Error bounds on a semi-discrete finite element approximation of the weak solution to a one phase moving-boundary system describing concrete carbonation

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Error bounds on a semi-discrete finite element approximation of the weak solution to a one phase moving-boundary system describing concrete carbonation

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Abstract

Galerkin approximations to solutions of a one-phase one-dimensional moving-boundary system describing the penetration of the carbonation of concrete are considered. The semi-discretization in space with piecewise linear finite elements is examined in order to obtain a priori and a posteriori error estimates for the semi-discrete fields of active concentrations and for the position of the moving-reaction interface. The main feature of the problem is that the non-linear coupling of the system occurs due to the presence of the moving boundary and non-linearity of the products by reaction.

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1 Introduction

In many real-world applications we frequently need to determine both the a priori unknown domain, where the problem is stated, as well as the solution itself. Such problems are typically named moving or free boundary problems. A particularly important problem of this kind refers to the determination of the depth at which molecules of gaseous carbon dioxide succeed to penetrate concrete-based structures. The phenomenon is of particular importance if we think of the concrete structures durability. The main feature of the process is that gaseous carbon dioxide from the ambient air penetrates through the porous fabric of the unsaturated concrete, dissolves in pore water and reacts with calcium hydroxide, which is available by dissolution from the solid matrix. Calcium carbonate and water are therefore formed via the reaction mechanism

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

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The physicochemical process associated with (1) is called concrete carbonation. Although this chemical reaction seems to be harmless (i.e., not corrosive), it may produce unwanted microstructural changes, and hence, it represents one of the most important reaction-diffusion scenarios which can essentially affect the service life of concrete-based structures. Note that, in combination with ingress of aggressive ion species (like chloride or sulfate), the carbonation typically facilitates corrosion, and hence, spalling of the concrete may occur. We refer to [Cha98] and references therein for details on concrete carbonation.

The present work represents a pre-study in what the investigation of semi-discrete variants for two-phase moving sharp-interface carbonation models is concerned. The one dimensional form of this problem is obtained by thinking of the slab $[0, L]$ ($L > 0$) (to which the model, which we state in section 2, refers) to be away from corners or any other type of geometric irregularities. Solving the moving-boundary model means in our case the calculation of the involved mass concentrations and determination of the a priori unknown position of the moving boundary (here: sharp-reaction front).

Several moving-boundary models have been recently proposed in [BKM03a, BKM03b, M06b] (and analyzed by the author in [M08]) to numerically illustrate the carbonation penetration into a large class of concrete-based materials. In the present framework, we follow other aims: We use the standard continuous time Galerkin method (see, for instance, [Joh94, IT03, Tho97] for an introduction to the subject) to investigate a semi-discrete FEM approximation. Specifically, we examine the semi-discretization in space with piecewise linear finite elements in order to investigate a few qualitative features of the ad hoc FEM approximation that we have employed in chapter 4 of [M08]. Now, our goal is to prove that the spatially semi-discrete solutions converge to the solution of the carbonation model in question when the mesh size decreases to zero. The error estimates will show an order of convergence of $O(h)$ for the FEM semi-discretization of the model, where $h$ denotes the maximum mesh size.

The a posteriori error estimate, which we also point out in this frame, may be of use when implementing 1D adaptive FEM schemes to solve moving-interface carbonation models. It is worth noticing that in [SM05] heuristic a posteriori estimates of the approximation error were used in order to calculate adaptively with ALBERTA (cf. [SS05]) the 2D penetration of an aggressive reaction front in concrete.

With our theoretical a posteriori estimate we hope to contribute to the understanding of 1D adaptive simulations of concrete carbonation when the carbonated and uncarbonated parts are separated by moving boundaries. The 2D case remains open for further study for both the moving-boundary scenario and when the model is formulated in fixed domains.

The paper is organized in the following fashion: We state our problem in section 2. A few remarks on the system (3)-(11), which represents the moving-boundary problem in study, are given in section 3. Section 4 collects technical preliminaries and section 5 presents the main assumptions on which our error analysis relies. Along the lines of this section, we prepare a suitable functional framework and the concept of weak solution that we use in the sequel. In section 6, we state the main results of this paper, whereas in sections 7 and section 8 we

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1 With the terminology from [M08], we prepare the basic framework for the error analysis of the full semi-discrete $P_1$ model.

