A MOVING-BOUNDARY PROBLEM FOR CONCRETE CARBONATION: GLOBAL EXISTENCE AND UNIQUENESS OF WEAK SOLUTIONS∗

ADRIAN MUNTEAN† AND MICHAEL BÖHM‡

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 results are a (global) existence- and uniqueness theorem, and non-trivial lower and upper estimates for the velocity of the moving boundary.

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 as a moving-boundary surface in the solid. We include simulation results showing that the model captures the qualitative behaviour of the carbonation process.

Key words. moving-boundary problem, reaction-diffusion equations, Stefan-like problem with kinetic condition, a priori estimates, lower and upper bounds, concrete carbonation

AMS subject classifications. Primary, 35 R 35; Secondary, 74 F 25, 35 D 05

1. Introduction. We study a two phase moving-boundary system with kinetic condition arising in the modeling of the concrete corrosion. Starting from the problem formulated in [30], we show existence, uniqueness and practical upper and lower bounds for the solution to a coupled PDEs-ODE system. 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, 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 (forming the protective pH ambient) into calcite. The loss of protection means in this context that once the calcium hydroxide is reacted away, the concrete-based material can be easily attacked by sulfate or chloride ions [9, 3, 13, 26], 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 [40, 34, 26], as

\[
\mathrm{CO}_2(g \rightarrow \text{aq}) + \mathrm{Ca(OH)}_2(\text{aq}) \overset{\text{H}_2\text{O}}{\rightarrow} \mathrm{CaCO}_3(\text{aq}) + \text{H}_2\text{O}.
\] (1.1)

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†Centre for Analysis, Scientific computing and Applications (CASA), Department of Mathematics and Computer Science, Technical University of Eindhoven, The Netherlands (a.muntean@tue.nl).
‡Centre for Industrial Mathematics (ZeTeM), Department of Mathematics and Computer Science, University of Bremen, Germany (mbohm@math.uni-bremen.de).
The phenomenology of the process is apparently simple: Molecules of gaseous CO\textsubscript{2} from the atmosphere penetrate the concrete via the unsaturated porous matrix. After entering the air part of the pores, CO\textsubscript{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. Ca(OH)\textsubscript{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\textsubscript{3} are the reaction products. CaCO\textsubscript{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 Ca(OH)\textsubscript{2} into CaCO\textsubscript{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\textsubscript{2} penetration in concrete structures accurately. More details on this important durability issue can be found in [12, 13, 30] 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 type of reaction interface

penetrate 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 [28, 32, 30] 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 [10, 11], e.g.), can not 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 ([33], e.g.), polymer industry ([1, 41], e.g.) or life sciences ([16], e.g.) may be tackled by conceptually close moving-boundary modeling strategies. The modeling, analysis and simulation of alike non-equilibrium scenarios in two and three space dimensions are sources rich in open problems.

The paper is organized as follows. In section 2 we describe the moving-boundary model 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 results. The bulk of the proofs is given in section 4. The aim of section 5 is to illustrate numerically a simple carbonation scenario, which is modeled as mentioned in 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 [32]. They constitute a part of the results from the PhD thesis [30] 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 [40]. 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 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 $t \in [0, T]$ 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 initialisation of carbonation coupled with carbonation in the interior, which leads to different models [15]. 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 [17, 18] to somehow related subjects involving conditions like $s_0 = 0$. 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 $\Omega_1(t) := [0, s(t)]$; $\bar{u}_3 := [\text{Ca(OH)}_2(\text{aq})]$ 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 $I := I_1 \cup \{4\} \cup I_2$, where $I_1 := \{1, 2, 5\}$ points out the active concentrations in $\Omega_1(t)$ and $I_2 := \{3, 6\}$ 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 $\bar{u}_i(x, t), i \in I$ and the interface position $s(t)$ which

![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.](image-url)
satisfy for all \( t \in S_T \) the equations

\[
\begin{align*}
(\phi_w \bar{u}_i)_t + (D_\nu \phi_w \bar{u}_{i,x})_x &= f_{\text{Henry}, i}, x \in \Omega_1(t), i \in \{1, 2\}, \\
(\phi_w \bar{u}_3)_t + (D_\lambda \phi_w \bar{u}_{3,x})_x &= f_{\text{Diss}, x} \in \Omega_2(t), \\
(\phi_w \bar{u}_4)_t &= f_{\text{Prec}, x} + f_{\text{React}, x} = s(t) \in \Gamma(t), \\
(\phi_w \bar{u}_5)_t + (D_\eta \phi_w \bar{u}_{5,x})_x &= 0, x \in \Omega_1(t), \\
(\phi_w \bar{u}_6)_t + (D_\eta \phi_w \bar{u}_{6,x})_x &= 0, x \in \Omega_2(t).
\end{align*}
\] (2.1)

The initial and boundary conditions are \( \phi_w \nu_{12} \bar{u}_i(x, 0) = \dot{u}_{i0}(x), \ i \in \mathcal{I}, x \in \Omega(0), \phi_w \nu_{12} \bar{u}_i(0, t) = \lambda_i(t), i \in \mathcal{I}_1, \dot{u}_{i,x}(L, t) = 0, i \in \mathcal{I}_2 \), where \( t \in S_T \). Specific to our problem, we impose the following interface conditions

\[
\begin{align*}
[j_1 \cdot n]_{\Gamma(t)} &= -\tilde{\eta}_T(s(t), t) + s'(t)[\phi_w \bar{u}_3]_{\Gamma(t)}, \\
[j_i \cdot n]_{\Gamma(t)} &= -\tilde{\eta}_T(s(t), t) + s'(t)[\phi_w \bar{u}_i]_{\Gamma(t)}, i \in \{2, 5, 6\}, \\
[j_3 \cdot n]_{\Gamma(t)} &= -\tilde{\eta}_T(s(t), t) + s'(t)[\phi_w \bar{u}_3]_{\Gamma(t)},
\end{align*}
\] (2.2)

\[
s'(t) = \frac{\tilde{\eta}_T(s(t), t)}{\phi_w \bar{u}_3(s(t), t)} = \frac{\gamma T(s(t), t)}{s(0) = s_0},
\] (2.3)

where \( \nu_{12} = \nu_{32} := 1, \nu_{22} := \frac{\phi_w}{\phi_w}, \nu_{52} = \nu_{62} := \frac{1}{\phi_w}, \nu_{\ell} := 1 \ (i \in \mathcal{I}, \ell \in \mathcal{I} - \{2\}) \), \( \delta_{ij} \ (i, j \in \mathcal{I}) \) is Kronecker’s symbol, \( j_i := -D_\eta \nu_{\ell} \phi_w \bar{u}_i \) \( (i, \ell \in \mathcal{I}_1 \cup \mathcal{I}_2) \) are the corresponding effective diffusive fluxes and \( \alpha > 0 \). Here \( D_\nu, \Lambda \) and \( s_0 \) are strictly positive constants, \( \lambda_i \) are prescribed in agreement with the environmental conditions to which \( \Omega \) a part of a concrete sample (cf. Fig. 2.1 (b)) - is exposed, see [37, 13]. An argument for the boundary conditions (2.2) is based on the so-called pillow lemma (see [24]). The initial conditions \( \dot{u}_{i0} > 0 \) are determined by the chemistry of the cement. The hardened mixture of aggregate, cement and water (i.e. the concrete) imposes 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, 40]) is valid. The productions terms \( f_{\text{Henry}, i}, f_{\text{Diss}, \nu}, f_{\text{Prec}, \nu} \) and \( f_{\text{React}, \nu} \) are sources or sinks by Henry-like interfacial transfer mechanisms, dissolution, precipitation, and carbonation reactions. Typical examples are:

\[
\begin{align*}
(f_{\text{Henry}})(0, t) &= (-1)^i P_i (\phi_w \nu_{12} \bar{u}_1 - Q_i \phi_w \nu_{12} \bar{u}_2) (P_i > 0, Q_i > 0), i \in \{1, 2\}, \\
(f_{\text{Diss}})(0, t) &= -S_{3,\text{diss}} (\phi_w \nu_{12} \bar{u}_3 - u_{3,eq}), S_{3,\text{diss}} > 0, f_{\text{Prec}} := 0, f_{\text{React}} := \tilde{\eta}_T.
\end{align*}
\] (2.4)

In (2.4), \( \tilde{\eta}_T(s(t), t) \) denotes the carbonation reaction rate. It is defined in the following fashion: Let \( \bar{u} = (\bar{u}_1, \ldots, \bar{u}_6)^t \) be the vector of concentrations and \( M_A \) the set of parameters \( \Lambda := (\Lambda_1, \ldots, \Lambda_m)^t \) chosen to describe the reaction rate. For our purposes, it suffices at this moment to assume that \( M_A \) is a non-empty compact subset of \( \mathbb{R}^m \). We introduce the function

\[
\tilde{\eta}_T: \mathbb{R}^6 \times M_A \to \mathbb{R}_+ \text{ by } \tilde{\eta}_T(u(x, t), \Lambda) := k \phi_w \nu_{12} \bar{u}_1(x, t) \bar{u}_3(x, t), x = s(t).
\] (2.5)

In (2.5), \( m := 3 \) and \( \Lambda = \{p, q, k \phi_w\} \in \mathbb{R}^3 \). We define the reaction rate \( \tilde{\eta}_T(s(t), t) \) and the term \( \tilde{\psi}_T(s(t), t) \) in (2.3) by

\[
\tilde{\eta}_T(s(t), t) := \tilde{\eta}_T(\bar{u}(s(t), t), \Lambda), \tilde{\psi}_T(s(t), t) := \tilde{\psi}_T(\bar{u}(s(t), t), \Lambda), \Lambda,
\] (2.6)

where \( \tilde{\eta}_T \) is given by (2.5) and represents the classical power-law ansatz [22]. In the engineering literature, there is a whole variety of reaction rates used in the context
of carbonation ([15, 34, 36]); (2.5), with \( p > 0 \) and \( q > 0 \), is 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 \textit{a priori} unknown.

The system (2.1)-(2.6) forms the \textit{sharp-interface carbonation model}. We abbreviate it as \((P_\Gamma)\). The model consists of a coupled semi-linear system of parabolic equations that has a moving \textit{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 (2.3). The interface conditions require further explanation. The term \( \tilde{\eta}_R(s(t),t) \approx \frac{1}{2} s'(t) \) denotes the number of grams per volume and time that is transported by diffusion to the interface \( \Gamma(t) \). In (2.2), \( \pm \phi \omega \bar{u}(s(t),t)s'(t) \) 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. [5], section 1.2.E, e.g.

The law (2.3), which we call \textit{kinetic or non-equilibrium} condition, governs the dynamics of the reaction interface. (2.3) is exact for the 1D case and has been derived via \textit{first principles} in [30]. We need the kinetic condition to complete the model formulation. We rely on (2.3) 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 bring about a blow up in concentration (see [23, 31], 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 [16, 41, 43].

The present setting is only applicable when the reaction rate is very rapid and the diffusion of the gaseous \( \text{CO}_2 \) is sufficiently slow, or in other terms, when the characteristic time of the carbonation reaction is much smaller than the characteristic time of 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)-(2.6) 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 \textit{a priori} clear what actually happens at \( \Gamma(t) \) with the reactants. For our case, complete reaction at \( \Gamma(t) \) would immediately imply the case of \textit{infinitely fast} chemical reaction in which the reactants practically vanish at \( \Gamma(t) \) (see [14], e.g.) We refer the reader to [35, 38] for concrete reaction-diffusion scenarios, where discontinuities in concentrations at moving boundaries arise.

3. Main results.

3.1. Preliminaries. For each \( i \in I_1 \cup I_2 \), we denote \( H_i := L^2(a,b) \) and set \([a,b] = [0,1]\) for \( i \in I_1 \) and \([a,b] = [1,2]\) for \( i \in I_2 \). Moreover, \( \mathcal{H} := \prod_{i \in I_1 \cup I_2} H_i \), \( V_i = \{ u \in H^1(a,b) : u_i(a) = 0 \}, \) \( i \in I_1 \), \( V_i := H^1(a,b), i \in I_2 \), and \( V = \prod_{i \in I_1 \cup I_2} V_i \). In addition, \( |\cdot| := |||\cdot|||_{L^2(a,b)} \) and \(||\cdot|| := |||\cdot|||_{H^1(a,b)} \). If \( (X_i : i \in I) \) is a sequence of given
where \( \eta \) and \( \lambda \) are given in (3.10) and (3.11), respectively.

