needed to establish the L^∞ -estimates on u_3 and u_5 . It says that the equilibrium concentration of $\text{Ca}(\text{OH})_2(\text{aq})$ is uniformly bounded by 1 and the diffusion of moisture should be sufficiently strong to spread away the water produced by reaction (1.1). (C2) suggests that the transfer of CO_2 from the air phase into the pore water is fast. It is used to get the L^∞ -estimates on u_1 and u_2 .

By (A) and (B), we deduce that $\eta_\Gamma(0, \Lambda) = 0$ for all $\Lambda \in M_\Lambda$. For all $\bar{u} \in \mathbb{R}^6$ there is an ϵ -neighborhood $\mathcal{U}_\epsilon(\bar{u})$ and a positive constant $C_\eta = C_\eta(\Lambda, \lambda, \epsilon, T_{\text{fin}})$ such that the inequality

$$\eta_\Gamma(\bar{u}(s(t), t), \Lambda) \leq C_\eta |\bar{u}(s(t), t)| \quad (3.33)$$

holds for all $t \in S_T$. (3.33) can be reformulated as

$$\eta_\Gamma(1, t) \leq C_\eta |u(1, t)| \quad \text{for all } t \in S_T. \quad (3.34)$$

Note also that there exists a function $c_g = c_g(C_\eta)$ such that

$$|e(s', u(1), \varphi(1))| \leq c_g |u(1)| |\varphi(1)| \quad \text{for all } \varphi \in \mathbb{V} \quad (3.35)$$

and a constant $c_f = c_f(C_\eta, K_1) > 0$ such that

$$|b_f(u, s, \varphi)| \leq c_f (|u_{3,eq}|_\infty^2 + |u|^2 + |\varphi|^2) \quad \text{for all } \varphi \in \mathbb{V}, \quad (3.36)$$

where $K_1 > 0$ is a constant depending on the material parameters entering f_i ($i \in \mathcal{I}$), i.e. P_1 , P_2 , Q_1 , Q_2 , and $S_{3,\text{diss}}$. The exact structure of c_g , c_f and K_1 is dictated by the definition of the production terms f_i and g_i ($i \in \mathcal{I}$), see (3.17) and (3.16). Since $\psi_\Gamma(1, t)$ has essentially the same structure as $\eta_\Gamma(1, t)$, it also satisfies (A) and (B).

3.3. Local solvability

We have the following results.

Theorem 3.2. Assume the hypotheses (A)–(C2) and let the conditions (3.18)–(3.23) be satisfied. If $s \in W^{1,4}(S_\delta)$ with $s' \geq 0$ a.e. in S_δ and $s(0) = s_0$ is given, then the problem (3.3)–(3.14) admits a unique weak solution in the sense of Definition 3.1 (formulated for given s).

Proof. Although this problem is non-linear, it is rather a standard transmission problem. The existence and uniqueness of the weak solutions can be shown as for the model problems presented in [38,40], and therefore, we omit the proof. $\square$

Theorem 3.3. Assume the hypotheses (A)–(C2) and let the conditions (3.18)–(3.23) be satisfied. Then we have:

- (i) $0 \leq u_i(y, t) + \lambda_i(t) \leq k_i$ a.e. $y \in [a, b]$ ($i \in \mathcal{I}_1 \cup \mathcal{I}_2$) for all $t \in S_\delta$. Moreover, $0 \leq v_4(t) \leq k_4$ a.e. $t \in S_\delta$, where v_4 is defined by (3.13);
- (ii) $v_4, s \in W^{1,\infty}(S_\delta)$.

Theorem 3.4 (Local Existence and Uniqueness). Assume the hypotheses (A)–(C2) and let the conditions (3.18)–(3.23) be satisfied. Then it exists a $\delta \in]0, T[$ such that the problem (3.3)–(3.14) admits a unique local solution on S_δ in the sense of Definition 3.1.

3.4. Return to the physical domain

Using inverse Landau transformation corresponding to (3.1) and (3.2), we map the solution back to the physical domain. We have

Proposition 3.5 (Change of Coordinates). Assume that the hypotheses of Theorem 3.4 are satisfied. Additionally, if $u_{3,eq} \in W^{1,2}(S_\delta)$, $\hat{u}_0 \in H^1(0, s_0)^{|\mathcal{I}_1|} \times H^1(s_0, L)^{|\mathcal{I}_2|}$, $\hat{u}_0$ and λ satisfy the compatibility conditions (3.5), then the solution $(\hat{u}, v_4, s)$ acts in the physical x - t plane and

$$(\hat{u}, v_4, s) \in \left[\prod_{i \in \mathcal{I}_1 \cup \mathcal{I}_2} H^1(S_\delta, \hat{H}_i(t)) \right] \times W^{1,4}(S_\delta)^2, \quad (3.37)$$

where $\hat{H}_i(t) := L^2(0, s(t))$ for $i \in \mathcal{I}_1$ and $\hat{H}_i(t) := L^2(s(t), L)$ for $i \in \mathcal{I}_2$.

Proof. We employ the inverse Landau transformations. The rest of the proof relies on a lifting regularity argument, integration by parts, and change of variables in the Bochner integral; see the proof of Proposition 3.4.17 in [27] for details. $\square$

3.5. Global solvability

The main result of this paper is the next theorem.

Theorem 3.6 (Global Solvability). Assume that the hypotheses of Theorem 3.4 are satisfied. Then for arbitrary $T^* > 0$ either the problem (3.3)–(3.14) has a solution on $S_{T^*} :=]0, T^*]$ or $s(t) \rightarrow L$ as $t \rightarrow T'$ for some $0 < T' \leq T^*$.

Proof. Let us fix $T^* > 0$. Theorem 3.4 states the existence of a unique weak solution in the time interval $S_\delta =]0, \delta[$ with $\delta > 0$. The same argument can be repeated to gain the existence (and uniqueness) of the weak solution with respect to time intervals like $]k\delta, (k+1)\delta[$, where the free factor $k \in \mathbb{N}$ satisfies the property $k+1 < \frac{1}{\delta}T^*$. The last time subinterval on which the solution is proved to exist is $]k_m\delta, T^*]$, where $k_m := \sup\{k \in \mathbb{N}: k+1 < \frac{1}{\delta}T^*\}$. Since the uniqueness is granted on each of the intervals $]0, \delta[, \dots,]k\delta, (k+1)\delta[, \dots,](k_m-1)\delta, k_m\delta[$, it actually holds on the whole $]0, T^*]$. $\square$

Theorem 3.6 indicates that the function $s(t)$, which is describing the position of the moving boundary, belongs to $W^{1,\infty}(\mathbb{R}^+)$. In principle, two conceptually distinct situations can happen: (1) $s(t) \rightarrow s(T')$ as $t \rightarrow T'$, where $T' > 0$ is given by

$$s(T') = L \quad (3.38)$$

(cf. [4,5]); or (2) the moving interface stops before reaching $x = L$, for instance, due to a complete consumption of one of the reactants (here: $\text{Ca}(\text{OH})_2$). Note that both situations are physically reasonable. However, in order to understand mathematically how the global solutions to (3.3)–(3.14) precisely behave, more estimates (especially decay estimates and/or regularity/concavity of $s(t)$) are needed. In this sense, we expect that our global solvability result can be refined very much in the spirit of [18,20], where the authors completely described the behavior of fast and slow global solutions for the case of a one-phase Stefan-like problem with super-linear reaction term.

4. Proofs

This section is organized in the following manner: We obtain a series of positivity, L^∞ - and energy estimates in Section 4.1. Section 4.2 contains the proof of the local existence of solutions.

4.1. Basic estimates. Proof of Theorem 3.3

The first lemma contains several inequalities which are needed for following the estimates. It may be proved by essentially standard methods.

Lemma 4.1 (Some Basic Estimates). Let $\xi > 0$, $\theta \in [\frac{1}{2}, 1]$, $c_\xi > 0$ and $s \in W^{1,1}(S_\delta)$.

(i) There exists a constant $\hat{c} = \hat{c}(\theta) > 0$ such that

$$|u_i|_\infty \leq \hat{c}|u_i|^{1-\theta} \|u_i\|^\theta \quad (4.1)$$

for all $u_i \in V_i$, where $i \in \mathcal{I}_1 \cup \mathcal{I}_2$.

(ii) There exists a constant $c_\xi > 0$ such that

$$|u_i|^{1-\theta} \|u_i\|^\theta \leq \xi \|u_i\| + c_\xi |u_i| \quad (4.2)$$

for all $u_i \in V_i$, where $i \in \mathcal{I}_1 \cup \mathcal{I}_2$.