2 In this paper, an isothermal model was employed to simulate the process, the moving front being defined using the concept of carbonation degree.
prove them. Finally, we draw a few conclusions and further remarks in section 9.

2 Statement of the problem

We analyze a semi-discrete finite element method to approximate the solution of a moving-boundary system modeling CO$_2$ penetration in concrete. In order to write down the mass-balance equations we denote the mass concentrations of the active species as follows:

Let $u_1$ and $u_2$ be the concentration of CO$_2$(g) and CO$_2$(aq), respectively. $u_3$ refers to the CaCO$_3$(aq) concentration, while $u_4$ denotes the Ca(OH)$_2$(aq) concentration. Finally, $u_5$ represents the moisture concentration produced by (1) in the reacted phase.

The problem reads: Find the concentrations vector $u = u(x, t) \ (x \in \Omega_1(t) = [0, s(t)], t \in S_T = [0, T]$ with $T > 0$) and the position $s(t)$ ($t \in S_T$) of the interface $\Gamma(t) = \{x = s(t) : t \in S_T\}$ such that the couple $(u, s)$ satisfies the following set of model equations$^3$:

\begin{align*}
  u_{1,t} - D_1 u_{1,xx} &= P_1(u_1 u_3 - u_1) \quad \text{in } \Omega_1(t) \quad (2) \\
  u_{2,t} - D_2 u_{2,xx} &= -P_2(u_2 u_3 - u_1) \quad \text{in } \Omega_1(t) \quad (3) \\
  u_{3,t} &= S_{3,\text{dist}}(u_{3,eq} - u_3) \quad \text{at } \Gamma(t) \quad (4) \\
  u_{4,t} - D_4 u_{4,xx} &= 0 \ (t \in \{4, 5\}), \quad \text{in } \Omega_1(t), \quad (5)
\end{align*}

initial conditions

\begin{align*}
  u_i(0, x) &= u_{i,0}(x) \quad \text{in } \Omega_i(0) \ (i \in \{1, 2, 3, 4, 5\}), \quad (6)
\end{align*}

and boundary conditions

\begin{align*}
  u_i(t, 0) &= \lambda_i(t), \quad t \in S_T \ (i \in \{1, 2, 4, 5\}) \quad (7) \\
  -D_1 u_{1,x}(s(t), t) &= \eta_T(u(s(t), t) + s'(t)u_1(s(t), t)) \quad (8) \\
  -D_2 u_{2,x}(s(t), t) &= \eta_T(u(s(t), t) + s'(t)u_2(s(t), t)) \quad (9) \\
  -D_4 u_{4,x}(s(t), t) &= \eta_T(u(s(t), t) + s'(t)u_4(s(t), t)) \quad (t \in \{4, 5\}) \quad (10)
\end{align*}

The couple $(u, s)$ also needs to satisfy the relations

\begin{align*}
  s'(t) = \eta_T(u(s(t), t)), \quad t \in S_T \quad (t(0) = s_0) \quad (11)
\end{align*}

in order to close the system.

To formulate (2)-(11), a set of model parameters are employed. In the sequel, we assume the following restrictions on these parameters

Assumption (1) Select

\begin{align*}
  &D_1, P_1, Q_1, \lambda_i, u_{3,eq}, S_{3,\text{dist}} \in \mathbb{R}_+^+ \ (i \in \{1, 2, 4, 5\}, j \in \{1, 2\}) \quad (12) \\
  &\lambda_i, u_{3,eq} : S_T \to \mathbb{R}_+^+, \ u_{i,0} : \Omega_i(0) \to \mathbb{R}_+^+ \ (i \in \{1, 2, 3, 4, 5\}) \text{ are given functions,} \quad (13)
\end{align*}

$^3$The underlying model represents a simplified case of a more general moving sharp-interface model, which was developed in [Munk].
\begin{equation}
\begin{aligned}
s_0 &> 0, \\
s_0 &\leq s(t) \leq L,
\end{aligned}
\end{equation}

where \(L\) is the precise length of the 1D geometry in question.