We reformulate the system (2.1)-(2.6): Let \( \hat{\mu}_i := \phi \phi_a \bar{\mu}_a, i \in \{1, 3, 4\}, \hat{\mu}_2 := \phi \phi_a \bar{\mu}_2, \hat{\mu}_i := \phi \hat{\mu}_i, i \in \{5, 6\} \) and write down (\( P_T \)) on fixed domains. As result of this procedure, we obtain the transformed model (3.3)-(3.13).

Let \( t \in S_T \) be arbitrarily fixed. In our setting, the fixed-domain transformations [27] read:

\[
\begin{align*}
(3.1) \quad & (x, t) \in [0, s(t)] \times \bar{S}_T \longrightarrow (y, t) \in [a, b] \times \bar{S}_T, y = \frac{x}{s(t)} \quad \text{for } i \in \mathcal{I}_1, \\
(3.2) \quad & (x, t) \in [s(t), L] \times \bar{S}_T \longrightarrow (y, t) \in [a, b] \times \bar{S}_T, y = a + \frac{x - s(t)}{L - s(t)} \quad \text{for } i \in \mathcal{I}_2.
\end{align*}
\]

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

\[
\begin{align*}
(3.3) \quad & (u_i + \lambda_i)_t - \frac{1}{s^2(t)} (D_{i,y}^1)_{i,y}(u, \lambda) + y s'(t) s(t) u_i, i \in \mathcal{I}_1, \\
(3.4) \quad & (u_i + \lambda_i)_t - \frac{1}{(L - s(t))^2} (D_{i,y}^2)_{i,y}(u, \lambda) + (2 - y) s'(t) s(t) u_i, i \in \mathcal{I}_2,
\end{align*}
\]

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

\[
(3.5) \quad u_0(0) = \lambda(0), \quad \text{and hence } \hat{u}_i(0) = 0 \quad \text{for } i \in \mathcal{I}_1
\]

The transformed initial, boundary and interface conditions are

\[
\begin{align*}
(3.6) \quad & u_i(y, 0) = u_{i,0}(y), i \in \mathcal{I}_1 \cup \mathcal{I}_2, u_i(a, t) = 0, i \in \mathcal{I}_1, u_i(b, t) = 0, i \in \mathcal{I}_2, \\
(3.7) \quad & \frac{-D_1}{s(t)} u_{1,y}(1) = \eta^1(1) + s'(1)(u_1(1) + \lambda_1), \\
(3.8) \quad & \frac{-D_2}{s(t)} u_{2,y}(1) = s'(1)(u_2(1) + \lambda_2), \\
(3.9) \quad & \frac{-D_3}{L - s(t)} u_{3,y}(1) = -\eta^3(1) + s'(1)(u_3(1) + \lambda_3), \\
(3.10) \quad & \frac{-D_4}{s(t)} u_{5,y}(1) + \frac{D_5}{L - s(t)} u_6, y(1) = \eta^5(1), u_5(1) + \lambda_5 = u_6(1) + \lambda_6,
\end{align*}
\]

where \( \eta^r(1) \) denotes the reaction rate that acts in the \( y-t \) plane. This is defined by

\[
(3.11) \quad \eta^r(1, t) := \tilde{\eta}^r(\bar{u}(y, t), t + \lambda(t), \Lambda), y \in [0, 1],
\]

for given \( \Lambda \in M_A \) and \( \tilde{\eta}^r \) as in (2.5). \( \psi^r(1, t) \) is defined analogously. We also mention that \( u_{i,0}(y) = \hat{u}_{i,0}(x) - \lambda_i(0), \) where \( x = y s_0, \) \( y \in [0, 1] \) 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

\[
(3.12) \quad s'(t) = \psi^1(1, t) \quad \text{and } v_4'(t) = f_4(v_4(t)) \quad \text{a.e. } t \in S_T,
\]
where \( v_4(t) := \dot{u}_4(s(t), t) \) for \( t \in S_T \), complete the model formulation. Furthermore, we take

\[
(3.13) \quad s(0) = s_0, v_4(0) = \dot{u}_{40}.
\]

Let \( \varphi := (\varphi_1, \varphi_2, \varphi_3, \varphi_5, \varphi_6) \in V \) be an arbitrary test function and take \( t \in S_T \).

To write down the weak formulation of (3.3)-(3.13) in a compact form, we introduce the notation:

\[
(3.14) \quad \begin{cases}
a(s, u, \varphi) := \frac{1}{r} \sum_{i \in T_1} (D_i u_{i,y}, \varphi_{i,y}) + \frac{1}{L_{s}} \sum_{i \in T_2} (D_i u_{i,y}, \varphi_{i,y}), \\
b_f(u, s, \varphi) := s \sum_{i \in T_1} (f_i(u), \varphi_i) + (L - s) \sum_{i \in T_2} (f_i(u), \varphi_i), \\
e(s', u, \varphi) := \sum_{i \in T_1 \cup T_2} g_i(s, s', u(1)) \varphi_i(1), \\
h(s', u, \varphi) := s' \sum_{i \in T_1} (yu_{i,y}, \varphi_i) + s' \sum_{i \in T_2} ((2 - y) u_{i,y}, \varphi_i),
\end{cases}
\]

for any \( u \in V \) and \( \lambda \in W^{1,2}(S_T) \). The term \( a(\cdot) \) incorporates the diffusive part of the model, \( b_f(\cdot) \) comprises volume productions, \( e(\cdot) \) sums 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 \( g_i(i \in T_1 \cup T_2) \) are given by

\[
(3.15) \quad \begin{cases}
g_1(s, s', u) := \eta \gamma(1, t) + s'(t) u_1(1), \\
g_2(s, s', u) := s'(t) u_2(1), \\
g_3(s, s', u) := \eta \gamma(1, t) - s'(t) u_3(1), \\
g_4(s, s', u) := \eta \gamma(1, t), \\
g_5(s, s', u) := 0,
\end{cases}
\]

whereas the volume terms \( f_i (i \in T) \) are defined as

\[
(3.16) \quad \begin{cases}
f_1(u) := P_1(Q_1 u_2 - u_1), \\
f_2(u) := -P_2(Q_2 u_2 - u_1), \\
f_3(u) := S_{diss}(u_3, e_q - u_3), \\
f_4(u) := 0.
\end{cases}
\]

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

\[
\begin{align*}
(3.17) \quad \lambda & \in W^{1,2}(S_T), \\
(3.18) \quad u_{3,e_q} & \in L^\infty(S_T), \quad u_{3,e_q}(t) \geq 0 \text{ a.e. } t \in S_T, \\
(3.19) \quad u_0 & \in L^\infty([a,b]), \\
(3.20) \quad \tilde{u}_{40} & \in L^\infty(0, s_0), \quad \tilde{u}_4(x, 0) > 0 \text{ a.e. } x \in [0, s_0], \\
(3.21) \quad s_0 & > 0, \quad L_0 < L < +\infty, \quad s_0 < L_0, \\
(3.22) \quad \min\{S_{diss}, P_1, Q_1, P_2, Q_2, D_0 (l \in \mathcal{T}_1 \cup \mathcal{T}_2)\} & > 0.
\end{align*}
\]

We denote

\[
(3.23) \quad m_0 := \min\{s_0, L - L_0\}, \quad M_0 := \max\{L_0, L - s_0\}.
\]

Set

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

and, for fixed \( \Lambda \in M_A \), we take

\[
(3.25) \quad M_{\gamma} := \max_{\bar{u} \in \mathcal{K}} \{\eta \gamma(\bar{u}, \Lambda)\}.
\]
In (3.24) we set
\[
\begin{align*}
\begin{cases}
    k_i := \max \{u_{i0}(y) + \lambda_i(t), \lambda_i(t) : y \in [a,b], t \in \bar{S}_T \}, & i = 1, 2, 3, 6, \\
    k_4 := \max \{u_{40}(x) + M_{\eta} T : x \in [0, s(t)], t \in \bar{S}_T \}, \\
    k_5 := \max \{u_{50}(y) + \lambda_5(t), \lambda_6(t), \kappa : y \in [a,b], t \in \bar{S}_T \}, \\
    k_6 := k_5,
\end{cases}
\end{align*}
\]  
where
\[
(3.27) \quad \kappa := \frac{L_0}{D_5 - M_{\eta} LL_0} \left( M_{\eta} + \frac{L}{2} |\lambda_5|_\infty + 1 \right).
\]

**Definition 3.1. (Local Weak Solution)** We call the triple \((u, v_4, s)\) a local weak solution to problem (3.3)-(3.13) if there is a \(\delta \in [0, T]\) with \(S_\delta := [0, \delta]\) such that
\[
(3.28) \quad s_0 < s(\delta) \leq L_0,
\]
\[
(3.29) \quad v_4 \in W^{1,4}(S_\delta), \quad s \in W^{1,4}(S_\delta),
\]
\[
(3.30) \quad u \in W^1_2(S_\delta; \mathbb{V}; \mathbb{H}) \cap [\bar{S}_\delta \mapsto L^\infty(a, b)]^{I_1 \cup I_2},
\]
For all \(\varphi \in \mathbb{V}\) and a.e. \(t \in S_\delta\) we have
\[
(3.31) \quad \begin{cases}
    s \sum_{i \in I_1} (u_{i,t}(t), \varphi_i) + (L - s) \sum_{i \in I_2} (u_{i,t}(t), \varphi_i) + a(s, u, \varphi) \\
    + c(s', u + \lambda, \varphi) = b_f(u + \lambda, s, \varphi) + h(s', u, \varphi) \\
    - s \sum_{i \in I_4} (\lambda_{i,t}(t), \varphi_i) - (L - s) \sum_{i \in I_2} (\lambda_{i,t}(t), \varphi_i), \\
    s'(t) = \eta_{T}(1, t), \quad v_4'(t) = f_4(v_4(t)) \text{ a.e. } t \in S_\delta, \\
    u(0) = u_0 \in \mathbb{H}, s(0) = s_0, v_4(0) = \bar{u}_{40}.
\end{cases}
\]

### 3.2. Hypotheses on the model parameters.

The only assumptions that are needed are the following:

(A) Fix \(\Lambda \in M_\Lambda\). Let \(\bar{\eta}_T(u, \Lambda) > 0\), if \(\bar{u}_1 > 0\) and \(\bar{u}_3 > 0\), and \(\bar{\eta}_T(u, \Lambda) = 0\), otherwise. For any fixed \(\bar{u}_1 \in \mathbb{R}\), \(\bar{\eta}_T\) is bounded.

(B) The reaction rate \(\bar{\eta}_T : \mathbb{R}^d \times M_\Lambda \rightarrow \mathbb{R}_+\) is locally Lipschitz. This restricts the choice of \(p\) and \(q\) in (2.5).

(C1) \(1 > k_3 \geq \max_{S_T} \{|u_{3,eq}(t)| : t \in \bar{S}_T\}; D_5 - M_{\eta} L > 0;\)

(C2) \(P_1 Q_1 k_2 \leq P_1 k_1; \quad P_2 k_1 \leq P_2 Q_2 k_2;\)

(C3) \(Q_2 > Q_1.\)

(A)-(C) can be interpreted in the following way: (A) means that the reaction takes place if both \(\text{CO}_2(aq)\) and \(\text{Ca(OH)}_2(aq)\) 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 \(L^\infty\)-estimates on \(u_3\) and \(u_5\). It says that the equilibrium concentration of \(\text{Ca(OH)}_2(aq)\) 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) and (C3) are rather technical. They both suggest that the transfer of \(\text{CO}_2\) from the air phase into the pore water is fast. (C2) is used to get the \(L^\infty\)-estimates on \(u_1\) and
u_2, while (C3) prevents the vanishing of these two concentrations at the interface position.