(iii) Let $\varphi \in \mathbb{V}$ with $\varphi = (\varphi_1, \dots, \varphi_6)^t$, $t \in S_\delta$, $\hat{c}$ as in (i), and ξ, c_ξ as in (ii). Then we have for $i \in \mathcal{I}_1$ and $j \in \mathcal{I}_2$ the following inequalities:

$$\begin{aligned} \frac{|s'(t)|}{s(t)} (y\varphi_{i,y}, \varphi_i) &= \frac{1}{2} \frac{|s'(t)|}{s(t)} \{ \varphi_i(1)^2 - |\varphi_i|^2 \} \leq \frac{1}{2} \frac{|s'(t)|}{s(t)} \{ \hat{c}^2 |\varphi_i|^{2(1-\theta)} \|\varphi_i\|^{2\theta} - |\varphi_i|^2 \}; \\ \frac{|s'(t)|}{s(t)} |\varphi_i(1)|^2 &\leq \frac{|s'(t)|}{s(t)} |\varphi_i|_\infty^2 \leq \frac{\xi}{s^2(t)} \|\varphi_i\|^2 + c_\xi \hat{c}^{\frac{2}{1-\theta}} \times s(t)^{\frac{2\theta-1}{1-\theta}} |s'(t)|^{\frac{1}{1-\theta}} |\varphi_i|^2; \\ \frac{|\varphi_i(1)|^2}{s^2(t)} &\leq \frac{1}{s^2(t)} |\varphi_i|_\infty^2 \leq \hat{c}^2 s(t)^{2\theta-2} |\varphi_i|^{2(1-\theta)} (s(t)^{-1} \|\varphi_i\|)^{2\theta} \leq \frac{\xi}{s^2(t)} \|\varphi_i\|^2 + c_\xi \hat{c}^{\frac{2}{1-\theta}} |s(t)|^{\frac{2(\theta-1)}{1-\theta}} |\varphi_i|^2; \\ \frac{|\varphi_i(1)|^2}{s(t)} &\leq \frac{\xi}{s^2(t)} \|\varphi_i\|^2 + c_\xi \hat{c}^{\frac{2}{1-\theta}} |s(t)|^{\frac{2\theta-1}{1-\theta}} |\varphi_i|^2; \\ \frac{|s'(t)|}{L-s(t)} ((2-y)\varphi_{j,y}, \varphi_j) &= \frac{1}{2} \frac{|s'(t)|}{L-s(t)} |\varphi_j(1)|^2 + \frac{1}{2} \frac{|s'(t)|}{L-s(t)} |\varphi_j|^2. \end{aligned}$$

Proof. (i) The case $\theta \in]\frac{1}{2}, 1[$ follows from $H^\theta(a, b) \hookrightarrow C([a, b])$ and from an interpolation inequality (see Theorem 5.9 in [2], e.g.). The case $\theta = \frac{1}{2}$ is discussed in [40, Example 21.62, p. 285], e.g. To get (ii) we use Young's inequality. Young's inequality and the integration by parts are the necessary tools to prove (iii). For instance, the fact that for each $i \in \mathcal{I}_2$ we have $((2-y)\varphi_{i,y}, \varphi_i) = \varphi_i(1)^2 - (\varphi_i, (2-y)\varphi_{i,y}) + |\varphi_i|^2$ shows the last statement in (iii). $\square$

The special choice $\theta = \frac{1}{2}$ can be further used to simplify the estimates. By this choice, the sum $s(t)^{\frac{2\theta-1}{1-\theta}} + (L-s(t))^{\frac{2\theta-1}{1-\theta}}$ becomes 2. Note also that for any $\xi > 0$, there exists a constant $c_\xi > 0$ such that

$$|\varphi_i(z)|^2 \leq \xi \|\varphi_i\|^2 + c_\xi |\varphi_i|^2 \quad (4.3)$$

for any $\varphi_i \in V_i$ ($i \in \mathcal{I}_1 \cup \mathcal{I}_2$) and $z \in [a, b]$. (4.3) is a straightforward consequence of Lemma 4.1(i). (4.3) can also be proved without using the interpolation inequality (as in (i)) by adapting Lemma 1 of [37] or Lemma 1 of [15] to our setting.

Let K_1 be the following positive constant

$$K_1 := 1 + P_2 Q_2 + \max\{P_1 Q_1, P_2\} + c_\xi \left(\frac{3\hat{c}^2 M_{\eta_r}}{2} \right)^2 + c_\xi \hat{c}^4 D_3^2. \quad (4.4)$$

The constant K_1 is dependent on the material parameters explicitly shown in (4.4), but is independent of the solution and of the length of the time interval.

Theorem 4.2 (Positivity and L^∞ -Estimates). *Let the triple (u, v_4, s) as in Definition 3.1 satisfy the assumptions (A)–(C2). Then the following statements hold:*

- (i) (Positivity) $u_\ell(t) + \lambda_\ell(t) \geq 0$ in $\mathbb{V}_\ell$ ($\ell \in \mathcal{I}_1 \cup \mathcal{I}_2$) for all $t \in S_\delta$.
- (ii) (L^∞ -estimates) Let $\ell \in \mathcal{I}_1 \cup \mathcal{I}_2$ be arbitrarily fixed. There exists a constant $k_\ell > 0$ (see (3.27)) such that $u_\ell(t) + \lambda_\ell(t) \leq k_\ell$ in V_ℓ ($\ell \in \mathcal{I} - \{4\}$) for all $t \in S_\delta$.
- (iii) (Localization of the interface)

$$s_0 \leq s(t) \leq s_0 + \delta M_{\eta_r} \quad \text{for all } t \in S_\delta, \text{ where } M_{\eta_r} \text{ is given in (3.26).}$$

- (iv) (Positivity and boundedness of v_4 at $\Gamma(t)$)

$$0 < \hat{u}_{40} \leq v_4(t) \leq \hat{u}_{40} + \delta M_{\eta_r} \quad \text{for all } t \in S_\delta.$$

Proof. The key idea of dealing with (i) and (ii) is to choose appropriate test functions $\varphi \in \mathbb{V}$ in the weak formulation (3.32). We prove (i) and (ii) simultaneously by following the next steps:

- (Step 1) Get L^∞ -estimates on u_1, u_2 and u_3 (thus C_η becomes independent of u_1);
- (Step 2) Show the positivity of u_1, u_2 and u_3 ;
- (Step 3) Show the positivity of u_5 and u_6 ;
- (Step 4) Get L^∞ -estimates on u_5 and u_6 .

We adopt this strategy because of the presence of the term $-\eta_r(1)\varphi_1(1) - \eta_r(1)\varphi_3(1) + \eta_r(1)\varphi_5(1)$ at the r.h.s. of the weak formulation, while η_r has the properties stated in (2.6), (A) and (B). Let k_i ($i \in \mathcal{I}$) be as in (3.27). We show that these values are L^∞ -estimates that we are looking for.

Step 1: We start by looking for L^∞ -estimates of u_1 and u_2 . We put in (3.32) the test function $\varphi \in ((u_1 + \lambda_1 - k_1)^+, (u_2 + \lambda_2 - k_2)^+, 0, 0, 0)^t \in \mathbb{V}$. We therefore have

$$\begin{aligned} \frac{s}{2} \frac{d}{dt} |\varphi|^2 + \frac{1}{s} \sum_{i=1}^2 (D_i \varphi_{i,y}, \varphi_{i,y}) &\leq -[\eta_\Gamma + s'(u_1(1) + \lambda_1)] \varphi_1(1) \\ &\quad - s'(u_2(1) + \lambda_2) \varphi_2(1) + sP_1(Q_1 \varphi_2 - \varphi_1 + Q_1 k_2 - k_1, \varphi_1) \\ &\quad - sP_2(Q_2 \varphi_2 - \varphi_1 + Q_2 k_2 - k_1, \varphi_2) + s' \sum_{i=1}^2 (y \varphi_{i,y}, \varphi_i). \end{aligned} \quad (4.5)$$

Divide (4.5) by s and integrate by parts $\frac{s'}{s} \sum_{i=1}^2 (y \varphi_{i,y}, \varphi_i)$. By (C2), we obtain:

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} |\varphi|^2 + \frac{1}{s^2} \sum_{i=1}^2 (D_i \varphi_{i,y}, \varphi_{i,y}) + \frac{s'}{s} |\varphi(1)|^2 \\ \leq -\frac{\eta_\Gamma}{s} \varphi_1(1) - \frac{s'}{s} (k_1 \varphi_1(1) + k_2 \varphi_2(1)) + \max\{P_1 Q_1, Q_2\} |\varphi|^2 + \frac{s'}{s} |\varphi(1)|^2 - \frac{s'}{s} |\varphi|^2. \end{aligned}$$

Canceling the term $\frac{s'}{s} |\varphi(1)|^2$ and using the positivity of φ_1 , φ_2 and η_Γ , we are led to the inequality

$$\frac{1}{2} \frac{d|\varphi|^2}{dt} + \frac{1}{s^2} \sum_{i=1}^2 \|\sqrt{D_i} \varphi_i\|^2 \leq K_1 \sum_{i=1}^2 |\varphi_i|^2. \quad (4.6)$$

Applying Gronwall's inequality we obtain $u_i(t) + \lambda_i(t) \leq k_i$ ($i \in \{1, 2\}$) for all $t \in S_\delta$. To complete Step 1, we still need to estimate u_3 from above. For this purpose, let us choose $\varphi = (0, 0, (u_3 + \lambda_3 - k_3)^+, 0, 0)^t \in \mathbb{V}$, i.e. $\varphi_3 := (u_3 + \lambda_3 - k_3)^+ \in V_3$. By means of this test function, we obtain

$$\begin{aligned} (L-s)(u_3 + \lambda_3)_t, \varphi_3 + \frac{1}{L-s} D_3(u_{3,y}, \varphi_{3,y}) + \frac{D_3}{L-s} |\varphi_3(1)| \\ = \frac{D_3}{L-s} |\varphi_3(1)| - [\eta_\Gamma - s'(u_3(1) + \lambda_3)] \varphi_3(t) + (L-s) S_{3,\text{diss}}(u_{3,\text{eq}} - (u_3 + \lambda_3), \varphi_3) + s'((2-y)u_{3,y}, \varphi_3). \end{aligned} \quad (4.7)$$