Under Assumption (1), the model (2)-(11) consists of a weakly coupled system of semi-linear parabolic differential equations (2)-(10) to be simultaneously solved together with the non-local ode (11), which drives the reaction interface \(\Gamma(t)\). We refer to (11) as the non-linear kinetic condition that governs the movement of the reaction interface. Notice that once the domain \(\Omega(t)\) is determined, equation (4) decouples from the system and can be solved exactly. Although it produces no mathematical difficulties, we keep it in the system formulation mainly because of its physical meaning, see [Mun08] for details.

3 Further remarks on (2)-(11)

Let us also notice the following facts

1. Details on the modeling, analysis and simulation of the concrete carbonation based on the moving-boundary methodology are given in [Mun03, MB06a]. We only mention that, employing the same techniques from [Mun06], locally in time positive weak solutions to (2)-(11) exist, are unique and depend continuously on data and parameters, see section 5 (especially Theorem 5.3) for some details.

2. The system (2)-(11) does act exclusively refer to concrete carbonation. It can also be imagined as a first attempt to model sulfate attack on concrete pipes, see [BDJR98]. For similar reaction-diffusion scenarios arising in geochemistry, we refer to the book by Ortoleva [Ort94].

3. Conceptually, the classical problem of ice melting (the Stefan problem, see [Cra84]) is very often considered as prototype when formulating models like (2)-(11). At the numerical level, there exist many approaches dealing with the error analysis of the finite element approximation of the weak solution to the classical one-dimensional one-phase Stefan problem. To our knowledge, Nitsche (cf. [Nit78, Nie80]) was the first who analyzed the semi-discrete one-phase Stefan problem and obtained an optimal error estimate in the \(W^{1,\infty}\)-norm for the interface position. He employed the fixed-front technique of Landau [Lan60] in order to freeze the boundaries of the moving phase and examined the transformed one in the fixed-domain. For further developments of his working technique, we refer the reader to the series of papers by Pani and his collaborators [Pan93, PD91b, PD91a] and [JP95], e.g. The papers [LOS02, LL98, KG87] and [Yui90] are also related to this issue. In all these contributions, various \(L^{\infty}, L^3, H^1\) - and \(H^2\) - error estimates have been obtained for the case of linear and quasi-linear single equations provided that standard conditions are imposed across the moving interface. Standard means in this context that both no jump in the temperature (or in the concentration) and the Stefan condition (interfacial mass balance) were used to close the respective models. Nevertheless, much less is known about how to deal with the case of coupled systems of pdes when, additionally, one or several moving internal boundaries driven by kinetic conditions are present.
4. The technical apparatus, which we use to gain a priori and a posteriori error estimates for our setting, combines ideas from [CR05, Mun06] and [BS96] (chapter 12). We particularly trust some hints from the paper by Coubessat and Rappaz [CR05]. In the latter paper, the authors are concerned with the error analysis of a viscous Burgers equation, where the end of the moving domain is driven by a linear kinetic condition. In their setting, the main difficulty is to deal with the Burger's type non-linearity and with additional non-local terms, which typically arise due to the freezing of the moving boundary. In contrast to [CR05], we do not consider a single model equation but a strongly coupled weakly non-linear system. The latter fact complicates the analysis substantially.

4 Technical preliminaries

The error analysis to be carried out requires some basic results concerning the approximation properties of first-order polynomials and the of functions spaces used. These results are elementary. We collect them here without proofs.

Notation 4.1. (a) We employ the sets of indices:

\[ I_1 := \{1, 2, 4, 5\}, \quad I_2 := \{3\}, \quad I = I_1 \cup I_2. \tag{16} \]

(b) We denote \( u(t) := \frac{\partial u}{\partial t}(y, t) = u_\ell(y, t), u_y(y, t) := \frac{\partial u}{\partial y}(y, t) \) for \((y, t) \in \Omega \times \mathbb{R}_+\). Notice also that, sometimes, we omit to write explicitly the dependence of \(u, \ell, \partial, \) or the test function on the variables \(t, x\) and/or \(y\). Also, we sometimes neglect to write the dependence of \( s \) on \( t \). In particular, \( u(1) \) and \( u_y(1) \) replace \( e(1, t) \), \( u_\ell(1, t) \) and \( u_y(1, t) \).