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

\[
\tilde{\eta}_T(\tilde{u}(t), t, \Lambda) \leq C_\eta |\tilde{u}(s(t), t)|
\]

holds for all \( t \in S_T \). (3.32) can be reformulated as

\[
\eta_T(1, t) \leq C_\eta |u(1, t)| \quad \text{for all } t \in S_T.
\]

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

\[
|\epsilon(s', u(1), \varphi(1))| \leq c_g |u(1)| |\varphi(1)| \quad \text{for all } \varphi \in V
\]

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

\[
|b_f(u, s, \varphi)| \leq c_f \left( |u_3, c_g|^2 + |u|^2 + |\varphi|^2 \right) \quad \text{for all } \varphi \in V,
\]

where \( K_1 > 0 \) is a constant depending on the material parameters entering \( f_i \) (\( i \in I \)), i.e. \( P_i, P_2, Q_1, Q_2, \) and \( S_{\text{3, diss}} \). The exact structure of \( c_g, c_f, K_1 \) is dictated by the definition of the production terms \( f_i \) and \( g_i \) (\( i \in I \)), see (3.16) and (3.15). Since \( \psi_T(1, t) \) has essentially the same structure as \( \eta_T(1, t) \), 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 (3.17)-(3.22) be satisfied. If \( s \in W^{1,4}(S_\delta) \) with \( s' \geq 0 \) a.e. in \( S_\delta \) and \( s(0) = s_0 \) is given, then the problem (3.3)-(3.13) 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 however standard. The existence and uniqueness of the weak solutions can be shown as for the model problems presented in [42, 44], and therefore we omit the proof. \( \square \)

**Theorem 3.3** (Local Existence and Uniqueness). Assume the hypotheses (A)-(C2) and let the conditions (3.17)-(3.22) be satisfied. Then the following assertions hold:

(a) There exists a \( \delta \in [0, T] \) such that the problem (3.3)-(3.13) admits a unique local solution on \( S_\delta \) in the sense of Definition 3.1:

(b) \( 0 \leq u_i(y, t) + \lambda_i(t) \leq k_i \) a.e. \( y \in [a, b] \) (\( i \in \mathcal{I}_1 \cup \mathcal{I}_2 \)) for all \( t \in S_\delta \). Moreover, \( 0 \leq \tilde{u}_q(x, t) \leq k_4 \) a.e. \( x \in [0, s(t)] \) for all \( t \in S_\delta \);

(c) \( u_4, s \in W^{1, \infty}(S_\delta) \).

It is worth mentioning that if the assumptions of Theorem 3.3 hold, then we can additionally prove the estimate \( u_5(y, t) + \lambda_5(t) \leq k_5 y \) for a.e. \( y \in [0, 1] \) and all \( t \in S_\delta \); see Remark 3.4.7 of [30].

**Proposition 3.4** (Strict Lower Bounds). Assume that the hypotheses of Theorem 3.3 are satisfied. If, additionally, (C3) holds and the initial and boundary data are strictly positive, then there exists a range of reasonable parameters such that the positivity estimates stated in Theorem 3.3 (b) are strict for all times.

The main physical motivation why such range of parameters ensuring the existence of strict lower bounds (see Proposition 3.4) may be found is that the carbonation

\[\text{\footnotesize\[3.34\] \quad |e(s', u(1), \varphi(1))| \leq c_g |u(1)| |\varphi(1)| \quad \text{for all } \varphi \in V\]}

\[\text{\footnotesize\[3.35\] \quad |b_f(u, s, \varphi)| \leq c_f \left( |u_3, c_g|^2 + |u|^2 + |\varphi|^2 \right) \quad \text{for all } \varphi \in V,\]}

where \( K_1 > 0 \) is a constant depending on the material parameters entering \( f_i \) (\( i \in I \)), i.e. \( P_i, P_2, Q_1, Q_2, \) and \( S_{\text{3, diss}} \). The exact structure of \( c_g, c_f, K_1 \) is dictated by the definition of the production terms \( f_i \) and \( g_i \) (\( i \in I \)), see (3.16) and (3.15). Since \( \psi_T(1, t) \) has essentially the same structure as \( \eta_T(1, t) \), it also satisfies (A) and (B).
process can be viewed as a one-stage non-catalytic gas-solid reaction. By Theorem 3.3 (b) and Proposition 3.4, there exist constants \( \psi_{\min}, \psi_{\max} \in \mathbb{R}_+ \) such that

\[
0 < \psi_{\min} \leq \psi_{\Gamma}(1, t) \leq \psi_{\max} < \infty
\]

(3.36) for all \( t \in S_\delta \). By (2.5), \( \psi_{\max} \) is independent of \( \delta \) and we may take \( \psi_{\max} := M_{\eta_\Gamma} \) (see (3.25)). \( \psi_{\min} \) typically depends on \( \delta \).

**3.4. Global solvability.** We say that problem (3.3)-(3.13) is globally solvable, if for each \( L_0 \in [s_0, L] \) there is a solution on \([s_0, L_0]\) in the sense of Definition 3.1. The case \( L_0 = L \) is excluded for similar reasons as \( s_0 = 0 \); see the corresponding note in section 2.

In order to obtain the global solvability of our problem, we start with assuming that the hypotheses of Proposition 3.4 hold. In this case, for an arbitrarily fixed \( L_0 \in [s_0, L] \) there is a moment \( T_{\text{fin}} = T_{\text{fin}}(L_0) \in [0, \infty] \) such that

\[
s(T_{\text{fin}}) = L_0.
\]

(3.37) Thus \( T_{\text{fin}} \) denotes the time when \( \Gamma(t) \) has penetrated all of \([s_0, L_0]\). We refer to it as the final carbonation time or shut-down time of the process. Physically reasonable restrictions on the life span of the weak solution (hence, on \( T_{\text{fin}} \)) are given in Proposition 3.6 (iii). The next three results are direct consequences of Theorem 3.3 and Proposition 3.4.

**Proposition 3.5 (Strict Monotonicity of the Reaction Interface).** If the assumptions of Proposition 3.4 are satisfied, then the position \( s \in W^{1, \infty}(S_\delta) \) of the interface \( \Gamma(t) \) is strictly monotone increasing on \( S_\delta \).

Proof. The conclusion is straightforward if one combines the definition of \( s' \) and the strict positivity of concentrations. \( \Box \)

**Proposition 3.6 (Practical Estimates).** Let \((u, v, s)\) be the unique local solution to (3.3)-(3.13) that fulfills the hypotheses of Proposition 3.4. Then the following estimates hold:

(i) \( \psi_{\min} \leq s'(t) \leq \psi_{\max} \) for all \( t \in S_\delta \);
(ii) \( s_0 \leq s(t) \leq s_0 + \psi_{\max}t \) for all \( t \in S_\delta \);
(iii) \( \frac{L - s_0}{\psi_{\max}} < T_{\text{fin}} < \frac{L - s_0}{\psi_{\min}} \), where \( T_{\text{fin}} \) satisfies (3.37);
(iv) If \( \Omega_1(t) = \{ x \in [0, L]; \hat{u}_3(x, t) > 0 \} \), \( t \in S_{T_{\text{fin}}} \), then \( \Omega_1(t_1) \subset \Omega_1(t_2) \) for \( t_1 < t_2, t_1, t_2 \in S_{T_{\text{fin}}} \).

Here \( \psi_{\min} \) and \( \psi_{\max} \) are as in (3.36).

Proof. By Theorem 3.3 (b) and Proposition 3.4, (i) and (ii) are straightforward. The equation for \( s' \) in (3.12) leads to \( T_{\text{fin}} - t_0 = \int_{s(t_0)}^{s(T_{\text{fin}})} \frac{1}{\psi_{\Gamma}(s)} ds \) with \( t_0 \in [0, T_{\text{fin}}] \), see [8]. We apply the mean-value theorem and estimate \( \psi_{\Gamma} \) from below by using the non-trivial uniform lower bounds on the reactants (i.e. on \( u_1 \) and \( u_3 \)), and afterwards from above, by means of the corresponding \( L^\infty \)-estimates and obtain (iii). By (3.12) and (i), one gets (iv). \( \Box \)

The statements of Proposition 3.6 have a clear practical meaning: the finite propagation speed is established in (i); (ii) points out a linear asymptotic behavior of the speed of the reaction interface with respect to time. This is only a rough estimate. Considering the investigations reported in [4, 6, 19, 39], we expect that better asymptotic estimates could be obtained. Inequalities in (iii) estimate \( T_{\text{fin}} \) from above and below. This is the time that reaction (1.1) needs to fully carbonate \([s_0, L_0]\). The upper bound is the most helpful indicator from the practical viewpoint. (iv) shows
that the carbonated zone progresses into the material; for somewhat similar situations see [25] (Corollary 2.5, pp. 284-285), [20] (Theorem 9.1, pp. 84-87) or [21] (Corollary 2.4), e.g.

**Theorem 3.7** (Global Solvability). Let \( L_0 \subset [0, L] \). Assume that the hypotheses of Proposition 3.4 are satisfied. Then the time interval \( S_{T_{\text{fin}}} := [0, T_{\text{fin}}] \) of global solvability of problem (3.3)-(3.13) is finite and is characterized by

\[
T_{\text{fin}} = s^{-1}(L_0).
\]

**Proof.** The finiteness of the length of the length of \( S_{T_{\text{fin}}} \) is a consequence of Proposition 3.6 (iii). The \( L^\infty \)-estimates of the concentrations together with their non-negativity imply that

\[
(u(y, t), v_4(t), s(t)) \in \prod_{i \in \mathcal{I}} [0, k_i] \times [s_0, s_0 + T_{\text{fin}} M_{\text{max}}],
\]

for all \( y \in [a, b] \) and \( t \geq 0 \). The strictly positive constant \( M_{\text{max}} \) is given by (3.26), while the value of \( T_{\text{fin}} \) obeys the \textit{a priori} estimate pointed out in Proposition 3.6 (iii). Note that the invariant region is independent of \( u, s, x \) or \( t \) and that \( T_{\text{fin}} \) can be \textit{a posteriori} calculated via (3.38). By the strict monotonicity of \( s \) (cf. Proposition 3.5) and \( W^1,\infty(S_{T_{\text{fin}}}) \hookrightarrow C(S_{T_{\text{fin}}}) \), we obtain (3.38). \( \square \)

### 3.5. Return to the physical domain.

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

**Proposition 3.8** (Change of Coordinates). Assume that the hypotheses of Theorem 3.3 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 \( \lambda \) satisfy the compatibility conditions (3.5), then the solution \((\hat{u}, v_4, s)\) acts in the physical \( x-t \) plane and

\[
(\hat{u}, v_4, s) \in \prod_{i \in \mathcal{I}_1 \cup \mathcal{I}_2} H^1(S_{T_{\text{fin}}}, \hat{H}_i(t)) \times W^{1,4}(S_{T_{\text{fin}}})^2,
\]

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 and change of variables in the Bochner integral; see the proof of Proposition 3.4.17 in [30] for details. \( \square \)

### 4. Proofs of the main results.

We prove the results stated in 3.3 and 3.4. This section is organized in the following manner: We obtain a series of positivity, \( L^\infty \)- and energy estimates in 4.1. Section 4.2 contains the proof of the local existence of solutions, while in section 4.3 we indicate a way to ensure the strict positivity of the active concentrations.

#### 4.1. Basic Estimates.

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 \( c_\xi > 0, \xi > 0, \theta \in [\frac{1}{2}, 1] \) and \( s \in W^{1,1}(S_\delta) \).

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

\[
|u_i|_\infty \leq \hat{c}|u_i|^{1-\theta}|u_i|^\theta
\]
for all $u_i \in V_i$, where $i \in \mathcal{I}_1 \cup \mathcal{I}_2$.

(ii) It holds

\begin{equation}
|u_i|^{1-\theta}||u_i||^{\theta} \leq \xi ||u_i|| + c_\xi |u_i| \tag{4.2}
\end{equation}

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

(iii) Let $\varphi \in \mathcal{V}$ with $\varphi = (\varphi_1, \ldots, \varphi_6)^t$, $t \in S_8$, $c$ as in (i), and $\xi, c_\xi$ as in (ii). Then we have for $i \in \mathcal{I}_1$ and $j \in \mathcal{I}_2$ the following inequalities:

\begin{align*}
|s'(t)|^{-y}(y\varphi_i, \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)} \left\{ \xi^2 |\varphi_i|^{2(1-\theta)} ||\varphi_i||^{2\theta} - |\varphi_i|^2 \right\}; \\
\frac{|s'(t)|}{s(t)}|\varphi_i(1)^2| &\leq \frac{|s'(t)|}{s(t)}||\varphi_i||^2 \leq \frac{\xi}{s^2(t)}||\varphi_i||^2 + c_\xi \hat{\varphi}_1^{(2\theta-1)} \times s(t)^{\frac{2\theta-1}{\theta}} |s'(t)|^{\frac{1}{\theta}} ||\varphi_i||^2; \\
\frac{|\varphi_i(1)|^2}{s^2(t)} &\leq \frac{1}{2 s(t)}||\varphi_i||^2 \leq \frac{1}{2 s^2(t)}|\varphi_i(1)|^2 \leq \xi^2 s(t)^{2\theta-2} |\varphi_i|^{2(1-\theta)} (s(t)^{1-1} ||\varphi_i||)^{2\theta}; \\
\frac{|s'(t)|}{L - s(t)} ((2 - y)\varphi_j, \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{align*}

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 [44] (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 $((2 - y)\varphi_i, \varphi_i) = \varphi_i(1)^2 - (\varphi_i, (2 - y)\varphi_i) + |\varphi_i|^2$ shows the last statement in (iii). \(\blacksquare\)

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

\begin{equation}
|\varphi_i(z)|^2 \leq \xi ||\varphi_i||^2 + c_\xi |\varphi_i|^2 \tag{4.3}
\end{equation}

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 [41] or Lemma 1 of [16] to our setting.