Dividing by $L-s$ and integrating afterwards by parts the expression $\frac{s'}{2(L-s)}((2-y)\varphi_{3,y}, \varphi_3)$, we have

$$\begin{aligned} \frac{1}{2} \frac{d|\varphi_3|^2}{dt} + \frac{1}{(L-s)^2} D_3 \|\varphi_3\|^2 = \frac{D_3}{(L-s)^2} |\varphi_3(1)|^2 - \frac{\eta_\Gamma}{L-s} \varphi_3(1) + \frac{s'}{L-s} (\varphi_3(1) + k_3) \varphi_3(1) \\ + S_{3,\text{diss}}(u_{3,\text{eq}} - k_3 - \varphi_3, \varphi_3) + \frac{s'(|\varphi_3(1)|^2 + |\varphi_3|^2)}{2(L-s)}. \end{aligned} \quad (4.8)$$

By (C1), we obtain

$$\begin{aligned} \frac{1}{2} \frac{d|\varphi_3|^2}{dt} + \frac{1}{(L-s)^2} D_3 \|\varphi_3\|^2 \leq \left[\frac{D_3}{(L-s)^2} + \frac{3s'}{2(L-s)} \right] |\varphi_3(1)|^2 + \frac{s'}{2} |\varphi_3|^2 \\ \leq \xi \frac{\|\varphi_3\|^2}{(L-s)^2} + \left[c_\xi \left[\hat{c}^2 \left(\frac{D_3}{(L-s)^2} + \frac{3s'}{2(L-s)} \right) (L-s)^{2\theta} \right]^{\frac{1}{1-\theta}} + \frac{s'}{2(L-s)} \right] |\varphi_3|^2. \end{aligned}$$

Via Gronwall's inequality we have that $u_3 + \lambda_3 \leq k_3$ for all $t \in S_\delta$, provided that $s' \in L^2(S_\delta)$. This is satisfied since for given u_1 the reaction rate η_Γ stays bounded, i.e. $s' \in L^\infty(S_\delta)$.

Until now we have shown the boundedness of u_1 and u_2 without requiring the boundedness of η_Γ . The boundedness of u_3 needs that of s' , and hence, η_Γ has to be bounded for fixed u_1 . The positivity of η_Γ is necessary in each step.

Step 2: We continue with proving the positivity property of u_1 and u_2 . Setting $\varphi := (-(u_1 + \lambda_1)^-, -(u_2 + \lambda_2)^-, 0, 0, 0)^t \in \mathbb{V}$, i.e. $\varphi_i := -(u_i + \lambda_i)^- \in V_i$ ($i \in \{1, 2\}$), we get:

$$\begin{aligned} \frac{s}{2} \frac{d|\varphi|^2}{dt} + \frac{1}{s} \sum_{i=1}^2 \|D_i \varphi_i\|^2 = -\eta_\Gamma \varphi_1(1) + s' |\varphi(1)|^2 + sP_1(Q_1(u_2 + \lambda_2), \varphi_1) - sP_1|\varphi_1|^2 - sP_2 Q_2(u_2 + \lambda_2, \varphi_2) \\ + sP_2(u_1 + \lambda_1, \varphi_2) + s' \sum_{i=1}^2 (y \varphi_{i,y}, \varphi_i). \end{aligned} \quad (4.9)$$

Noting that $\pm \eta_{\Gamma}(u_1(1) + \lambda_1)^{-} = 0$ and dividing the expression (4.9) by s , we obtain

$$\begin{aligned} \frac{1}{2} \frac{d|\varphi|^2}{dt} + \frac{1}{s^2} \sum_{i=1}^2 \|D_i \varphi_i\|^2 &\leq \frac{s'}{s} |\varphi(1)|^2 - P_1 |\varphi|^2 - P_2 Q_2 |\varphi_2|^2 + \min\{P_1 Q_1, P_2\} |\varphi|^2 + \frac{s'}{2s} \sum_{i=1}^2 (|\varphi_i(1)|^2 - |\varphi_i|^2) \\ &\leq \frac{3s'}{2s} |\varphi(1)|^2 + K_1 |\varphi|^2 \leq \xi \frac{\|\varphi\|^2}{s^2} + 2K_1 |\varphi|^2. \end{aligned} \quad (4.10)$$

Let $\xi \in]0, \min\{D_1, D_2\}]$. Gronwall's inequality shows the positivity property. Finally, we focus on showing the positivity of u_3 . We obtain this property as follows: With $\varphi := (0, 0, -(u_3 + \lambda_3)^{-}, 0, 0)^t \in \mathbb{V}$ or $\varphi_3 := -(u_3 + \lambda_3)^{-} \in V_3$, we are led to

$$\begin{aligned} \frac{L-s}{2} \frac{d}{dt} |\varphi_3|^2 + \frac{1}{L-s} \|\sqrt{D_3} \varphi_3\|^2 &= -\eta_{\Gamma} \varphi_3(1) - s' |\varphi_3(1)|^2 \\ &\quad + \frac{D_3}{L-s} |\varphi(1)|^2 + (L-s) S_{3,\text{diss}}[(u_{3,\text{eq}}, \varphi_3) + |\varphi_3|^2] + \frac{s'}{2} (|\varphi_3(1)|^2 + |\varphi_3|^2). \end{aligned} \quad (4.11)$$

Note that $-\eta_{\Gamma} \varphi_3(1) - \frac{s'}{2} |\varphi_3(1)|^2 \leq 0$ and $(L-s) S_{3,\text{diss}}(u_{3,\text{eq}}, \varphi_3) \leq 0$. Now, we employ again the interpolation and Young inequalities in (4.11) to obtain

$$\frac{1}{2} \frac{d}{dt} |\varphi_3|^2 + \frac{D_3}{(L-s)^2} \|\varphi_3\|^2 \leq \xi \frac{\|\varphi_3\|^2}{(L-s)^2} + \left(K_1 + \frac{s'}{2}\right) |\varphi_3|^2. \quad (4.12)$$

By $\xi \in]0, D_3[$ and the use of Gronwall's inequality, we complete this step.

Step 3: We recall here the arguments from Step 2. Since the proof is similar, we do not repeat it. Our choice of test function concerning this case is $\varphi = (0, 0, 0, -(u_5 + \lambda_5)^{-}, -(u_6 + \lambda_6)^{-})^t \in \mathbb{V}$. No additional restrictions on the model parameters are needed.

Step 4: We choose as test function $\varphi := (0, 0, 0, (u_5 + \lambda_5 - k_5(t+1))^+, (u_6 + \lambda_6 - k_6(t+1))^+)^t \in \mathbb{V}$. Assume also $\lambda_5 \in W^{1,\infty}(S_T)$ and take $k_6 \geq |\lambda_{5,t}|_{\infty}$. We have

$$\begin{aligned} \frac{s}{2} \frac{d}{dt} |\varphi_5|^2 + \frac{L-s}{2} \frac{d}{dt} |\varphi_6|^2 + \frac{D_5}{s} \|\varphi_5\|^2 + \frac{D_6}{L-s} \|\varphi_6\|^2 &\leq (L-s)(\lambda_{5,t} - k_6, \varphi_6) + s'(y u_{5,y}, \varphi_5) + s'((2-y) u_{6,y}, \varphi_6) \\ &\leq \frac{s'}{2} |\varphi_5(1)|^2 + \frac{s'}{2} |\varphi_6|^2 - \frac{s'}{2} |\varphi_5|^2. \end{aligned}$$

Using the interpolation inequality, the latter expression leads to

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} (s |\varphi_5|^2 + (L-s) |\varphi_6|^2) + \frac{D_5}{s} \|\varphi_5\|^2 + \frac{D_6}{L-s} \|\varphi_6\|^2 &\leq \frac{s'}{2} \|\varphi_5\| |\varphi_5| + \frac{s'}{2} |\varphi_6|^2 + \frac{s'}{2} |\varphi_5|^2 - \frac{s'}{2} |\varphi_5|^2 \\ &\leq \frac{D_5}{2s} \|\varphi_5\|^2 + \frac{|s'|^2 s}{2D_5} |\varphi_5|^2 + \frac{s'}{2(L-s)} ((L-s) |\varphi_6|^2). \end{aligned}$$

Then, we get

$$\frac{1}{2} \frac{d}{dt} (s |\varphi_5|^2 + (L-s) |\varphi_6|^2) + \frac{D_5}{2s} \|\varphi_5\|^2 + \frac{D_6}{2(L-s)} \|\varphi_6\|^2 \leq \frac{|s'|^2}{2D_5} (s |\varphi_5|^2) + \frac{s'}{2(L-s)} ((L-s) |\varphi_6|^2). \quad (4.13)$$

Gronwall's inequality shows that $u_5(t) + \lambda_5(t) \leq k_5(t+1)$ and $u_6(t) + \lambda_6 \leq k_6(t+1)$ for all $t \in S_{\delta}$ a.e. $y \in [a, b]$.