4.1 Function spaces and elementary inequalities

(i) Let us introduce the notation of spaces and norms to be considered here.

Set \( H = L^2(0, 1) = H_0, \quad \mathbb{H} = \bigcap_{\ell} H_\ell, \quad H^i = H^i \mathbb{H} \). The space \( H^i \) is equipped with the norm \( |u|_{H^i} := \left( \int_0^1 u(y)^2 \, dy \right)^{\frac{1}{2}} \) and with the scalar product

\[ (u, v)_{H^i} := \left( \int_0^1 u(y)v(y) \, dy \right) \] for all \( u, v \in H^i \). The product space \( \mathbb{H} \) is normed by \( |u|_{\mathbb{H}} := \left( \sum_{\ell} |u|_{H_\ell}^2 \right)^{\frac{1}{2}} \) for all \( u \in \mathbb{H} \) and equipped with the standard scalar product.

Denote \( V := \{ v \in H^1(0, 1) : v(0) = 0 \} := V_0, \quad V := \bigcap_{\ell} V_\ell, \quad V_i := V^{i/2} \). The space \( V_0 \) is endowed with the norm \( |u|_{V_0} = |u|_{H_0} \).

(ii) For reader's convenience, we also list a few elementary inequalities, which we extensively use in the sequel.

The inequality

\[ ab \leq \xi a^\ell + c_\ell b^\ell, \tag{17} \]

where \( \xi > 0, \quad c_\ell := \frac{1}{\ell} - \frac{1}{\ell} \frac{1}{\ell} > 0, \quad \frac{1}{\ell} + \frac{1}{\ell} = 1 \) with \( \ell \in \mathbb{N} \), is true for all \( a, b \in \mathbb{R}_+ \). (17) is referred to as the inequality of Young. We also make use of the following generalization of Young's inequality

\[ ab^{\theta} \leq \frac{\xi}{2} a^2 + \xi c_\ell b^\ell + c_\ell c_\ell c^\ell. \tag{18} \]
This holds for all $\theta \in [0,1]$ and $a, b, c \in \mathbb{R}$, where $c_1 := \frac{1}{2(1-\theta)}$ and $c_2$ is as in (17).

We obtain (18) by applying first the arithmetic-geometric mean for the numbers $a$ and $b$ with $\xi := 1-\theta$ and then by using (17) in the second term for the numbers $b^2$ and $c^2$ with $\frac{1}{2} = \theta$ and $\frac{1}{2} = 1-\theta$. If in (18) $\xi$ and $\xi$ belong to a compact subset of $\mathbb{R}_1$, then it results that $c_1$ and $c_2$ are strictly positive and bounded above.

The inequality

$$ |a + b|^p \leq \begin{cases} 
(1 + \xi)^{p-1} |a|^p + (1 + \xi)^{p-1} |b|^p & \text{for } p \in [1, \infty[, \\
|a|^p + |b|^p & \text{for } p \in ]0, 1[ 
\end{cases} 
$$

(19)

holds for arbitrary $a, b \in \mathbb{R}$ and $\xi > 0$.

Furthermore, let us consider $\xi > 0$, $c_1 > 0$ set as in (17), and $\theta \in [\frac{1}{2}, 1[$. Then there exists the constant $c = c(\theta) > 0$ such that

$$ |u_i|_\infty \leq c|u_i|^{1-\theta}|u_i|^\theta \leq c\|u_i\| + c_1|u_i|$$

for all $u_i \in V_i$, $i \in I_1$. (20)

We refer to (20) as interpolation or multiplicative inequality.

### 4.2 Useful basic facts from approximation theory

In section 5, we make use of the following piecewise-linear finite element discretization of the space interval $[0,1]$. Denote $J_m := \{0, \ldots, n\}$. For each $i \in J_m$, we denote $y_i := y_i(y_{i+1})$. We take $y_0 = 0 < y_1 < y_2 \ldots < y_{n+1} = 1$ and set $h_i = y_{i+1} - y_i$ for all $j \in J_m$. Let $h$ be the maximum mesh size, namely $h = \max_{i \in J_m} h_i$. Denote by $V_h := \{v \in C([0,1]) : v|_{[y_i, y_{i+1})} \in \Pi_1, j \in J_m\}$, where $\Pi_1$ represents the set of polynomials of degree one.