Let $K_1$ be the following positive constant

\begin{equation}
K_1 := 1 + P_2 Q_2 + \max\{P_1 Q_1, P_2 Q_2\} + c_\xi \left(\frac{3\xi^2 M_{w}}{2}\right)^{2} + c_\xi c^4 D^2.
\tag{4.4}
\end{equation}

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 3.2 (Positivity and $L^\infty$-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) $u(t) + \lambda(t) \geq 0$ in $V$ for all $t \in S_8$.

(ii) ($L^\infty$-estimates) Let $\ell \in \mathcal{I}_1 \cup \mathcal{I}_2$ be arbitrarily fixed. There exists a constant $k_\ell > 0$ (see (3.26)) such that $u_i(t) + \lambda_i(t) \leq k_\ell$ in $V_i$ ($\ell \in \mathcal{I} - \{4, 5\}$) for all $t \in S_8$. In addition, there exists a constant $k_5 > 0$ such that $u_5(t) \leq k_5 y$ a.e. $y \in [0, 1]$ and all $t \in S_8$. 


(iii) (Localization of the interface)
\[ s_0 \leq s(t) \leq s_0 + \delta M_{\eta} \text{ for all } t \in S_{\delta}, \text{ where } M_{\eta} \text{ is given in (3.26).} \]

(iv) (Positivity and boundedness of } u_3 \text{ at } \Gamma(t)\]
\[ 0 < \hat{\dot{u}}_{40} \leq u_4(t) \leq \hat{\dot{u}}_{40} + \delta M_{\eta} \text{ for all } t \in S_{\delta}. \]

Proof. The key idea of dealing with (i) and (ii) is to choose appropriate test functions \( \varphi \in V \) in the weak formulation (3.31). We prove (i) and (ii) simultaneously by following the next steps:

- **Step 1**: We start by looking for \( L^{\infty} \)-estimates on \( u_1, u_2 \) and \( u_3 \) (thus \( C_\eta \) 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 \( L^{\infty} \)-estimates on \( u_5 \) and \( u_6 \).

We adopt this strategy because of the existence of the term \(-\eta_1(1)\varphi_1(1) - \eta_1(1)\varphi_3(1) + \eta_1(1)\varphi_5(1))\) at the r.h.s. of the weak formulation, while \( \eta_1 \) has the properties stated in (2.5), (A) and (B). Let \( k_i (i \in I) \) be as in (3.26). We show that these values are \( L^{\infty} \)-estimates that we are looking for.

**Step 1**: We start by looking for \( L^{\infty} \)-estimates of \( u_1 \) and \( u_2 \). We put in (3.31) the test function \( \varphi \in ((u_1 + \lambda_1 - k_1)^+, (u_2 + \lambda_2 - k_2)^+, 0, 0, 0)^t \in V \). We therefore have

\[
\frac{s}{2} \frac{d}{dt} |\varphi|^2 + \frac{1}{s^2} \sum_{i=1}^{2} (D_i \varphi_{i,y}, \varphi_{i,y}) = -[\eta_1 + s'(u_1(1) + \lambda_1)] \varphi_1(1) - s'(u_2(1) + \lambda_2) \varphi_2(1) + sP_1(Q_1 \varphi_1 - \varphi_1 + Q_1 k_2 - k_1, \varphi_1) - sP_2(Q_2 \varphi_2 - \varphi_1 + Q_2 k_2 - k_1, \varphi_2) + s' \sum_{i=1}^{2} (y \varphi_{i,y}, \varphi_i).
\]

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:

\[
\frac{1}{2} \frac{d}{dt} |\varphi|^2 + \frac{1}{s} \sum_{i=1}^{2} (D_i \varphi_{i,y}, \varphi_{i,y}) + \frac{s'}{s} |\varphi(1)|^2 - \frac{\eta_1}{s} \varphi_1(1) - \frac{s'}{s} (k_1 \varphi_1(1) + k_2 \varphi_2(1)) + \max \{P_1 Q_1, P_2 Q_2\} |\varphi|^2 + \frac{s'}{s} |\varphi(1)|^2 - \frac{s'}{s} |\varphi|^2.
\]

Cancelling the term \( \frac{s'}{s} |\varphi(1)|^2 \) and using the positivity of \( \varphi_1, \varphi_2 \) and \( \eta_1 \), we are led to the inequality

\[
\frac{1}{2} \frac{d}{dt} |\varphi|^2 + \frac{1}{s} \sum_{i=1}^{2} ||D_i \varphi_i||^2 \leq K_1 \sum_{i=1}^{2} |\varphi|^2.
\]

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 \( \varphi = (0, 0, (u_3 + \lambda_3 - k_3)^+, 0, 0)^t \in V \), i.e. \( \varphi_3 := (u_3 + \lambda_3 - k_3)^+ \in V_3 \). By means of this test function, we obtain

\[
(L - s)((u_3 + \lambda_3,t), \varphi_3) + \frac{1}{L - s} D_3(u_3,y, \varphi_3,y) + \frac{D_3}{L - s} |\varphi_3(1)| = \frac{D_3}{L - s} |\varphi_3(1)| + \frac{\eta_1}{s} - s'(u_3(1) + \lambda_3) \varphi_3(t) + \frac{s'(2 - y) u_3,y, \varphi_3)}{L - s} S_{3, diss}(u_3, eq - u_3 + \lambda_3, \varphi_3) + s'((2 - y) u_3,y, \varphi_3).
\]
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
\[
\frac{1}{2} \frac{d}{dt} \|\varphi_3\|^2 + \frac{1}{(L - s)^2} D_3 \|\varphi_3\|^2 = \frac{D_3}{(L - s)^2} \|\varphi_3(1)\|^2 - \frac{\eta_\Gamma}{L - s} \varphi_3(1) + \frac{s'}{L - s} (\varphi_3(1) + k_3) \varphi_3(1)
\]
\[
+ S_{3,\text{diss}}(u_{3,eq} - k_3 - \varphi_3, \varphi_3) + \frac{s'}{2} \frac{(\|\varphi_3(1)\|^2 + \|\varphi_3\|^2)}{2(L - s)}.
\]
(4.8)
By (C1), we obtain
\[
\frac{1}{2} \frac{d}{dt} \|\varphi_3\|^2 + \frac{1}{(L - s)^2} D_3 \|\varphi_3\|^2 \leq \left[ \frac{D_3}{(L - s)^2} + \frac{3s'}{2(L - s)} \right] \|\varphi_3(1)\|^2 + \frac{s'}{2} \|\varphi_3\|^2
\]
\[
\leq \frac{\xi}{(L - s)^2} \left[ \epsilon^2 \left( \frac{D_3}{(L - s)^2} + \frac{3s'}{2(L - s)} \right)^2 \right] \frac{1}{1 + (L - s)^2} + \frac{s'}{2} \|\varphi_3\|^2.
\]
Via Gronwall’s inequality we have that $u_3 + \lambda_3 \leq k_3$ for all $t \in S_3$, provided that $s' \in L^\infty(S_t)$, i.e. for given $u_1$ the reaction rate $\tilde{\eta}_\Gamma$ stays bounded.
Until now we have shown the boundedness of $u_1$ and $u_2$ without requiring the boundedness of $\eta_\Gamma$. The boundedness of $u_3$ needs that of $s'$, and hence, $\eta_\Gamma$ has to be bounded for fixed $u_1$. The positivity of $\eta_\Gamma$ 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. $\varphi_1 := -(u_1 + \lambda_1)^- \in V_1 (i \in \{1, 2\})$, we get:
\[
\frac{s}{2} \frac{d}{dt} \|\varphi\|^2 + \frac{1}{s} \sum_{i=1}^{2} \|D_i \varphi_i\|^2 = -\eta_\Gamma \varphi_1(1) + s' \|\varphi(1)\|^2
\]
\[
+ s P_1(Q_1(u_1 + \lambda_2), \varphi_1) - s P_1(\varphi_1)^2 - s P_2 Q_2(u_2 + \lambda_2, \varphi_2)
\]
\[
+ s P_2(u_1 + \lambda_1, \varphi_2) + s' \sum_{i=1}^{2} (y \varphi_{i,y}, \varphi_i).
\]
(4.9)
Noting that $\pm \tilde{\eta}_\Gamma (u_1(1) + \lambda_1)^- = 0$ and dividing the expression (4.9) by $s$, we obtain
\[
\frac{1}{2} \frac{d}{dt} \|\varphi\|^2 + \frac{1}{s^2} \sum_{i=1}^{2} \|D_i \varphi_i\|^2 \leq \frac{s'}{s} \|\varphi(1)\|^2 - P_1(\varphi)^2 + P_2 Q_2(\varphi_2)^2
\]
\[
+ \min\{P_1 Q_1, P_2 Q_2\} \|\varphi\|^2 + \frac{s'}{2s} \sum_{i=1}^{2} (|\varphi_i(1)|^2 - |\varphi_i|^2)
\]
\[
\leq \frac{3s'}{2s} \|\varphi(1)\|^2 + K_1 \|\varphi\|^2 \leq \frac{\|\varphi\|^2}{s^2} + 2 K_1 \|\varphi\|^2.
\]
(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
\[
\frac{L - s}{2} \frac{d}{dt} |\varphi_3|^2 + \frac{1}{L - s} \|\sqrt{D_3} \varphi_3\|^2 = -\eta_\Gamma \varphi_3(1) - s' |\varphi_3(1)|^2
\]
\[
+ D_3 \frac{(\|\varphi_3(1)\|^2 + (L - s) S_{3,\text{diss}}([u_{3,eq}, \varphi_3] + \varphi_3^2) + \frac{s'}{2} (|\varphi_3(1)|^2 + |\varphi_3|^2)}.
\]
Note that $-\eta_t \varphi_3(1) - \frac{s'}{2} |\varphi_3(1)|^2 \leq 0$ and $(L-s) S_{3, dist}(u_3, \varphi_3) \leq 0$. Now, we employ again the interpolation and Young inequalities in (4.11) to obtain

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

By $\xi \in [0, D_3(\text{and the use of Gronwall’s inequality, we complete this step})]$

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 $\varphi = (0, 0, 0, -(u_5 + \lambda_5)^-, -(u_6 - \lambda_6)^\dagger) \in V$. No additional restrictions on the model parameters are needed.

Step 4: As test function we put $\varphi := (0, 0, 0, (u_5 + k_5 y)^+, (u_6 - k_6)^\dagger) \in V$. By $\varphi_5(1) = \varphi_6(1)$, Cauchy-Schwarz’ inequality, and the embeddings $H^1(S_5) \hookrightarrow C(\hat{S}_5)$, $H^1(S_6) \hookrightarrow H^\perp(S_6)$ and $H^1(S_6) \hookrightarrow L^\infty(S_6)$ imply the following estimates:

\begin{align*}
\frac{s}{2} \frac{d|\varphi_5|^2}{dt} + \frac{L - s}{2} \frac{d|\varphi_6|^2}{dt} + \frac{D_5}{s} |||\varphi_5||^2 \\
+ \frac{k_5 D_5}{s} |||\varphi_5|| + \frac{D_6}{L - s} |||\varphi_6||^2 \leq M_m ||\varphi_5||_\infty - \frac{s}{2} (\lambda_{5,t}, \varphi_5) \\
+ s' \frac{|\varphi_5(1)|^2 - s' |\varphi_6|^2}{2} + s' \frac{|\varphi_6(1)|^2 + s' |\varphi_6|^2}{2} \\
+ k_5 s' L |\varphi_5||_\infty + \frac{s}{2} \lambda_{5,t} |\varphi_5||_\infty \\
\leq (M_m + \frac{L}{2} |\lambda_{5,t} + k_5 M_m L||\varphi_5|| + \xi \frac{||\varphi_5||^2}{s^2} \\
+ \left[ s' + K_1 (s' s^2) \frac{1}{m} \right] (||\varphi_5||^2 + ||\varphi_6||^2).
\end{align*}

(4.13)

Choose $\xi \in [0, s_0 k_5 D_5]$ and recall the definition of $k_5$ (cf. (3.26)), then

\begin{equation}
(4.14) \quad M_m + \frac{L}{2} |\lambda_{5,t}||_\infty + k_5 M_m L \leq \frac{k_5 D_5}{L_0}
\end{equation}

is fulfilled. Application of Gronwall’s inequality shows that $u_5(t) \leq k_5 y$ and $u_6(t) \leq k_6$ for all $t \in S_5$ a.e. $y \in [a, b]$.