Steps 1–4 complete the proof of (i) and (ii). The definitions of s' and v'_4 together with the statement (ii) prove (iii) and (iv). $\square$

Lemma 4.3 (Energy Estimates). Assume that (A)–(C2) hold and let the triple (u, v_4, s) be as in Definition 3.1. The following statements hold a.e. in S_{δ} :

$$|u(t) + \lambda(t)|^2 \leq \alpha(t) \exp\left(\int_0^t \beta(\tau) d\tau\right); \quad (4.14)$$

$$\int_0^t \|u(\tau) + \lambda(\tau)\|^2 d\tau \leq d_0^{-1} \alpha(t) \exp\left(\int_{t_0}^t \beta(\tau) d\tau\right), \quad (4.15)$$

where

$$d_0 := \min\left\{\min_{i \in \mathcal{I}_1} \frac{s_0 D_i}{L^2 m_0}, \min_{i \in \mathcal{I}_2} \frac{(L-L_0) D_i}{(L-s_0)^2 m_0}\right\}, \quad m_0 \text{ as in (3.24)}. \quad (4.16)$$

The factors $a(t)$, $\alpha(t)$ and $\beta(t)$ are given by

$$a(t) := \frac{s'(t)}{2} + \frac{(s'(t))^2}{2} + \frac{(L-s(t))^2 K_2}{2}, \quad (4.17)$$

$$\alpha(t) := |\varphi(0)|^2 + \frac{2}{m_0} \int_0^t a(\tau) d\tau, \quad (4.18)$$

$$\beta(t) := \left[\frac{s'(t)}{2} + K_2 \left(2 + \frac{D_3}{L-s(t)} + \frac{s'(t)}{2} \right)^2 \right] \frac{1}{m_0}, \quad (4.19)$$

whereas

$$K_2 := 1 + (S_{3,\text{diss}}|u_{3,\text{eq}}|_\infty)^2 + \frac{LP_1 Q_1}{2} + c_\xi \hat{c}^4. \quad (4.20)$$

Furthermore, we have

$$u \in L^2(S_\delta, \mathbb{V}), \quad u_{,t} \in L^2(S_\delta, \mathbb{V}^*), \quad u \in C(\bar{S}_\delta, \mathbb{H}). \quad (4.21)$$

Proof. Inserting the test function $\varphi := u + \lambda \in \mathbb{V}$ in the variational formulation (3.32), we find the energy estimates (4.14) and (4.15) in the following way: By

$$\frac{s}{2} \sum_{i \in \mathcal{I}_1} \frac{d}{dt} |\varphi_i(t)|^2 + \frac{L-s}{2} \sum_{i \in \mathcal{I}_2} \frac{d}{dt} |\varphi_i(t)|^2 + a(s, \varphi, \varphi) + e(s', \varphi, \varphi) = b_f(\varphi, s, \varphi) + h(s', \varphi, y, \varphi) \quad \text{for } t \in S_\delta, \quad (4.22)$$

it yields

$$\begin{aligned} & \frac{s}{2} \sum_{i \in \mathcal{I}_1} \frac{d}{dt} |\varphi_i(t)|^2 + \frac{L-s}{2} \sum_{i \in \mathcal{I}_2} \frac{d}{dt} |\varphi_i(t)|^2 + \frac{s_0}{s^2} \sum_{i \in \mathcal{I}_1} D_i \|\varphi_i\|^2 + \frac{L-L_0}{(L-s)^2} \sum_{i \in \mathcal{I}_2} D_i \|\varphi_i\|^2 \\ & \leq -\eta_r \varphi_1(1) - s'(|\varphi_1(1)|^2 + |\varphi_2(1)|^2) - \eta_r \varphi_3(1) + s'|\varphi_3(1)|^2 + \eta_r |\varphi_5(1)| + \frac{D_3}{L-s} |\varphi_3(1)|^2 \\ & \quad + sP_1 Q_1 (\varphi_2, \varphi_1) - sP_1 |\varphi_1|^2 - sP_2 Q_2 |\varphi_2|^2 + sP_2 (\varphi_1, \varphi_2) + (L-s)S_{3,\text{diss}}|u_{3,\text{eq}}|_\infty |\varphi_3| - (L-s)S_{3,\text{diss}}|\varphi_3|^2 \\ & \quad + \frac{s'}{2} \sum_{i \in \mathcal{I}_1} (|\varphi_i(1)|^2 - |\varphi_i|^2) + \frac{s'}{2} \sum_{i \in \mathcal{I}_2} (|\varphi_i(1)|^2 + |\varphi_i|^2) \\ & \leq s'|\varphi_3(1)|^2 + s'|\varphi_5(1)| + \frac{D_3}{L-s} |\varphi_3(1)|^2 + \frac{LP_1 Q_1}{2} (|\varphi_1|^2 + |\varphi_2|^2) \\ & \quad + \frac{LP_2}{2} (|\varphi_1|^2 + |\varphi_2|^2) + (L-s)S_{3,\text{diss}}|u_{3,\text{eq}}|_\infty |\varphi_3| + \frac{s'}{2} \sum_{i \in \mathcal{I}_1 \cup \mathcal{I}_2} |\varphi_i(1)|^2 + \frac{s'}{2} \sum_{i \in \mathcal{I}_2} |\varphi_i|^2 \\ & \leq \frac{(s')^2}{2} + \frac{[(L-s)S_{3,\text{diss}}|u_{3,\text{eq}}|_\infty]^2}{2} + \left(1 + \frac{D_3}{L-s} + \frac{s'}{2}\right) \sum_{i \in \mathcal{I}_1 \cup \mathcal{I}_2} |\varphi_i(1)|^2 + \left(\frac{LP_1 Q_1}{2} + \frac{s'}{2} \frac{LP_2}{2}\right) \sum_{i \in \mathcal{I}_1 \cup \mathcal{I}_2} |\varphi_i|^2. \end{aligned} \quad (4.23)$$

We employ the interpolation inequality to bound the term

$$\left(1 + \frac{D_3}{L-s} + \frac{s'}{2}\right) \sum_{i \in \mathcal{I}_1 \cup \mathcal{I}_2} |\varphi_i(1)|^2$$

from above by

$$\begin{aligned} & \left(1 + \frac{D_3}{L-s} + \frac{s'}{2}\right) s^{2\theta} \sum_{i \in \mathcal{I}_1} \hat{c}^2 \left(\frac{\|\varphi_i\|}{s} \right)^{2\theta} |\varphi_i|^{2(1-\theta)} + \left(1 + \frac{D_3}{L-s} + \frac{s'}{2}\right) (L-s)^{2\theta} \sum_{i \in \mathcal{I}_2} \hat{c}^2 \left(\frac{\|\varphi_i\|}{L-s} \right)^{2\theta} |\varphi_i|^{2(1-\theta)} \\ & \leq \xi \sum_{i \in \mathcal{I}_1} \frac{\|\varphi_i\|^2}{s^2} + \xi \sum_{i \in \mathcal{I}_2} \frac{\|\varphi_i\|^2}{(L-s)^2} + c_\xi \sum_{i \in \mathcal{I}_1 \cup \mathcal{I}_2} \left[1 + \frac{D_3}{L-s} + \frac{s'}{2} \right]^{\frac{1}{1-\theta}} \left[s^{\frac{2\theta}{1-\theta}} + (L-s)^{\frac{2\theta}{1-\theta}} \right] |\varphi_i|^2. \end{aligned} \quad (4.24)$$

Set $\theta = \frac{1}{2}$. We then obtain

$$\begin{aligned} & \frac{s}{2} \sum_{i \in \mathcal{I}_1} \frac{d}{dt} |\varphi_i(t)|^2 + \frac{L-s}{2} \sum_{i \in \mathcal{I}_2} \frac{d}{dt} |\varphi_i(t)|^2 + \frac{s_0}{s^2} \sum_{i \in \mathcal{I}_1} D_i \|\varphi_i\|^2 + \frac{L-L_0}{(L-s)^2} \sum_{i \in \mathcal{I}_2} D_i \|\varphi_i\|^2 \\ & \leq \xi \sum_{i \in \mathcal{I}_1} \frac{\|\varphi_i\|^2}{s^2} + \xi \sum_{i \in \mathcal{I}_2} \frac{\|\varphi_i\|^2}{(L-s)^2} + a(t) + \beta(t) |\varphi(t)|^2. \end{aligned} \quad (4.25)$$

Set $\xi \in]0, \min_{i \in \mathcal{I}_1 \cup \mathcal{I}_2} \{s_0 D_i, (L-L_0) D_i\}]$. In order to be able to apply Gronwall's inequality to the term $\frac{s}{2} \sum_{i \in \mathcal{I}_1} \frac{d}{dt} |\varphi_i(t)|^2 + \frac{L-s}{2} \sum_{i \in \mathcal{I}_2} \frac{d}{dt} |\varphi_i(t)|^2$, we proceed as in Step 4 from the previous proof, eventually tuning the structure of $\beta(t)$. We obtain then the estimate (4.14), where the factors $a(t)$, $\alpha(t)$ and $\beta(t)$ are given as in (4.17)–(4.19). Choose d_0 as in (4.16) and note also that $d_0 > 0$. The proof of (4.15) relies on (4.14) and integration by parts. To get (4.21), the Bochner measurability and integrability of u and $u_{,t}$ need to be discussed in the similar way as in Lemma 26.1 in [38, pp. 395–396] and Remark 27.1 in [38, p. 405]. If $u \in L^2(S_\delta, \mathbb{V})$ and $u_{,t} \in L^2(S_\delta, \mathbb{V}^*)$, then $u \in \mathbb{W}_2^1(S_\delta; \mathbb{V}, \mathbb{H})$. The embedding $\mathbb{W}_2^1(S_\delta; \mathbb{V}, \mathbb{H}) \hookrightarrow C(\bar{S}_\delta; \mathbb{H})$ shows the second part of (4.21). $\square$

4.2. Proof of Theorem 3.4

The proof relies on the use of Banach's fixed-point principle.