Assume $u_0 \in V$. In the sequel, $u_{0,h}$ denotes the Lagrange interpolant of $u_0 \in V$ in $V_h$, and respectively, for each $i \in I_1$, $u_{0,i}$ represents the interpolant of $u_0 \in V_i$ in $V_i$. Hence, we have $\|u_{0,h}\|_V \leq \|u_0\|_V$. Set $V_h := V_h^{[2]}$.

If $u_{0,i} \in H^1(0,1)$ for all $i \in I_1$, then by classical interpolation results (see [John93] or Lemma 4.2 below) we obtain

$$ \|u_0 - u_{0,h}\| \leq ch^3\|u_0\|_{H^2(0,1)}. $$

(31)

where $c$ is a strictly positive constant independent of $h$.

Let us denote by $I_h^i$ ($i \in I_1$) the interpolation operator

$$ I_h^i : C([0,1]) \rightarrow V_h \text{ defined by } (I_h^i u)(y) := \sum_{j \in J_m} u(y_j) \psi_j(y), y \in [0,1]. $$

Let $P_h^i$ ($i \in I_1$) be the orthogonal projection of $H_i$ onto $V_h$, which is defined by

$$ (P_h^i u_i - u_i, \psi) = 0 \text{ for all } \psi \in V_h \text{ and } u_i \in H_i. $$

Since $P_h^i u_i$ is the best approximation of $u_i$ in $V_h$ with respect to the $L^2$-norm, we have

$$ |P_h^i u_i - u_i| \leq |I_h^i u_i - u_i| \leq c h^3\|u_i\|_{H^2(0,1)}, \text{ for all } u_i \in H^1 \cap H^2, $$

(22)

where $H^1 \cap H^2 := \{\varphi \in H^1(0,1) : \varphi(0) = \varphi(1) = 0\}$. For each $i \in I_1$, let $R_h^i : H_0^1(0,1) \rightarrow V_h$ be the orthogonal projection with respect to the energy inner product $(\nabla u_i, \nabla \varphi)$. With other words, $a(R_h^i u_i - u_i, \varphi) = 0$ for
all $\varphi \in V_h$ and $u_i \in H^2_0(0,1)$, where $a(u_i, \varphi) := \langle \nabla u_i, \nabla \varphi \rangle$. The operator $R_h = (R^1_h, R^2_h, R^3_h, R^4_h)$ is the elliptic (Ritz) operator. Note also that $R_h u$ is the finite element approximation of the solution of the corresponding elliptic problem with the solution $u$. Finally, we recall the following classical interpolation result:

**Lemma 4.2 (Lagrange Interpolant)** Assume $\theta \in [\frac{1}{2}, 1]$ and take $\varphi \in H^2(0,1)$. Let $R_h$ denote Riesz' projection operator. Then there exists the strictly positive constants $\gamma_1$, $\gamma_2$ and $\gamma_3$ such that the Lagrange interpolant $R_h \varphi$ of $\varphi$ satisfies the following estimates:

(i) $|\varphi - R_h \varphi| \leq \gamma_1 h^\theta |\varphi|_{H^2(0,1)}$;

(ii) $||\varphi - R_h \varphi|| \leq \gamma_2 h |\varphi|_{H^2(0,1)}$;

(iii) $|\varphi(1) - R_h(1)\varphi(1)| \leq \gamma_3 h^{1-\theta} |\varphi|_{H^2(0,1)}$.

**Proof.** (i) and (ii) are classical results, see Theorem 5.5, p.55 in [LT03] (or [Joh94], e.g.). The proof of (iii) follows combining (i), (ii) and the multiplicative inequality (20). More precisely, we set $\gamma_3 := c_1^{-1/2} \gamma_2$, whereas $c > 0$ is cf. (20) and $\theta \in [\frac{1}{2}, 1]$. 

In sections 7 and 8, we use Lemma 4.2 with the choice $\mathcal{R}_h := H^1_0$ and $\varphi := \varphi_i \in V_i \cap H^2(0,1) = H^2 \cap H^1$ for $i \in I_i$.