Steps 1-4 complete the proof of (i) and (ii). The definitions of $s'$ and $u_4$ together with the statement (ii) prove (iii) and (iv). \(\Box\)

Condition (4.14) is sufficient to prevent a possible blow up in the concentration $u_5$. It basically says that, in order to avoid a blow up situation, the water produced at $\Gamma(t)$ should diffuse sufficiently quickly away from the interface.

**Lemma 4.3 (Energy Estimates).** Assume that (A)-(C2) hold and let the triple $(u, u_4, s)$ be as in Definition 3.1. The following statements hold a.e. in $S_5$:

\begin{align*}
(4.15) \quad |u(t) + \lambda(t)|^2 \leq \alpha(t) \exp \left( \int_0^t \beta(\tau) d\tau \right); \\
(4.16) \quad |u(t) + \lambda(t)|^2 \leq \alpha(t) + \int_0^t \beta(s) \alpha(s) \exp \left( \int_s^t \beta(\tau) d\tau \right) ds; \\
(4.17) \quad \int_0^t |u(t) + \lambda(t)|^2 d\tau \leq \frac{1}{2} \alpha(t) \exp \left( \int_0^t \beta(\tau) d\tau \right),
\end{align*}
where

\[ d_0 := \min \left\{ \min_{i \in I_1} \frac{s_0 D_i}{L^2 m_0}, \min_{i \in I_2} \frac{(L - L_0) D_i}{(L - s_0)^2 m_0} \right\}, m_0 \text{ as in } (3.23). \]

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

\[
  a(t) := \frac{(s'(t))^2}{2} + \frac{(L - s(t))^2 K_2}{2},
\]

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

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

whereas

\[
  K_2 := 1 + (S_{3,\text{diss}}|u_3,\xi|\infty)^2 + \frac{LP_1 Q_1}{2} + c\varepsilon^4.
\]

Furthermore, we have

\[
  u \in L^2(S_\delta, \mathcal{V}), u_{x,t} \in L^2(S_\delta, \mathcal{V}^*), u \in C(S_\delta, \mathbb{H}).
\]

**Proof.** Inserting the test function \( \varphi := u + \lambda \in \mathcal{V} \) in the variational formulation (3.31), we find the energy estimates (4.16) and (4.17) in the following way: By

\[
  \frac{s}{2} \sum_{i \in I_1} \frac{d}{dt} |\varphi_i(t)|^2 + \frac{L - s}{2} \sum_{i \in I_2} \frac{d}{dt} |\varphi_i(t)|^2 + a(s, \varphi, \varphi)
\]

\[
  + \varepsilon(s', \varphi, \varphi) = b_f(\varphi, s, \varphi) + h(s', \varphi, \varphi) \text{ for } t \in S_\delta,
\]

it yields

\[
  \frac{m_0}{2} \frac{d}{dt} |\varphi(t)|^2 + \frac{s_0}{s^2} \sum_{i \in I_1} D_i |\varphi_i|^2 + \frac{L - L_0}{(L - s)^2} \sum_{i \in I_2} D_i |\varphi_i|^2
\]

\[
  \leq -\eta s |\varphi_1| - s(1 - |\varphi_1(1)|^2 + |\varphi_1(1)|^2) - \eta s |\varphi_1(1)| + s' |\varphi_1(1)|^2
\]

\[
  + \frac{D_3}{L - s} |\varphi_3(1)|^2
\]

\[
  + sP_1 Q_1 (\varphi_2, \varphi_1) - P_1 |\varphi_2|^2 - sP_2 Q_2 |\varphi_2|^2 + sP_2 (\varphi_1, \varphi_2)
\]

\[
  + (L - s) S_{3,\text{diss}}|u_3,\xi|\infty|\varphi_3| - (L - s) S_{3,\text{diss}}|\varphi_3|^2
\]

\[
  + \frac{s'}{2} \sum_{i \in I_4} (|\varphi_i(1)|^2 - |\varphi_i|^2) + \frac{s'}{2} \sum_{i \in I_2} (|\varphi_i(1)|^2 + |\varphi_i|^2)^2
\]

\[
  \leq s' |\varphi_3(1)|^2 + s' |\varphi_3(1)| + \frac{D_3}{L - s} |\varphi_3(1)|^2 + \frac{LP_1 Q_1}{2} \left( |\varphi_1|^2 + |\varphi_2|^2 \right)
\]

\[
  + \frac{LP_2}{2} \left( |\varphi_1|^2 + |\varphi_2|^2 \right) + (L - s) S_{3,\text{diss}}|u_3,\xi|\infty|\varphi_3|
\]

\[
  + \frac{s'}{2} \sum_{i \in I_1 \cup I_2} |\varphi_i(1)|^2 + \frac{s'}{2} \sum_{i \in I_2} |\varphi_i|^2
\]
We employ the interpolation inequality to bound the term (4.25) from above by 

\[ \left(1 + \frac{D_3}{L-s} + \frac{s'}{2}\right) \sum_{i \in I_1 \cup I_2} |\varphi_i(1)|^2 \]

from above by

\[
\left(1 + \frac{D_3}{L-s} + \frac{s'}{2}\right) \sum_{i \in I_1} s^{2\theta} \left( \frac{||\varphi_i||}{s} \right)^{2\theta} \left| \varphi_i \right|^{2(1-\theta)} + \left(1 + \frac{D_3}{L-s} + \frac{s'}{2} \right) (L-s)^{2\theta} \sum_{i \in I_2} s^{2\theta} \left( \frac{||\varphi_i||}{L-s} \right)^{2\theta} \left| \varphi_i \right|^{2(1-\theta)} \\
\leq \xi \sum_{i \in I_1} s^{2\theta} \frac{||\varphi_i||^2}{\theta} + \xi \sum_{i \in I_2} \frac{||\varphi_i||^2}{(L-s)^2} + \xi \sum_{i \in I_2} \frac{||\varphi_i||^2}{(L-s)^2} \\
+ c_\xi \sum_{i \in I_1 \cup I_2} \left[ 1 + \frac{D_3}{L-s} + \frac{s'}{2} \right] \left[ s^{2\theta} + (L-s)^{2\theta} \right] |\varphi_i|^2 .
\]

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

\[
\frac{d}{dt} \frac{m_0}{2} |\varphi(t)|^2 + \frac{s_0}{s^2} \sum_{i \in I_1} D_i |\varphi_i|^2 + \frac{L-L_0}{(L-s)^2} \sum_{i \in I_2} D_i |\varphi_i|^2 \\
\leq \xi \sum_{i \in I_1} \frac{||\varphi_i||^2}{s^2} + \xi \sum_{i \in I_2} \frac{||\varphi_i||^2}{(L-s)^2} + a(t) + \beta(t) |\varphi(t)|^2 .
\]

Set \( \xi \in ]0, \min_{i \in I_1 \cup I_2} \{ s_0 D_i, (L-L_0) D_i \} [ \). We obtain via Gronwall’s inequality the estimate (4.15), where the factors \( a(t), \alpha(t) \) and \( \beta(t) \) are given as in (4.19)-(4.21). Gronwall’s inequality yields (4.16). Choose \( d_0 \) as in (4.18) and note also that \( d_0 > 0 \). The proof of (4.17) relies on (4.15) and integration by parts. To get (4.23), we have to discuss the Bochner measurability and integrability of \( u \) and \( u_t \) in the same way as in Lemma 26.1 in [42], pp.395-396 and Remark 27.1 in [42], p.405. If \( u \in L^2(S_\delta, \mathbb{V}) \) and \( u_t \in L^2(S_\delta, \mathbb{V}^*) \), then \( u \in \mathcal{W}^1_2(S_\delta; \mathbb{V}, \mathbb{H}) \) (see [44] for this space). The embedding \( \mathcal{W}^1_2(S_\delta; \mathbb{V}, \mathbb{H}) \hookrightarrow C(S_\delta) \) shows the second part of (4.23).

4.2. Proof of Theorem 3.3. The proof relies on the use of Banach’s fixed-point principle.

Proof. The set

\[ M(S_\delta) := \{ r \in W^{1,4}(S_\delta) : r(t) \in [s_0, M_{\eta \delta} + s_0] \} \]

for all \( t \in S_\delta, r'(t) \geq 0 \) for a.e. \( t \in S_\delta, |r'|_{L^1(S_\delta)} \leq \delta M_{\eta \delta} \}

equipped with the metric

\[ \rho(r_1, r_2) = |r'_2 - r'_1|_{L^1(S_\delta)} \text{ for all } r_1, r_2 \in M(S_\delta) \]
is a non-empty closed subset of $W^{1,4}(S_d)$. $(M(S_d), \rho)$ forms a complete metric space. We show that the map

$$\mathcal{T} : M(S_d) \to W^{1,4}(S_d),$$

$$\mathcal{T} : s \mapsto (u, v_4) \text{ cf. } ((3.31), (3.12)) \text{ (see also Theorem 3.2)}$$

is a strictly contractive self-map, provided

$$0 < \delta \leq \delta_0 \text{ (see (4.58) for the choice of } \delta_0).$$

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

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

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

Set $w := w_2 - w_1$, where $w_i := (w_{i1}, w_{i2}, w_{i3}, w_{i4}, w_{i5}, w_{i6})^t$, $\lambda_i := (\lambda_{i1}, \lambda_{i2}, \lambda_{i3}, \lambda_{i4}, \lambda_{i5}, \lambda_{i6})^t$, $w_{ij} := u_{ij} - \lambda_{ij}$ $(i \in \{1, 2\}, j \in I_1 \cup I_2$). Furthermore, we set $\Delta \psi_T(t) := \psi_T(s_2(t), t) - \psi_T(s_1(t), t)$, $\Delta \eta_T(t) := \eta_T(s_2(t), t) - \eta_T(s_1(t), t)$, $\Delta s(t) := s_2(t) - s_1(t)$, $\Delta s'(t) := s_2'(t) - s_1'(t)$, $\Delta r(t) := r_2(t) - r_1(t)$, $\Delta r'(t) := r_2'(t) - r_1'(t)$ and $\Delta v_4 = v_{42} - v_{41}$.