Proof of Theorem 3.4. The set

$$M(S_\delta) := \{r \in W^{1,4}(S_\delta): r(t) \in [s_0, M_{\eta_\Gamma} \delta + s_0] \text{ for all } t \in S_\delta, r'(t) \geq 0 \text{ a.e. } t \in S_\delta, |r'|_{L^4(S_\delta)} \leq \delta M_{\eta_\Gamma}\} \quad (4.26)$$

equipped with the metric

$$\rho(r_1, r_2) = |r'_2 - r'_1|_{L^4(S_\delta)} \quad \text{for all } r_1, r_2 \in M(S_\delta)$$

is a non-empty closed subset of $W^{1,4}(S_\delta)$. $(M(S_\delta), \rho)$ forms a complete metric space. We show that the map

$$\mathcal{T} : M(S_\delta) \rightarrow W^{1,4}(S_\delta), \quad (4.27)$$

$$\mathcal{T} : s \mapsto (u, v_4) \quad \text{cf. (3.32), (3.12)} \quad (\text{see also Theorem 3.2})$$

$$\mapsto r \quad \text{with } r'(t) = \psi_\Gamma(1, t), \quad r(0) = r_0, \quad (4.28)$$

is a strictly contractive self-map, provided

$$0 < \delta \leq \delta_0 \quad (\text{see (4.35) for the choice of } \delta_0). \quad (4.29)$$

By Theorem 3.2, $\mathcal{T}$ does indeed map $M(S_\delta)$ into $W^{1,4}(S_\delta)$. Because of $r(t) = s_0 + \int_0^t \psi_\Gamma(1, \tau) d\tau$, yields $r' \in L^4(S_\delta)$. By $r \in W^{1,\infty}(S_\delta) \hookrightarrow W^{1,p}(S_\delta)$ for all $1 \leq p \leq \infty$, it results that $r \in W^{1,4}(S_\delta)$. By (3.12) and the positivity of concentrations, we get that $r' \geq 0$ a.e. in S_δ . Furthermore, the L^∞ -estimates on concentrations ensure that $|r'|_{L^4(S_\delta)} \leq M_{\eta_\Gamma} \delta$.

We show: $\mathcal{T}$ is strictly contractive. To this end, let $s_i \in M(S_\delta)$, $i = 1, 2$, and $r_i = \mathcal{T}(s_i)$, where

$$\mathcal{T} : s_i \mapsto (u_i, v_{4i}) \mapsto r_i, \quad i = 1, 2.$$

Set $w := w^2 - w^1$, where $w := (w_1, w_2, w_3, w_5, w_6)^t$ with $w_i = w_i^2 - w_i^1$ and $w^i := (w_{i1}, w_{i2}, w_{i3}, w_{i5}, w_{i6})^t$ ($i \in \{1, 2\}$). Furthermore, let $\lambda_i := (\lambda_{i1}, \lambda_{i2}, \lambda_{i3}, \lambda_{i5}, \lambda_{i6})^t$, $w_{ij} := u_{ij} - \lambda_{ij}$ ($i \in \{1, 2\}$, $j \in \mathcal{I}_1 \cup \mathcal{I}_2$). Furthermore, we set $\Delta \psi_\Gamma(t) := \psi_\Gamma(s_2(t), t) - \psi_\Gamma(s_1(t), t)$, $\Delta \eta_\Gamma(t) := \eta_\Gamma(s_2(t), t) - \eta_\Gamma(s_1(t), t)$, $\Delta s(t) := s_2(t) - s_1(t)$, $\Delta s'(t) := s'_2(t) - s'_1(t)$, $\Delta r(t) := r_2(t) - r_1(t)$, $\Delta r'(t) := r'_2(t) - r'_1(t)$ and $\Delta v_4 = v_{41} - v_{42}$.

The key idea of the proof relies on the fact that $\mathcal{T}$ improves integrability, i.e. $\mathcal{T} : W^{1,2}(S_\delta) \rightarrow W^{1,4}(S_\delta)$.

By (A) and (3.12), we note that

$$\int_{S_\delta} |\Delta r'(\tau)|^4 d\tau = \int_{S_\delta} |\Delta \psi_\Gamma(\tau)|^4 d\tau \leq C_\eta \int_{S_\delta} |w(1, \tau)|^4 d\tau.$$

Applying the interpolation inequality¹ (4.1) with $\theta = \frac{1}{2}$, we get

$$\int_{S_\delta} |\Delta r'(\tau)|^4 d\tau \leq C_\eta \hat{c}^4 \sup_{t \in \bar{S}_\delta} |w(t)|^2 \int_{S_\delta} \|w(\tau)\|^2 d\tau. \quad (4.30)$$

¹ The same argument shows that Δv_4 belongs to $W^{1,4}(S_\delta)$.

We want to bound the quantities $\sup_{t \in S_\delta} |w(t)|^2$ and $\int_{S_\delta} \|w(\tau)\|^2 d\tau$ from above. To this end, we subtract the variational formulation (3.32) written for w^2 from that one written for w^1 , where in both expressions we use the test function $w = w^2 - w^1 \in \mathbb{V}$. It yields

$$\begin{aligned} & s_2 \sum_{i \in \mathcal{I}_1} \frac{1}{2} \frac{d}{dt} |w_i(t)|^2 + (L - s_2) \sum_{i \in \mathcal{I}_2} \frac{1}{2} \frac{d}{dt} |w_i(t)|^2 + \frac{1}{s_2} \sum_{i \in \mathcal{I}_1} \|\sqrt{D_i} w_i\|^2 + \frac{1}{(L - s_2)} \sum_{i \in \mathcal{I}_2} \|\sqrt{D_i} w_i\|^2 \\ & \leq -\Delta s \sum_{i \in \mathcal{I}_1} (w_{1i,t}, w_i) + \Delta s \sum_{i \in \mathcal{I}_2} (w_{1i,t}, w_i) + \frac{1}{s_2} \sum_{i \in \mathcal{I}_1} |\sqrt{D_i} w_i(1)|^2 \\ & \quad + \frac{1}{L - s_2} \sum_{i \in \mathcal{I}_2} |\sqrt{D_i} w_i(1)|^2 + \frac{\Delta s}{s_1 s_2} \sum_{i \in \mathcal{I}_1} D_i (w_{1i,y}, w_{i,y}) - \frac{\Delta s}{(L - s_1)(L - s_2)} \sum_{i \in \mathcal{I}_2} D_i (w_{1i,y}, w_{i,y}) \\ & \quad - e(s'_1, w_1, w) + e(s'_2, w_2, w) + b_f(w_2, s_2, w) - b_f(w_1, s_1, w) + h(s'_2, w_{2,y}, w) - h(s'_1, w_{1,y}, w) \\ & \leq \sum_{\ell=1}^5 J_\ell, \end{aligned} \quad (4.31)$$

where we are given

$$\begin{aligned} J_1 &:= -\Delta s \sum_{i \in \mathcal{I}_1} (w_{1i,t}, w_i) + \Delta s \sum_{i \in \mathcal{I}_2} (w_{1i,t}, w_i), \\ J_2 &:= \frac{\Delta s}{s_1 s_2} \sum_{i \in \mathcal{I}_1} (D_i w_{1i,y}, w_{i,y}) - \frac{\Delta s}{(L - s_1)(L - s_2)} \sum_{i \in \mathcal{I}_2} (D_i w_{1i,y}, w_{i,y}), \\ J_3 &:= b_f(w_2, s_2, w) - b_f(w_1, s_1, w), \\ J_4 &:= e(s'_1, w_1, w) - e(s'_2, w_2, w) + \frac{1}{s_2} \sum_{i \in \mathcal{I}_1} |\sqrt{D_i} w_i(1)|^2 + \frac{1}{L - s_2} \sum_{i \in \mathcal{I}_2} |\sqrt{D_i} w_i(1)|^2, \\ J_5 &:= h(s'_2, w_{2,y}, w) - h(s'_1, w_{1,y}, w). \end{aligned}$$

To estimate J_ℓ ($\ell \in \{1, \dots, 5\}$), we repeatedly use Lemma 4.1 and Theorem 4.2 together with the application of Cauchy-Schwarz's and Young's inequalities. To shorten further the notation, we employ the positive constant

$$K_3 := 1 + c_\xi \sum_{i \in \mathcal{I}_1 \cup \mathcal{I}_2} D_i^2 + \frac{P_1 Q_1 + P_2}{2} + k_3^2 + S_{3,\text{diss}} |u_{3,\text{eq}}|_\infty^2 + (P_2 k_1)^2 + (P_1 Q_1 k_2)^2 + c_\xi (1 + \bar{k}^2) + c_\xi c_{\bar{\xi}} c^2 \hat{c}^2. \quad (4.32)$$

It is worth noticing that K_3 is bounded above, invariant with respect to t and depends on the choice of L , L_0 , s_0 , c_ξ , $c_{\bar{\xi}}$, $\hat{c}$, θ , k_i and D_i ($i \in \mathcal{I}_1 \cup \mathcal{I}_2$).