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

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

$$\int_{S_d} |\Delta r'((\tau) \|^4 d\tau = \int_{S_d} |\Delta \psi_T((\tau) \|^4 d\tau \leq C^n \int_{S_d} |w(1, \tau) \|^4 d\tau.$$

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

$$\int_{S_d} |\Delta r'((\tau) \|^4 d\tau \leq C_n \varepsilon^4 \sup_{t \in S_d} |w(t)| \int_{S_d} ||w(\tau)||^2 d\tau.$$

We want to bound the quantities $\sup_{t \in S_d} |w(t)|^2$ and $\int_{S_d} ||w(\tau)||^2 d\tau$ from above. To this end, we subtract the variational formulation (3.31) written for $w_2$ from that one written for $w_1$, where in both expressions we use the test function $w = w_2 - w_1 \in V$. It yields

$$s_2 \sum_{i \in I_1} \frac{1}{2} \frac{d}{dt} |w_i(t)|^2 + (L - s_2) \sum_{i \in I_2} \frac{1}{2} \frac{d}{dt} |w_i(t)|^2 + \frac{1}{s_2} \sum_{i \in I_1} ||D_i w_i||^2$$

$$+ \frac{1}{(L - s_2)} \sum_{i \in I_2} ||D_i w_i||^2$$

\(^2\)The same argument shows that $\Delta v_4$ belongs to $W^{1,4}(S_d)$.\)
\[ \leq -\Delta s \sum_{i \in I_1} (w_{1i,t}, w_i) + \Delta s \sum_{i \in I_2} (w_{1i,t}, w_i) \]
\[ + \frac{1}{s_2} \sum_{i \in I_2} |\sqrt{D_i} w_i(1)|^2 \]
\[ + \frac{1}{L - s_2} \sum_{i \in I_2} |\sqrt{D_i} w_i(1)|^2 + \frac{\Delta s}{s_1 s_2} \sum_{i \in I_1} D_i (w_{1i,y}, w_{i,y}) \]
\[ - \frac{\Delta s}{(L - s_1)(L - s_2)} \sum_{i \in I_2} D_i (w_{1i,y}, w_{i,y}) \]
\[ + e(s'_1, w_1, w) - e(s'_2, w_2, w) + b_f(w_2, s_2, w) - b_f(w_1, s_1, w) \]
\[ + h(s'_2, w_{2,y}, w) - h(s'_1, w_{1,y}, w) \leq \sum_{\ell=1}^5 J_\ell, \]

where we are given

\[ J_1 := -\Delta s \sum_{i \in I_1} (w_{1i,t}, w_i), \]
\[ J_2 := \frac{\Delta s}{s_1 s_2} \sum_{i \in I_1} (D_i w_{1i,y}, w_{i,y}) - \frac{\Delta s}{(L - s_1)(L - s_2)} \sum_{i \in I_2} (D_i w_{1i,y}, w_{i,y}), \]
\[ J_3 := b_f(w_2, s_2, w) - b_f(w_1, s_1, w), \]
\[ J_4 := e(s'_1, w_1, w) - e(s'_2, w_2, w) + \frac{1}{s_2} \sum_{i \in I_2} |\sqrt{D_i} w_i(1)|^2 \]
\[ + \frac{1}{L - s_2} \sum_{i \in I_2} |\sqrt{D_i} w_i(1)|^2, \]
\[ J_5 := h(s'_2, w_{2,y}, w) - h(s'_1, w_{1,y}, w). \]

To estimate \( J_\ell (\ell \in \{1, \ldots, 5\}) \), 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

\[ K_3 := 1 + \epsilon \sum_{i \in I_1 \cup I_2} D_i + \frac{P_1 Q_1 + P_2}{2} + k_3^2 + S_{3, \text{diss}} |u_{3,eq}|^2_{\infty} \]
\[ + (P_2 k_1)^2 + (P_1 Q_1 k_2)^2 + 2\epsilon \varepsilon^2 L^2 \tilde{c}^4 + \epsilon \tilde{c} (1 + \bar{k}^2) + \epsilon \bar{c} \epsilon \varepsilon^2 \tilde{c}^2, \]

where \( \tilde{c} = \tilde{c}(C_\eta, k_1, k_2, k_3) \geq 3C_\eta + 3M_{\eta r} + k_1 + k_2 + k_3^2 + \frac{L - L_2 + \delta a}{\varepsilon (L - L_2)} \sum_{i \in I_1 \cup I_2} D_i \). It is worth noticing that \( K_3 \) is bounded above, invariant with respect to \( t \) and depends on the choice of \( L, L_0, s_0, c_\xi, c_\tilde{c}, \tilde{c}, \theta, k_1 \) and \( D_i \) \((i \in I_1 \cup I_2)\).

We proceed with finding out an upper margin of \( \sum_{\ell=1}^5 |J_\ell| \). The bound of \( |J_1| \) is

\[ |J_1| \leq \frac{|\Delta s|^2}{2} |w_{1i,t}|^2 + \frac{|w|^2}{2}. \]

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

\[ |J_2| \leq \frac{|\Delta s|}{s_1 s_2} \sum_{i \in I_1} D_i |w_{1i}| |w_i| + \frac{|\Delta s|}{(L - s_1)(L - s_2)} \sum_{i \in I_2} D_i |w_{1i}| |w_i| \]
There exists a constant $\text{Fix}$ (4.38)

Rearranging the last two expressions, we obtain

\[
20 \leq \xi \sum_{i \in \mathcal{I}_1} \left( \frac{\|w_i\|^2}{s_2^2} + \xi \sum_{i \in \mathcal{I}_2} \frac{\|w_i\|^2}{(L - s_2)^2} + c_\xi \left( \sum_{i \in \mathcal{I}_1} \left( \frac{D_1 \|w_{1i}\|}{s_1^2} \right)^2 + \sum_{i \in \mathcal{I}_2} \left( \frac{D_1 \|w_{1i}\|}{(L - s_1)^2} \right)^2 \right) \right) |\Delta s|^2
\]

\[
\leq \xi \sum_{i \in \mathcal{I}_1} \frac{\|w_i\|^2}{s_2^2} + \xi \sum_{i \in \mathcal{I}_2} \frac{\|w_i\|^2}{(L - s_2)^2} + K_3 \left( \frac{1}{s_1^2} + \frac{1}{(L - s_1)^2} \right) \|w_1\|^2 |\Delta s|^2
\]

\[
|J_3| \leq \frac{|\Delta s|^2}{2} + \left[ (P_1 Q_1 k_2)^2 + (P_2 k_1)^2 + \frac{P_1 Q_1 + P_2}{2} \right] (|w_1|^2 + |w_2|^2)
\]

(4.36) \quad + \frac{|\Delta s|^2}{2} + S_{\text{dist}}^2 |w_3|^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.

To bound $|J_4|$, we use (A) and the special structure of the boundary term $c(s', w_i, w)$.
We obtain

\[
|J_4| \leq \left| \Delta \eta w_1(1) + s'_2 w_1(1)^2 + \Delta s' k_1 w_1(1) + s'_2 w_1(1)^2 + \Delta s' k_1 w_2(1) \\
+ \Delta \eta w_3(1), - s'_2 w_3(1)^2 + \Delta s' k_3 w_3(1) - \Delta \eta w_5(1) \right| (-1)
\]

\[
+ \left( \frac{1}{s_0} + \frac{1}{L - L_0} \right) \sum_{i \in \mathcal{I}_1 \cup \mathcal{I}_2} D_i |w_i(1)|^2
\]

(4.37) \quad \leq \frac{3}{2} |\Delta s'|^2 \xi \sum_{i \in \mathcal{I}_1} \frac{||w_i||^2}{s_2^2} + \xi \sum_{i \in \mathcal{I}_2} \frac{||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

\[
J_{51} := s_2 \frac{s'_2}{s'_2} \sum_{i \in \mathcal{I}_1} (yw_{2i,y}, w_i) - s_1 \frac{s'_1}{s_1} \sum_{i \in \mathcal{I}_1} (yw_{1i,y}, w_i)
\]

\[
J_{52} := (L - s_2) \frac{s'_2}{L - s_2} \sum_{i \in \mathcal{I}_2} ((2 - y)w_{2i,y}, w_i) - (L - s_1) \frac{s'_1}{L - s_1} \sum_{i \in \mathcal{I}_2} ((2 - y)w_{1i,y}, w_i).
\]

Rearranging the last two expressions, we obtain

\[
\frac{1}{L} |J_{51}| \leq \left( \frac{|\Delta s'|}{s_2} + \frac{s'_1}{s_1 s_2} |\Delta s| \right) \sum_{i \in \mathcal{I}_1} |(yw_{2i,y}, w_i)| + \frac{s'_1}{s_1} \sum_{i \in \mathcal{I}_1} |(yw_{i,y}, w_i)|,
\]

\[
\frac{1}{L} |J_{52}| \leq \left( \frac{|\Delta s'|}{L - s_2} + \frac{s'_1}{(L - s_1)(L - s_2)} |\Delta s| \right) \sum_{i \in \mathcal{I}_2} |((2 - y)w_{2i,y}, w_i)|
\]

(4.38) \quad + \frac{s'_1}{L - s_1} \sum_{i \in \mathcal{I}_2} |((2 - y)w_{i,y}, w_i)|.

Fix $i \in \mathcal{I}_1$ arbitrarily. Let us now estimate each of the terms $J_{5k}$ ($k \in \{1, 2\}$). We have

\[
(yw_{2i,y}, w_i) = w_{2i}(1)w_i(1) - \int_0^1 w_{2i}w_i dy - \int_0^1 yw_{2i}w_{i,y} dy.
\]

There exists a constant $c = c(\tilde{k}) > 0$ such that

\[
|(yw_{2i,y}, w_i)| \leq c|w_i(1)| + |w_{2i}||w_i| + |w_{2i}||w_i|.
\]

(4.39)
To deal with the last two terms in (4.40), we use the following strategy:

\[ \frac{|\Delta s'|}{s_2} |(yw_{2i}, w_i)| \quad \text{and} \quad \frac{s'_i}{s_1 s_2} |\Delta s||yw_{2i}, w_i| \]

as follows:

\[ \frac{|\Delta s'|}{s_2} |(yw_{2i}, w_i)| \leq c\bar{c}|\Delta s'| \left( \frac{|w_i|}{s_2} \right)^\theta |w_1|^{1-\theta} s_2^{\theta-1} + \frac{|\Delta s'|^2}{2} + \bar{k}_2 \left( \frac{|w_i|}{s_2} \right)^2 \\
+ c\bar{c}\bar{k} \left( \frac{|w_i|}{s_2} \right)^2 + \xi \left( \frac{s'_i}{s_1} \right)^2 k^2 |\Delta s|^2. \]

By Lemma 4.1 (in which we set \( \theta = \frac{1}{2} \)), we gain the estimate

\[ \frac{s'_i}{s_1} |(yw_{2i}, w_i)| \leq \xi \left( \frac{|w_i|}{s_2} \right)^2 + K_3 \left( \frac{s'_i}{s_1} \right)^2 s_2^2 |w_i|^{2}. \]

Collecting the last three inequalities for all \( i \in I_1 \), we obtain

\[ \frac{1}{L} |J_{51}| \leq \sum_{i \in I_1} \left[ |\Delta s|^2 \left( \frac{1}{2} + K_3 \left( \frac{s'_i}{s_1} \right)^2 \right) + |\Delta s'|^2 \left( \frac{1}{2} + K_3 \right) + 3\xi \left( \frac{|w_i|}{s_2} \right)^2 \right] \\
+ K_3 \left( \frac{1}{s_2} + \left( \frac{s'_i}{s_1} \right)^2 \right) \sum_{i \in I_1} |w_i|^2 \\
+ \sum_{i \in I_1} \left[ \frac{c\bar{c}s'_i}{s_1 s_2^{1-\theta}} |\Delta s| \left( \frac{|w_i|}{s_2} \right)^\theta |w_1|^{1-\theta} \right. \left. + c\bar{c}|\Delta s'| \left( \frac{|w_i|}{s_2} \right)^\theta |w_1|^{1-\theta} s_2^{\theta-1} \right] |w_i|^2. \]

To deal with the last two terms in (4.40), we use the following strategy:

\[ \sum_{i \in I_1} \frac{c\bar{c}s'_i}{s_1 s_2^{1-\theta}} |\Delta s| \left( \frac{|w_i|}{s_2} \right)^\theta |w_1|^{1-\theta} \leq \xi |\Delta s|^2 + \\
+ \xi c\xi \sum_{i \in I_1} \left( \frac{|w_i|}{s_2} \right)^2 + c\bar{c}c\xi (c\bar{c})^{\frac{1}{\theta}} \left( \frac{s'_i}{s_1 s_2^{1-\theta}} \right) \sum_{i \in I_1} |w_i|^2. \]

The last term is estimated in the same manner. We obtain

\[ \frac{1}{L} |J_{51}| \leq |\Delta s|^2 \left( 2 + 2\bar{c} + 4K_3 \left( \frac{s'_i}{s_1} \right)^2 \right) + |\Delta s'|^2 \left( 2 + 2\bar{c} + 4K_3 \right) + \\
+ \xi (3 + 2\bar{c}^2) \sum_{i \in I_1} \left( \frac{|w_i|}{s_2} \right)^2 + \\
+ K_3 \left( \frac{1}{s_2} \left( 1 + \frac{1}{s_2} \right) \left( \frac{s'_i}{s_1} \right)^2 \left( \frac{s_2}{s_2} + \frac{1}{s_2} \right) \right) \sum_{i \in I_1} |w_i|^2. \]
The bound on $|J_{52}|$ follows similarly. This reads

$$\frac{1}{L}|J_{52}| \leq (1 + \bar{\xi} + 2K_3)|\Delta s'|^2 + \left(1 + \bar{\xi} + 2K_3 \left(\frac{s'_1}{L - s_1}\right)^2\right) |\Delta s|^2 +$$

$$+ \xi \left(3 + 2c_{\bar{\xi}}\right) \sum_{i \in I_2} \frac{||w_i||^2}{(L - s_2)^2} +$$

$$+ K_3 \left[\frac{1}{L - s_2} + \frac{1}{(L - s_2)^2} + \frac{(s'_1)^2}{(L - s_1)(L - s_2)} + \left(s'_1 \frac{1}{L - s_1}\right)^2\right] \times$$

$$\times \left(\frac{1}{L - s_2} + (L - s_2)^2\right) \sum_{i \in I_2} |w_i|^2.$$