We proceed with finding out an upper margin of $J := \sum_{\ell=1}^5 |J_\ell|$. Firstly, for any $\xi > 0$, we have

$$\begin{aligned} \int_0^t |J_1| d\tau & \leq \left| \int_0^t \Delta s \sum_{i \in \mathcal{I}_1} (w_{1i,t}, w_i) d\tau \right| + \left| \int_0^t \Delta s \sum_{i \in \mathcal{I}_2} (w_{1i,t}, w_i) d\tau \right| \\ & \leq |\Delta s|_{L^\infty(S_t)} \int_0^t \sum_{i \in \mathcal{I}_1 \cup \mathcal{I}_2} \|w_i\| \|w_{1i,t}\|_{\mathbb{V}^*} d\tau \\ & \leq \xi \sum_{i \in \mathcal{I}_1} \int_0^t \left(\frac{D_i}{s_2} \|w_i\|^2 + \frac{s_2}{4\xi D_i} |\Delta s|_{L^\infty(S_t)}^2 |w_{1i,t}|_{\mathbb{V}^*}^2 \right) d\tau \\ & \quad + \xi \sum_{i \in \mathcal{I}_2} \int_0^t \left(\frac{D_i}{L - s_2} \|w_i\|^2 + \frac{L - s_2}{4\xi D_i} |\Delta s|_{L^\infty(S_t)}^2 |w_{1i,t}|_{\mathbb{V}^*}^2 \right) d\tau. \end{aligned}$$

By Cauchy-Schwarz and the arithmetic-geometric means inequalities, we obtain

$$\begin{aligned} |J_2| & \leq \frac{|\Delta s|}{s_1 s_2} \sum_{i \in \mathcal{I}_1} D_i \|w_{1i}\| \|w_i\| + \frac{|\Delta s|}{(L - s_1)(L - s_2)} \sum_{i \in \mathcal{I}_2} D_i \|w_{1i}\| \|w_i\| \\ & \leq \xi \sum_{i \in \mathcal{I}_1} \frac{D_i \|w_i\|^2}{s_2^2} + \xi \sum_{i \in \mathcal{I}_2} \frac{D_i \|w_i\|^2}{(L - s_2)^2} + \frac{1}{4} \left(\sum_{i \in \mathcal{I}_1} \frac{D_i \|w_{1i}\|^2}{s_1^2 s_2} + \sum_{i \in \mathcal{I}_2} \frac{D_i \|w_{1i}\|}{(L - s_1)^2 (L - s_2)} \right) |\Delta s|^2 \\ & \leq \xi \sum_{i \in \mathcal{I}_1} \frac{D_i \|w_i\|^2}{s_2^2} + \xi \sum_{i \in \mathcal{I}_2} \frac{D_i \|w_i\|^2}{(L - s_2)^2} + \frac{K_4}{4} \left(\frac{1}{s_0^3} + \frac{1}{(L - L_0)^3} \right) \|w^1\|^2 |\Delta s|^2, \end{aligned}$$

$$|J_3| \leq \frac{|\Delta s|^2}{2} + \left[(P_1 Q_1 k_2)^2 + (P_2 k_1)^2 + \frac{P_1 Q_1 + P_2}{2} \right] (|w_1|^2 + |w_2|^2) \\ + \frac{|\Delta s|^2}{2} + S_{3,\text{diss}}^2 |u_{3,\text{eq}}|_{\infty}^2 |w_3|^2 + \frac{|\Delta s|^2}{2} + k_3^2 |w_3|^2 \leq \frac{3}{2} |\Delta s|^2 + K_3 |w|^2,$$

where K_3 is given by (4.32) and $K_4 := \sum_{i \in \mathcal{I}_1 \cup \mathcal{I}_2} D_i$. To bound $|J_4|$, we use (A) and the special structure of the boundary term $e(s', w_i, w)$. We obtain

$$|J_4| \leq |\Delta \eta_r| |w_1(1)| + s'_2 w_1(1)^2 + |\Delta s' k_1| |w_1(1)| + s'_2 w_1(1)^2 + |\Delta s' k_1| |w_2(1)| \\ + |\Delta \eta_r| |w_3(1)| + s'_2 w_3(1)^2 + |\Delta s' k_3| |w_3(1)| + |\Delta \eta_r| |w_5(1)| + \left(\frac{1}{s_0} + \frac{1}{L - L_0} \right) \sum_{i \in \mathcal{I}_1 \cup \mathcal{I}_2} D_i |w_i(1)|^2 \\ \leq \frac{3}{2} |\Delta \eta_r|^2 + \xi \sum_{i \in \mathcal{I}_1} \frac{D_i \|w_i\|^2}{s_2^2} + \xi \sum_{i \in \mathcal{I}_2} \frac{D_i \|w_i\|^2}{(L - s_2)^2} + K_3 |w|^2.$$

We split the term J_5 into two components J_{51} and J_{52} such that $J_5 = J_{51} + J_{52}$, where

$$J_{51} := s'_2 \sum_{i \in \mathcal{I}_1} (y w_{2i,y}, w_i) - s'_1 \sum_{i \in \mathcal{I}_1} (y w_{1i,y}, w_i), \\ J_{52} := s'_2 \sum_{i \in \mathcal{I}_2} ((2 - y) w_{2i,y}, w_i) - s'_1 \sum_{i \in \mathcal{I}_2} ((2 - y) w_{1i,y}, w_i).$$

It is easy to see that

$$|J_{51}| \leq |\Delta s'| \sum_{i \in \mathcal{I}_1} \|w_{2i}\| \|w_i\| + \frac{|s'_1|}{2} \sum_{i \in \mathcal{I}_1} (|w_i(1)|^2 + |w_i|^2) \leq |\Delta s'| \sum_{i \in \mathcal{I}_1} \|w_{2i}\| \|w_i\| + \frac{|s'_1|}{2} \sum_{i \in \mathcal{I}_1} (\|w_i\| \|w_i\| + |w_i|^2), \\ |J_{52}| \leq |\Delta s'| \sum_{i \in \mathcal{I}_1} \|w_{2i}\| \|w_i\| + \frac{|s'_1|}{2} \sum_{i \in \mathcal{I}_2} (\|w_i\| \|w_i\| + |w_i|^2).$$

Hence, it holds that

$$|J_5| \leq \frac{5}{2} |\Delta s'|^2 + \frac{1}{2} \|w^2\|^2 |w|^2 + \frac{1}{4} \sum_{i \in \mathcal{I}_1} \frac{D_i}{s_2} \|w_i\|^2 + \frac{1}{4} \sum_{i \in \mathcal{I}_1} \frac{D_i}{L - s_2} \|w_i\|^2 \\ + \frac{1}{4} \sum_{i \in \mathcal{I}_1} \frac{s_2}{D_i} |s'_1|^2 |w_i|^2 + \frac{1}{4} \sum_{i \in \mathcal{I}_1} \frac{L - s_2}{D_i} |s'_1|^2 |w_i|^2 + \frac{1}{2} \sum_{i \in \mathcal{I}_1 \cup \mathcal{I}_2} |s'_1|^2 |w_i|^2.$$

On the other hand, we have

$$\int_0^t \left(s_2 \sum_{i \in \mathcal{I}_1} \frac{1}{2} \frac{d}{dt} |w_i(t)|^2 + (L - s_2) \sum_{i \in \mathcal{I}_2} \frac{1}{2} \frac{d}{dt} |w_i(t)|^2 \right) d\tau \\ = -\frac{1}{2} \sum_{i \in \mathcal{I}_1} \int_0^t s'_2 |w_i(t)|^2 d\tau + \frac{1}{2} \sum_{i \in \mathcal{I}_2} \int_0^t s'_2 |w_i(t)|^2 d\tau + \frac{s_2(t)}{2} \sum_{i \in \mathcal{I}_1} |w_i(t)|^2 + \frac{L - s_2(t)}{2} \sum_{i \in \mathcal{I}_2} |w_i(t)|^2.$$

Hence, we obtain

$$\frac{s_2(t)}{2} \sum_{i \in \mathcal{I}_1} |w_i(t)|^2 + \frac{L - s_2(t)}{2} \sum_{i \in \mathcal{I}_2} |w_i(t)|^2 + \frac{1}{2s_2} \sum_{i \in \mathcal{I}_1} \int_0^t D_i \|w_i(\tau)\|^2 d\tau + \frac{1}{2(L - s_2)} \sum_{i \in \mathcal{I}_2} \int_0^t D_i \|w_i(\tau)\|^2 d\tau \\ \leq \frac{1}{2} \int_0^t |s'_2| |w| d\tau + \sum_{i=1}^5 \int_0^t |J_i| d\tau.$$