Finally, it yields

$$\frac{1}{L}|J_5| \leq \left[3 + 3\bar{\xi} + 4K_3 \left(\frac{s'_1}{s_1}\right)^2 + 2K_3 \left(\frac{s'_1}{L - s_1}\right)^2\right] |\Delta s|^2 +$$

$$+ (3 + 3\bar{\xi} + 6K_3) |\Delta s'|^2$$

(4.42)

$$+ \xi \left(3 + 2c_{\bar{\xi}}\right) \left(\sum_{i \in I_1} \frac{||w_i||^2}{s_2^2} + \sum_{i \in I_2} \frac{||w_i||^2}{(L - s_2)^2}\right) + K_3 \chi_1(t)|w|^2,$$

where the expression of $\chi_1(t)$ is given by

$$\chi_1(t) := \frac{1}{s_2(t)} + \frac{1}{L - s_2(t)} + \frac{1}{s_2^2(t)} + \frac{1}{(L - s_2(t))^2} + \left(\frac{s'_1(t)}{s_1(t)}\right)^2 \left(\frac{2}{s_2(t)} + \frac{1}{s_2(t)}\right)$$

$$+ \left(\frac{s'_1(t)}{L - s_1(t)}\right)^2 \left(\frac{2}{L - s_2(t)} + \frac{1}{L - s_2(t)}\right) + \frac{(s'_1(t))^2}{(L - s_1(t))(L - s_2(t))},$$

for a.e. $t \in S_\bar{\xi}$. Summing up the bounds on $|J_i|$, it yields

(4.43)

$$|J| \leq a(t)|\Delta s|^2 + b(t)|\Delta s'|^2 + c(t)|w|^2$$

$$+ d(\xi, \bar{\xi}) \left(\sum_{i \in I_1} \frac{||w_i||^2}{s_2^2} + \sum_{i \in I_2} \frac{||w_i||^2}{(L - s_2)^2}\right) +$$

where the factors $a(t)$, $b(t)$ and $c(t)$ (with $t \in S_\bar{\xi}$) are defined by

$$a(t) := \frac{|w_{1,t}|^2}{2} + \frac{3}{2} + K_3 \left(\frac{1}{s_2^2(t)} + \frac{1}{(L - s_1(t))^2}\right) ||w_1(t)||^2$$

$$+ \left[3 + 3\bar{\xi} + 4K_3 \left(\frac{s'_1(t)}{s_1(t)}\right)^2 + 2K_3 \left(\frac{s'_1(t)}{L - s_1(t)}\right)^2\right],$$

$$b(t) := \frac{3}{2} + L(3 + 3\bar{\xi} + 6K_3),$$

$$c(t) := \frac{1}{2} + 2K_3 + LK_3 \chi_1(t),$$

and $d(\xi, \bar{\xi}) := 2\bar{\xi} + L\zeta(3 + 2c_{\bar{\xi}})$, where $c_{\bar{\xi}} = c_{\bar{\xi}}(\bar{\xi})$. Clearly, for any choice of $\xi > 0$ and $\bar{\xi} > 0$ there exist two real constants $\alpha_{\varepsilon_{\xi}}$ and $\beta_{\varepsilon_{\xi}}$ such that $0 < \alpha_{\varepsilon_{\xi}} < d(\xi, \bar{\xi}) < \beta_{\varepsilon_{\xi}}$.
On the other hand, there exists a constant $C = C(L, L_0, s_0, K_3, M_{nf}) \in \mathbb{R}_+^*$ such that

$$c(t) \leq C \text{ a.e. in } S_\delta.$$  \hspace{1cm} (4.44)

Insert (4.43) in (4.33). Choosing conveniently sufficiently small $\xi > 0$ and $\bar{\xi} > 0$, we are led to

$$|w(t)|^2 + d_0 \int_0^t ||w(\tau)||^2 d\tau \leq |w(0)|^2 + \int_0^t (a(\tau)|\Delta s(\tau)|^2 + b(\tau)|\Delta s'(\tau)|^2) d\tau$$  

$$+ \int_0^t c(\tau)|w(\tau)|^2 d\tau,$$  \hspace{1cm} (4.45)

where the strictly positive constant $d_0$ is given by

$$d_0 := \min \left\{ \min_{i \in I_1} \frac{s_0 D_i - d(\xi, \bar{\xi})}{L^2}, \min_{i \in I_2} \frac{(L - L_0) D_i - d(\xi, \bar{\xi})}{(L - s_0)^2} \right\}.$$  \hspace{1cm} (4.46)

We denote

$$N_1(t) := \frac{N_2(t)}{C} \quad \text{(with } C \text{ as in (4.44))},$$  

$$N_2(t) := c(t) N_3(t),$$  

$$N_3(t) := |w(0)|^2 + \int_0^t \left[ a(\tau)|\Delta s(\tau)|^2 + b(\tau)|\Delta s'(\tau)|^2 \right] d\tau.$$ 

The application of Gronwall’s inequality in (4.45) leads to

$$|w(t)|^2 \leq N_3(t) \exp \left( \int_0^t c(\tau) d\tau \right) \text{ a.e. } t \in S_\delta.$$  \hspace{1cm} (4.47)

It should be noted that the presence of the factors $||w_1(t)||^2$ and $|w_{1.1}|^2$ in the expression of $a(t)$ is not disturbing. Our only concern is to ensure, e.g., that $\int_0^t ||w_1(\tau)||^2|\Delta s(\tau)|d\tau$ stays bounded for a.e. $t \in S_\delta$. This follows due to the the energy estimate (4.17) and the inequality

$$\int_0^t \frac{d}{d\tau} \left( \int_0^\tau ||w_1(s)||^2 ds \right) |\Delta s(\tau)|^2 d\tau \leq |\Delta s(t)|^2 \int_0^t ||w_1(\tau)||^2 d\tau.$$ 

Also, it results that

$$\int_0^t ||w(\tau)||^2 d\tau \leq \frac{1}{d_0} (N_1(t) + N_3(t)) e^{Ct} \text{ a.e. } t \in S_\delta.$$  \hspace{1cm} (4.48)

Moreover, the inequality

$$|\Delta s(t)|^2 \leq t \int_0^t |\Delta s'(\tau)|^2 d\tau$$  \hspace{1cm} (4.49)

provides the estimate

$$\int_{S_\delta} |\Delta s(\tau)|^2 d\tau \leq \delta^2 \int_{S_\delta} |\Delta s'(\tau)|^2 d\tau.$$  \hspace{1cm} (4.50)
We show that
\begin{equation}
M_1 := \exp \left( \int_0^\delta c(\tau)d\tau \right) \left[ \max_{t \in S_\delta} \{ \delta^2 a(t) + b(t) \} \right]
\end{equation}
and
\begin{equation}
M_2 := \frac{2}{d_0} \exp(C \delta) \left[ \max_{t \in S_\delta} \{ \delta^2 a(t) + b(t) \} \right],
\end{equation}
satisfy
\begin{equation}
|w(t)|^2 \leq M_1 \sqrt{\delta} \left[ \int_0^t |\Delta s'(\tau)|^4 d\tau \right]^{\frac{1}{2}}
\end{equation}
and
\begin{equation}
\int_0^t ||w(\tau)||^2 d\tau \leq M_2 \sqrt{\delta} \left[ \int_0^t |\Delta s'(\tau)|^4 d\tau \right]^{\frac{1}{2}}.
\end{equation}

The constants $M_1$ and $M_2$ depend only on $\delta$, $\theta$, $S_0$, $L$, $L_0$, $C$, $c_\xi$, $c_\bar{\xi}$ and $k_i(i \in I)$.

The statements (4.53) and (4.54) follow in a straightforward way. On one hand, by (4.44), (4.49) and (4.50), we have
\begin{equation*}
|w(t)|^2 \leq N_3(t) \exp \left( \int_0^t c(\tau)d\tau \right) = \exp \left( \int_0^t c(\tau) d\tau \right) \times
\end{equation*}
\begin{equation*}
\times \left[ |w(0)|^2 + \int_0^t a(\tau)|\Delta s(\tau)|^2 + b(\tau)|\Delta s'(\tau)|^2 d\tau \right] \leq \exp \left( \int_0^t c(\tau)d\tau \right) \times
\end{equation*}
\begin{equation*}
\times \left[ \int_0^t [\delta^2 a(\tau) + b(\tau)] |\Delta s'(\tau)|^2 d\tau \right] \leq M_1 \sqrt{\delta} \left[ \int_0^t |\Delta s'(\tau)|^4 d\tau \right]^{\frac{1}{2}},
\end{equation*}
where $M_1$ satisfies (4.51). On the other hand, we use (4.47), (4.48), and the positivity of $N_1(t)$ and of $N_1'(t)$ (for a.e. $t \in S_\delta$), to establish
\begin{equation*}
\int_0^t ||w(\tau)||^2 d\tau \leq \frac{1}{d_0} \left( N_3(t) + \int_0^t N_2(\tau)e^{C\tau} d\tau \right)
\end{equation*}
\begin{equation*}
\leq \frac{1}{d_0} \left( N_3(t) + N_1(t) \right) e^{Ct}
\end{equation*}
\begin{equation*}
\leq \frac{2}{d_0} \exp(C t) \left[ \max_{t \in S_\delta} \{ \delta^2 a(t) + b(t) \} \right] \times
\end{equation*}
\begin{equation*}
\times \int_0^t |\Delta s'(\tau)|^2 d\tau \leq M_2 \int_0^t |\Delta s'(\tau)|^2 d\tau \leq M_2 \sqrt{\delta} \left[ \int_0^t |\Delta s'(\tau)|^4 d\tau \right]^{\frac{1}{2}},
\end{equation*}
where $M_2$ is given by (4.52). Combining (4.53), (4.54) in (4.32), it results that

$$
\int_{t_0}^{t} |\Delta r'(\tau)|^4 d\tau \leq M_3 \int_{t_0}^{t} |\Delta s'(\tau)|^4 d\tau,
$$

where the constant $M_3$ is given by

$$
M_3 := C_\eta \delta^4 M_1 M_2 \delta.
$$

We set

$$
\chi := \min\{C_\eta \delta^4 M_1 M_2, \frac{1}{\delta + 1}\},
$$

where we put

$$
0 < \delta \leq \frac{L_0}{M_{\eta^r}} := \delta_0.
$$

By (4.58), we ensure $s(\delta) \leq L_0$. Finally, using the Lipschitz constant $\delta \chi < 1$, the strict contractivity of the fixed-point operator $T$ is proven.

We now have the existence of a unique weak solution in the time interval $S_3 = [0, \delta[$. 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 $k + 1 < \frac{1}{4} T_{\text{fin}}$, where $T_{\text{fin}}$ is given by (3.37). This proves Theorem 3.3. Moreover, if $T_{\text{fin}} < +\infty$, then the last time interval on which the solution is proved to exist is $]k_m \delta, T_{\text{fin}}[$, where $k_m := \sup\{k \in \mathbb{N} : k + 1 < \frac{1}{4} T_{\text{fin}}\}$. Since the uniqueness is granted on each of the intervals $[0, \delta[$, $]k\delta, (k + 1)\delta[$, $]k_m \delta, k_m \delta[$, it actually holds on the whole $]0, T_{\text{fin}}[$. 

\[4.3.\] Sketch of the proof of Proposition 3.4. The idea of the proof is a refined version of the arguments that we have used to show the positivity of concentrations. We focus on getting lower bounds for $\text{Ca(OH)}_2(aq)$, $\text{CO}_2(aq)$ and $\text{CO}_2(g)$ concentrations and only tersely suggest how the lower bounds for the other concentrations are obtained.

We choose in the weak formulation (3.31) the test function

$$
\phi_i := \begin{cases} -|u_3 - u_3^* \gamma_3(t)|, & \text{for } i = 3 \\ 0, & \text{otherwise} \end{cases} \in V_i \text{ for all } i \in I_1 \cup I_2.
$$

In (4.59), the function $\gamma_3 \in C^1(S_3)$ has to be determined such that $\gamma_3'(t) \leq 0$ for all $t \in S_3$ and $\gamma_3(0) = 1$. On this way, we obtain the following identity

$$
(u_3 + \lambda_3)_+ \gamma_3 + \frac{D_3}{(L - s)^2} ||\phi_3||^2 = \frac{1}{L - s} (-\eta_t(u(1) + \lambda), \phi_3(1)) + s'(u_3(1) + \lambda_3, \phi_3(1)) + S_{2,\text{dis}}(u_3 + \lambda_3 - u_3, \phi_3) +
$$

$$
\frac{s'}{L - s} ((2 - y)\phi_3, \phi_3).
$$

We collect some of the terms in (4.60), add the positive term $\lambda \gamma_3(t) - \theta u_3^*, \phi_3$ to its right-hand side, and conveniently select $u_3^*$ within the interval $[0, \min_{S_3} \lambda_3(t)]$. The constants $\zeta > 0$ and $\theta > 0$ are chosen such that

$$
\zeta \gamma_3(t) - \theta > 0 \text{ for all } t \in [0, \infty] \text{ and } \lim_{t \to \infty} (\zeta \gamma_3(t) - \theta) > 0.
$$

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Thus, we obtain
\[ \frac{1}{2} \frac{d}{dt} |\varphi_3|^2 + \frac{D_3}{(L-s)^2} ||\varphi_3||^2 \leq \frac{1}{L-s} (\eta u(1) + \lambda) + \\
+ s'(u_3(1) + \lambda_3, \varphi_3(1)) + S_{3,\text{diss}} |\varphi_3|^2 + S_{3,\text{diss}} (\lambda_3 - u_3, \varphi_3) - \\
- (u_3^* \gamma_3'(t) + \lambda_3, \varphi_3) - (\zeta u_3^* \gamma_3(t) - \theta u_3^*, \varphi_3) + \frac{s'}{L-s} (2-y) \varphi_3, \varphi_3. \]
(4.62)

We state the following auxiliary result:

*Lemma 4.4.* Assume that the hypotheses of Theorem 3.3 are satisfied. Additionally, let \( \lambda_3 \in W^{1,2}(S_\delta) \) and set \( s := -S_{3,\text{diss}} + \zeta, \rho := \frac{1}{u_3} (\lambda_3 - S_{3,\text{diss}} \lambda_3 + S_{3,\text{diss}} u_3, \varphi_3) \), \( \chi := \rho - \theta \), where \( \zeta \) and \( \theta \) are positive constants satisfying (4.61). The following statements hold:

(i) If \( \lambda_3 = \text{const} \), and if

\[ \zeta \in \max \{ S_{3,\text{diss}}, \frac{\sigma \theta}{\theta - \rho} \}, +\infty \]

then the function

\[ \gamma_3(t) = -\frac{\chi}{\sigma} + \frac{\sigma + \chi}{\sigma} e^{-\sigma t} \]

for all \( t \in [0, \infty) \)

is the unique positive solution of the problem

\[ \gamma_3'(t) + \sigma \gamma_3(t) + \chi(t) = 0, \gamma_3'(t) < 0 \]

for all \( t \in [0, \infty) \) with \( \gamma_3(0) = 1 \).

(ii) If \( \lambda_3 = \lambda_3(t) \neq \text{const} \), \( \rho \in L^2(0, \infty) \), and

\[ \sigma - \sigma \int_0^t \chi(\tau)e^{\sigma \tau} d\tau + \chi(t)e^{\sigma t} > 0 \]

for all \( t \in [0, \infty) \),

then

\[ \gamma_3(t) = \left( 1 - \int_0^t \chi(\tau)e^{\sigma \tau} d\tau \right) e^{-\sigma t} \]

for all \( t \in S_\delta \)

is the unique positive solution of (4.65).

*Proof.* [of Lemma 4.4] The choice of the test function (4.64) (or (4.67)) relies on the sign restrictions \( \rho > 0 \), \( \sigma > 0 \), \( \chi < 0 \) as well as on (4.61), (4.63), and (4.66). These estimates support the existence and uniqueness of a strictly positive and bounded function \( \gamma_3 \). The statements (i) and (ii) follow by straightforward verification. \( \square \)

Now, with \( \gamma_3(t) \) as in Lemma 4.4 we force the fourth, fifth and sixth term from the right-hand side of (4.62) to vanish. Combining Young’s inequality and the interpolation inequality (4.1), we obtain:

\[ \frac{1}{2} \frac{d}{dt} ||\varphi_3||^2 + \frac{D_3}{(L-s)^2} ||\varphi_3||^2 \leq \frac{1}{L-s} ((2-y) \varphi_3, \varphi_3) \leq \frac{\xi}{2} ||\varphi_3||^2 + \frac{\delta}{2} e^{\xi} \delta ||\varphi_3||^2 \leq \frac{\xi}{2} ||\varphi_3||^2 + \frac{\delta}{2} e^{\xi} \delta ||\varphi_3||^2, \]

where we select \( \xi \in [0, 2D_3] \). Since \( \varphi_3(0) = 0 \), we can use Gronwall’s inequality to conclude that \( u_3 \geq u_3^* \gamma_3(t) > 0 \) for all \( t \in S_\delta \).

Note that the choice of \( \gamma_3 \) does not depend on \( \delta \).

We choose in the weak formulation (3.31) the test functions

\[ \varphi_i := \begin{cases} -[u_i - u_i^* \gamma_i(t)]^- & \text{for } i \in \{1, 2\} \\
0, & \text{otherwise} \end{cases} \in V_i \text{ for all } i \in I_1 \cup I_2. \]

(4.68)
Select $i \in \{1, 2\}$. In (4.68) $u_i^* > 0$ are given constants and the functions $\gamma_i \in C^1(\bar{S}_\delta)$ have to be determined such that $\gamma_i'(t) \leq 0$ for all $t \in S_\delta$ and $\gamma_i(0) = 1$. It makes sense to look for $u_i^*$ in the interval $[0, \min_{S_\delta} \lambda_i(t)]$. We want to determine the function $\gamma_i$ such that $u_i^* \gamma_i$ margins the concentration $u_i$ from below. Moreover, for sufficiently large time $t$ we want that $u_i^* \gamma_i(t)$ decreases to some strictly positive value. We have that

\[
(u_1 + \lambda_1)_t, \varphi_1 + \frac{D_1}{s^2}(u_{1,y}, \varphi_{1,y}) + \frac{1}{s}(\eta r(u + \lambda_1), \varphi_1(1)) + \frac{s'}{s}(u_1(1) + \lambda_1, \varphi_1(1)) = P_1(Q_1(u_2 + \lambda_2) - (u_1 + \lambda_1), \varphi_1) + y\frac{s'}{s}(u_{1,y}, \varphi_1),
\]

\[
(u_2 + \lambda_2)_t, \varphi_2 + \frac{D_2}{s^2}(u_{2,y}, \varphi_{2,y}) + \frac{s'}{s}(u_2(1) + \lambda_2, \varphi_2(1)) = -P_2(Q_2(u_2 + \lambda_2) - (u_1 + \lambda_1), \varphi_2) + y\frac{s'}{s}(u_{2,y}, \varphi_2).
\]

Taking $\varphi_i$ as in (4.68), we obtain

\[
\frac{1}{2} \frac{d}{dt} |\varphi_1|^2 + \frac{D_1}{s^2}||\varphi_1||^2 = -\frac{1}{s}(\eta r(u + \lambda_1), \varphi_1(1)) - \frac{s'}{s} |\varphi_1(1)|^2
\]

\[
+ y\frac{s'}{s}(\varphi_{1,y}, \varphi_1) - \frac{s'}{s}(u_i^* \gamma_i(1) + \lambda_1, \varphi_1(1)) - (\lambda'_1 + P_1 \lambda_1 - P_1 Q_1 \lambda_2, \varphi_1)
\]

(4.69)

\[
- (u_i^* \gamma_1', \varphi_1) + P_1 Q_1(u_i^* \gamma_2(t), \varphi_1) - P_1(u_i^* \gamma_1(t), \varphi_1) + P_1(Q_1 \varphi_2 - \varphi_1, \varphi_1)
\]

and respectively,

\[
\frac{1}{2} \frac{d}{dt} |\varphi_2|^2 + \frac{D_2}{s^2}||\varphi_2||^2 = -\frac{s'}{s} |\varphi_2(1)|^2 + y\frac{s'}{s}(\varphi_{2,y}, \varphi_2) - \frac{s'}{s}(u_i^* \gamma_2(t), \lambda_2, \varphi_2(1))
\]

\[
- (\lambda'_2 + P_2 Q_2 \lambda_2 - P_2 \lambda_1, \varphi_2) - (u_i^* \gamma_2', \varphi_2) + P_2 Q_2(-u_i^* \gamma_2(t), \varphi_2)
\]

(4.70)

\[
+ P_2(u_i^* \gamma_1(t), \varphi_2) - P_2(Q_2 \varphi_2 - \varphi_1, \varphi_2).
\]

We make use of the next auxiliary result:

**Lemma 4.5.** Assume that (C3) and the hypotheses of Theorem 3.3 are satisfied. Additionally, let $\lambda_1 \in C^2(\bar{S}_\delta)$, $\lambda_2 \in C^1(\bar{S}_\delta)$, $u_i^* > 0$ and $u_i^* > 0$. The problem (4.71)-(4.73)

\[
\gamma_1' - P_1 Q_1 \frac{u_2}{u_1^*} \gamma_2 + P_1 \gamma_1 = -\frac{\lambda'_1 + P_1 \lambda_1 - P_1 Q_1 \lambda_2}{u_1^*},
\]

(4.71)

\[
\gamma_2' + P_2 Q_2 \gamma_2 - \frac{P_2 u_2}{u_1^*} \gamma_1 = -\frac{\lambda'_2 + P_2 Q_2 \lambda_2 - P_2 \lambda_1}{u_2^*},
\]

(4.72)

\[
\gamma_1(0) = \gamma_2(0) = 1, \gamma'_i \leq 0 \text{ in } S_\delta.
\]

(4.73)

has a unique positive solution in $C^1(\bar{S}_\delta) \times C^1(\bar{S}_\delta)$.

**Proof.** [of Lemma 4.5] The idea of the proof is rather simple: We formulate (4.71)-(4.73) as a second-order non-homogeneous differential equation. We solve this explicitly. Explicit ranges of model parameters are needed in order to ensure (4.73). The conclusion of the lemma follows by straightforward verification. \[ \Box \]

By Lemma 4.5, several terms from (4.69) and (4.70) cancel out. More precisely, the first four terms as well as the last one on the right-hand side of (4.69) remain, but the other vanish. On the right-hand side of (4.70), the first three terms and the last one stay, but the rest of them vanish. In this way, we obtain once more the
inequalities employed for the positivity of the concentrations \( u_1 \) and \( u_2 \). We conclude via the same Gronwall-type argument that

\[
u_1 > u_{1*}^r \gamma_1(t) \quad \text{and} \quad u_2 > u_{2*}^r \gamma_2(t) \quad \text{for a.e. } t \in S_5.
\]

Since reaction (1.1) produces water, there is no difficulty to show that the initial conditions \( \hat{u}_{50} \) and \( \hat{u}_{60} \) are the strict lower bounds of \( u_5 \) and \( u_6 \).

5. Illustration of \( \text{CO}_2 \) 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 [13]. 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 (\( P_\Gamma \)). 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 [30], while a priori and a posteriori error estimates for the semi-discrete approximation are derived in [29]. The plots in Fig. 5.1–5.2 show the solution of (\( P_\Gamma \)). Observe that steep concentration 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 $\eta_r$ and on the range of the effective diffusion coefficient of CO$_2$(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 CO$_2$(g) produces a significant increase in the penetration depth. In Fig. 5.3 (b), we observe that if CO$_2$(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 CO$_2$(g) molecules is to be expected. Another issue is illustrated in Fig. 5.4 and Table 5.1. Namely, we use the standard set of parameters (see [30] (appendix D)) to compare the numerical lower bounds with the theoretical lower bounds in the case of Ca(OH)$_2$(aq) concentration.

For the chosen parameter set, where we additionally select $u^*_3/5 = 10^{-3}$ and take $\gamma_3(t)$ as in (4.64), the theoretical lower bounds underestimate the numerical ones along the whole computation time. This underestimation of the lower bounds yields an overestimation of the final time of the process $T_{\text{fin}}$. Also, we observe a decrease in time of the numerical lower bound for Ca(OH)$_2$(aq), see the broken curve in Fig. 5.4. This effect is mainly due to the continuous depletion of alkaline species by carbonation. On the other hand, a slight increase in time of the theoretical lower bound on the
same species can be noticed in Fig. 5.4 (the continuous curve). The latter effect is a direct consequence of the influence of the production term by dissolution.

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.

REFERENCES

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