Then, putting $\xi = \frac{3}{8}$ and $D_0 := \min\{D_i: i \in \mathcal{I}_1 \cup \mathcal{I}_2\}$, we get

$$\frac{s_2(t)}{2} \sum_{i \in \mathcal{I}_1} |w_i(t)|^2 + \frac{L - s_2(t)}{2} \sum_{i \in \mathcal{I}_2} |w_i(t)|^2 + \frac{1}{8} \sum_{i \in \mathcal{I}_1} \int_0^t \frac{D_i}{s_2} \|w_i(\tau)\|^2 d\tau + \frac{1}{8} \sum_{i \in \mathcal{I}_2} \int_0^t \frac{D_i}{(L - s_2)} \|w_i(\tau)\|^2 d\tau \\ \leq \frac{1}{2} \int_0^t |s'_2| |w|^2 d\tau + \left(\frac{c_\xi L}{D_0} \int_0^t |w_{1,\tau}^1| d\tau + \frac{K_3}{s_0^3} \int_0^t \|w_{1i}\|^2 d\tau \right) |\Delta s|_{L^\infty(s_\tau)}$$

$$\begin{aligned}
& + \frac{3}{2} \int_0^t |\Delta s|^2 d\tau + \left(2K_3 + \frac{1}{2}\right) \int_0^t (1 + \|w^2\|^2) |w|^2 d\tau + \frac{3}{2} \int_0^t |\Delta \eta_I|^2 d\tau \\
& + \frac{5}{2} \int_0^t |\Delta s'|^2 d\tau + \left(\frac{L}{4D_0} + \frac{1}{2}\right) \int_0^t |s'_1|^2 |w|^2 d\tau.
\end{aligned}$$

Here, we put $\nu_0 := \min\{\frac{s_0}{2}, \frac{L-L_0}{2}\}$, $a(t) = 1 + |s'_2(t)| + \|w^2(t)\|^2 + |s'_1(t)|^2$, and

$$K_5 := 2K_3 + \frac{1}{2} + \frac{4L}{4D_0} + \frac{c_\xi L}{D_0} \int_0^\delta |w_{,\tau}|_{V^*}^2 d\tau + \frac{K_3}{s_0^3} \int_0^\delta \|w^1\|^2 d\tau. \quad (4.33)$$

Note that Lemma 4.3 implies $K_5 < \infty$. Furthermore, it holds that

$$\begin{aligned}
& \nu_0 |w(t)|^2 + \frac{D_0}{4L} \int_0^t \|w\|^2 d\tau \\
& \leq K_5 \int_0^t a(\tau) |w(\tau)|^2 d\tau + K_5 \delta \int_0^t |\Delta s'|^2 d\tau + \frac{3}{2} \int_0^t \left(\int_0^\tau |\Delta s'(p)| dp \right)^2 d\tau + \frac{3}{2} \int_0^t |\Delta \eta_I|^2 d\tau + \frac{5}{2} \int_0^t |\Delta s'|^2 d\tau. \quad (4.34)
\end{aligned}$$

Theorem 4.2(ii) implies that for some positive constant K_6 we have $|\Delta \eta_I(\tau)| \leq K_6 |w(\tau, 1)|$ for any $\tau \in S_t$. Therefore,

$$\nu_0 |w(t)|^2 + \frac{D_0}{8L} \int_0^t \|w\|^2 d\tau \leq K_7 \int_0^t a(\tau) |w(\tau)|^2 d\tau + K_7 \int_0^t |\Delta s'|^2 d\tau,$$

where $K_7 = K_5 + \frac{9}{2} K_6^2 \hat{c}^2 + K_5 \delta + \frac{3}{2} \delta^{\frac{3}{2}} + \frac{5}{2}$. Applying now Gronwall's inequality, we obtain

$$\nu_0 |w(\tau)|^2 + \frac{D_0}{8L} \int_0^t \|w\|^2 d\tau \leq \int_0^t K_7 |\Delta s'|^2 d\tau \exp\left(\int_0^t \frac{K_7}{\nu_0} a(\tau) d\tau\right)$$

so that

$$\begin{aligned}
& \int_{S_\delta} |r'(\tau)|^4 d\tau \leq C_\eta \hat{c}^4 \sup_{S_\delta} |w(t)|^2 \int_{S_\delta} \|w(\tau)\|^2 d\tau \\
& \leq C_\eta \hat{c}^4 \frac{8L}{\nu_0 D_0} \exp\left(\int_0^t \frac{K_7}{\nu_0} a(\tau) d\tau\right) \left(\int_0^t K_7 |\Delta s'|^2 d\tau\right)^2 \\
& \leq K_8 \delta \int_0^t |\Delta s'|^4 d\tau,
\end{aligned}$$

where $K_8 := C_\eta \hat{c}^4 \frac{1}{\nu_0} \frac{8L}{D_0} K_7^2 \exp(\int_0^t \frac{K_7}{\nu_0} a(\tau) d\tau)$. Choose now δ_0 such that

$$0 < \delta_0 < \frac{1}{K_8}. \quad (4.35)$$

This shows the strict contractivity of the fixed-point operator $\mathcal{T}$. $\square$

5. Illustration of CO₂ penetration in a concrete wall

We consider an 18 years old concrete wall made of Portland cement (CEM 1), whose chemistry and outdoor exposure conditions are described in Table 3.1 of [12]. The indicator test emphasizes a thin macroscopic front penetrating the material and separating carbonated from non-carbonated phases; see Fig. 1.1. We employ a FEM Galerkin scheme to approximate the weak solution to (P_I) . We proceed as follows: We immobilize the moving boundary and discretize the PDE system in space. Afterwards, we integrate the obtained stiff ODE system in time using MATLAB. The numerical procedure is explained in detail in Chapter 4 of [27], while *a priori* and *a posteriori* error estimates for the semi-discrete approximation are derived for the one-phase case in [26]. The plots in Figs. 5.1–5.2 show the solution of (P_I) . Observe that steep concentration

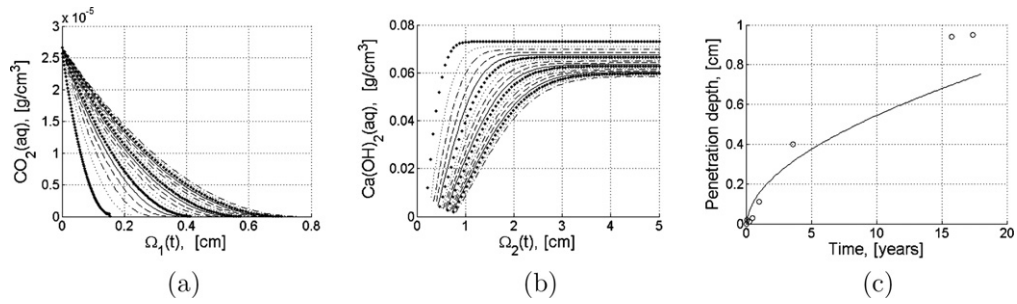


Fig. 5.1. (a) + (b) $\text{CO}_2(\text{aq})$ and $\text{Ca}(\text{OH})_2(\text{aq})$ profiles vs. space. Each curve refers to time $t = i$ years, $i \in \{1, \dots, 18\}$. (c) Interface position vs. the experimental points "o" after $T_{\text{fin}} = 18$ years of exposure.

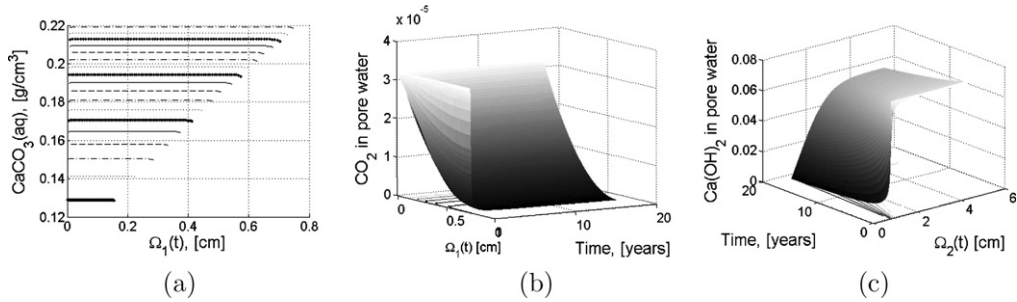


Fig. 5.2. (a) $\text{CaCO}_3(\text{aq})$ profiles vs. space. Each curve refers to time $t = i$ years, $i \in \{1, \dots, 18\}$. (b) + (c) Concentration of $\text{CO}_2(\text{aq})$ and $\text{Ca}(\text{OH})_2(\text{aq})$ vs. time and space.

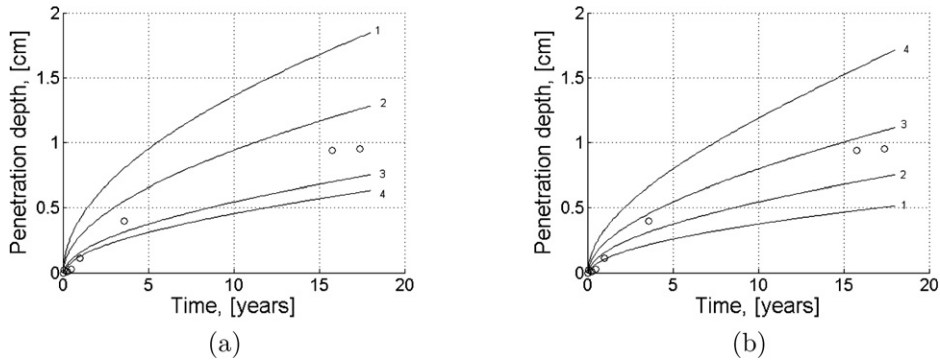


Fig. 5.3. (a) Interface position vs. the experimental points "o" when varying the reaction order $p = 1.5, 1.3, 1, 0.9$ while $q = 1$. (b) Interface position vs. the experimental points "o" when varying the effective dimensional diffusion coefficient of $\text{CO}_2(\text{g})$ as follows: $\frac{D_2}{2}$, D_2 , $2D_2$ and $4D_2$.

gradients arise near $\Gamma(t)$ (cf. Fig. 5.1(b), Fig. 5.2(c), e.g.) and the calculated interface position is in the experimental range, see Fig. 5.1(c) and Fig. 5.3. Furthermore, Fig. 5.2(a) shows a gradual increase in the concentration of $\text{CaCO}_3(\text{aq})$ within $\Omega_1(t)$. It visualizes the expansion of $\Omega_1(t)$ and also points out the shrinking of $\Omega_2(t)$. The results in Fig. 5.3 indicate a strong dependence of the penetration speed on the structure of the reaction rate $\tilde{\eta}_r$ and on the range of the effective diffusion coefficient of $\text{CO}_2(\text{g})$. Changing the partial reaction order p from 0.9 to 1.5 produces a significant increase of the reaction rate, which finally results in a higher penetration depth. The penetration depth obtained with $p = 1.5$ is at least twice bigger than that obtained for $p = 1$ (compare the curve 1 with the curve 4 in Fig. 5.3(a)). Alterations of the exponent q may lead to drastic changes in the penetration depth as well. An increase in the effective diffusivity of $\text{CO}_2(\text{g})$ produces a significant increase in the penetration depth. In Fig. 5.3(b), we observe that if $\text{CO}_2(\text{g})$ encounters difficulties to travel to the reaction zone, then the speed of this zone is correspondingly smaller. On the other hand, if the matrix has large pores, then a fast advancement of $\text{CO}_2(\text{g})$ molecules is to be expected.

6. Conclusions

We formulate a moving-boundary model to describe the penetration of a sharp-reaction interface in concrete. Results concerning the global existence and uniqueness of positive weak solutions to the proposed model are presented. A simulation example illustrates the typical behavior of active concentrations and interface penetration into a concrete wall. The

model shows qualitatively good results when the numerical solution is compared with measured penetration depth profiles. The setting can be extended (with minor modifications) to account for more reaction interfaces simultaneously penetrating an unsaturated reactive mineral material.

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References

- [1] G. Meyer, A. Fasano, M. Primicerio, On a problem in the polymer industry: Theoretical and numerical investigation of swelling, *SIAM J. Math. Anal.* 17 (1986).
- [2] R.A. Adams, J.F. Fournier, *Sobolev Spaces*, 2nd ed., Pure Appl. Math. Ser., Academic Press, Amsterdam, 2003.
- [3] D. Agreba-Driollet, F. Diele, R. Natalini, A mathematical model for the sulfur dioxide aggression to calcium carbonate stones: Numerical approximation and asymptotic analysis, *SIAM J. Appl. Math.* 64 (2004) 1636–1667.
- [4] T. Aiki, H. Imai, Global existence of solutions to one-phase Stefan problems for semilinear parabolic equations, *Ann. Mat. Pura Appl.* (4) 175 (1998) 327–337.
- [5] T. Aiki, personal communication, 2008.
- [6] V. Alexiades, A.D. Solomon, *Mathematical Modeling of Melting and Freezing Processes*, Hemisphere Publishing Group, Washington, Philadelphia, London, 1993.
- [7] J. Bear, *Dynamics of Fluids in Porous Media*, Dover Publications Inc., New York, 1972.
- [8] M. Böhm, J. Devinny, F. Jahani, G. Rosen, O a moving-boundary system modeling corrosion of sewer pipes, *Appl. Math. Comput.* 92 (1998) 247–269.
- [9] M. Böhm, R.E. Showalter, Diffusion in fissured media, *SIAM J. Math. Anal.* 16 (1985) 500–509.
- [10] M. Böhm, R.E. Showalter, A nonlinear pseudoparabolic diffusion equation, *SIAM J. Math. Anal.* 16 (1985) 980–999.
- [11] L.M. Brieger, F.H. Wittmann, Numerical simulation of concrete carbonation, in: F.H. Wittmann (Ed.), *Werkstoffwissenschaften und Bausanierung. Berichtstand zum 2. Int. Koll.*, Technische Akademie Esslingen, 1986, pp. 635–640.
- [12] D. Bunte, Zum Karbonatisierungsbedingten Verlust der Dauerhaftigkeit von Aussenbauteilen aus Stahlbeton, PhD thesis, TU Braunschweig, 1994.
- [13] J.R. Cannon, A. Fasano, Boundary value multidimensional problems in fast chemical reactions, *Arch. Ration. Mech. Anal.* 53 (1974) 1–13.
- [14] T. Chaussadent, États de lieux et réflexions sur la carbonatation du béton armé, tech. report, Laboratoire Central de Ponts et Chaussées, 1999.
- [15] P. Colli, A. Visintin, A free boundary problem of biological interest, *Math. Methods Appl. Sci.* 11 (1989) 79–93.
- [16] A. Fasano, M. Primicerio, General free-boundary problems for the heat equation, II, *J. Math. Anal. Appl.* 58 (1977) 202–231.
- [17] A. Fasano, M. Primicerio, General free-boundary problems for the heat equation, III, *J. Math. Anal. Appl.* 59 (1977) 1–14.
- [18] M. Fila, Ph. Souplet, Existence of global solutions with slow decay and unbounded free boundary for a superlinear Stefan problem, *Interfaces Free Bound.* 3 (2001) 337–344.
- [19] G.F. Froment, K.B. Bischoff, *Chemical Reactor Analysis and Design*, 2nd ed., Wiley Ser. Chem. Eng., John Wiley and Sons, New York, Chichester, Brisbane, Toronto, Singapore, 1990.
- [20] H. Ghidouche, Ph. Souplet, D. Tarzia, Decay of global solutions, stability and blowup for a reaction–diffusion problem with free boundary, *Proc. Amer. Math. Soc.* 129 (3) (2001) 781–792.
- [21] Z. Guan, X.-J. Wang, Existence and blow-up of solutions to two-phase nonequilibrium problems, *SIAM J. Math. Anal.* 27 (1996) 1038–1048.
- [22] M.E. Gurtin, *Thermomechanics of Evolving Phase Boundaries in the Plane*, Clarendon Press, Oxford, 1993.
- [23] J. Kropp, Relations between transport characteristics and durability, in: J. Kropp, H.K. Hilsdorf (Eds.), *Performance Criteria for Concrete Durability*, RILEM Report 12, E and FN Spon Editions, 1995, pp. 97–137.
- [24] H.G. Landau, Heat conduction in a melting solid, *Q. Appl. Mech. Math.* 8 (1950) 81–94.
- [25] S.A. Meier, M.A. Peter, A. Muntean, M. Böhm, Dynamics of the internal reaction layer arising during carbonation of concrete, *Chem. Eng. Sci.* 162 (2007) 1125–1137.
- [26] A. Muntean, Error bounds on a semi-discrete finite element approximation of the weak solution to a one-phase moving-boundary system describing concrete corrosion, *Int. J. Numer. Anal. Model.* 5 (3) (2008) 353–372.
- [27] A. Muntean, *A Moving-Boundary Problem: Modeling, Analysis and Simulation of Concrete Carbonation*, PhD thesis, Faculty of Mathematics, University of Bremen, Germany, Cuvillier Verlag, Göttingen, 2006.
- [28] A. Muntean, Concentration blow up in a two-phase non-equilibrium model with source term, *Meccanica* 42 (2007) 409–411.
- [29] A. Muntean, M. Böhm, Dynamics of a moving reaction interface in a concrete wall, in: J.F. Rodrigues, et al. (Eds.), *Free and Moving Boundary Problems. Theory and Applications*, in: *Internat. Ser. Numer. Math.*, vol. 154, Birkhäuser, Basel, 2006, pp. 317–326.
- [30] P.J. Ortoleva, *Geochemical Self-Organization*, Oxford Monogr. Geol. Geophys., vol. 23, Oxford Univ. Press, NY, Oxford, 1994.
- [31] V.G. Papadakis, C.G. Vayenas, M.N. Fardis, Physical and chemical characteristics affecting the durability of concrete, *ACI Mater. J.* 88 (1991) 186–196.
- [32] A. Rouzaud, One-dimensional modeling of coupled heat and mass transfer at solid/liquid moving interface, *J. Crystal Growth* 104 (1990) 701–712.
- [33] A.V. Sætta, B.A. Schrefler, R.V. Vitaliani, The carbonation of concrete and the mechanism of moisture, heat and carbon dioxide flow through porous materials, *Cement Concrete Res.* 23 (1993) 761–772.
- [34] K. Sisomphon, Influence of pozzolanic material additions on the development of the alkalinity and the carbonation behaviour of composite cement pastes and concretes, PhD thesis, TU Hamburg-Harburg, 2004.
- [35] S.L. Sobolev, Two-temperature Stefan problem, *Phys. Lett. A* 197 (1995).
- [36] H.F.W. Taylor, *Cement Chemistry*, Thomas Telford Publishing, London, 1997.
- [37] A. Visintin, Stefan problem with a kinetic condition at the free boundary, *Ann. Mat. Pura Appl.* 146 (1987) 97–122.
- [38] J. Wloka, *Partial Differential Equations*, Cambridge Univ. Press, Cambridge, 1992.
- [39] W. Xie, Phase transition in binary systems and the binary alloy problem, *Math. Methods Appl. Sci.* 15 (1992) 205–221.
- [40] E. Zeidler, *Nonlinear Functional Analysis and Its Applications. Linear Monotone Operators*, vol. II/A, Springer-Verlag, Berlin, 1990.