### 5 Fixed-domain formulation. More notations, assumptions and auxiliary results

By the transformation

$$y = \frac{s}{s(t)}
$$

we map the moving domain $\Omega(t)$ into $[0,1]$ for each $t \in S_T$. We perform (23) for (2)-(11), but keep (4) unchanged. Since the calculations are obvious, we omit to write the classical formulation of the transformed system and will only give its weak form in (46).

In what follows, we refer to the concentrations vector acting in the domain whose boundaries are fixed, which is originally defined as $u(s,t)$ in the original domain $\hat{\Omega}(t)$, as $u(y,t)$. We also keep the same actation for the position of the interface, namely $s(t)$. Let $\hat{\varphi} := (\varphi_1, \varphi_2, \varphi_3, \varphi_4)^T \in V$ be an arbitrary test function and take $i \in S_T$. We let $a(\cdot)$ denote the transport part of the model, $b_f(\cdot)$ and $c(\cdot)$ comprise various volume and surface productions, and $h(\cdot)$ incorporate a non-local term, whose presence is due to the use of (23), viz.

$$
a(s,u,\varphi) := \frac{1}{s} \sum_{i \in I_i} \langle D_i u_i, \varphi_i \rangle,
$$

$$
b_f(u,s,\varphi) := s \sum_{i \in I_i} \langle f_i(u), \varphi_i \rangle,
$$

$$
e(s',u,\varphi) := \sum_{i \in I_i} g_i(s',u(1)) \varphi(1),
$$

$$
h(s',u_y,\varphi) := \sum_{i \in I_i} s'(y u_i, \varphi_i),
$$

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where the production terms \( f \) and \( g \) are given by

\[
\begin{align*}
    f_1(u) & := P_1(Q_1 u_1 - u_1), \\
    f_2(u) & := -P_2(Q_2 u_2 - u_1), \\
    f_3(u) & := f_5(u) = 0, \\
    g_1(s', u) & := \eta \left( 1, t \right) + s' \left| u_1(1, t) \right|, \\
    g_2(s', u) & := s'(t) u_3(1, t), \\
    g_3(s', u) & := \eta \left( 1, t \right).
\end{align*}
\]

Set

\[
    \mathcal{K} := \prod_{i \in \mathcal{I}_1 \cup \mathcal{I}_2} [0, k_i],
\]

and, for fixed \( A \in \mathcal{M}_A \), we take

\[
    \mathcal{M}_\eta := \max_{u \in \mathcal{K}} \{ \eta \left( u, A \right) \}. \tag{25}
\]

In (24), we set

\[
    \begin{cases}
        k_i := \max\{ u_{i0}(y) + \lambda_i(t), \lambda_i(t) : y \in [0, 1], t \in \mathcal{S}_T \}, i = 1, 2, 4, \\
        k_3 := \max\{ u_{30}(y) + \lambda_3(t), \lambda_3(t), \kappa : y \in [0, 1], t \in \mathcal{S}_T \},
    \end{cases} \tag{26}
\]

where

\[
    \kappa := \frac{L_0}{D_5 - \mathcal{M}_\eta L_0} \left( M_\eta + \frac{L_1}{2} \lambda_{5A} + 1 \right). \tag{27}
\]

The only assumptions that are needed to describe the reaction rate \( \eta \) are contained in the items (A) and (B) of the next Assumption.

**Assumption (II)**

Consider

(A) Fix \( A \in \mathcal{M}_A \). Let \( \eta \left( u, A \right) > 0 \) if \( u_1 > 0 \) and \( u_2 > 0 \), and \( \eta \left( u, A \right) = 0 \), otherwise. Moreover, for any fixed \( u_1 \in \mathbb{R} \) the reaction rate \( \eta \) is bounded.

(B) The reaction rate \( \eta \) is locally Lipschitz.

(C1) \( 1 > k_3 \geq \max_{\mathcal{S}_T} \{ |u_{3eq}(t)| : t \in \mathcal{S}_T \}; D_5 - \mathcal{M}_\eta L > 0 \);

(C2) \( P_1 Q_1 k_3 \leq P_1 k_3; P_3 k_3 \leq P_3 Q_3 k_2 \);

(C3) \( Q_3 > Q_1 \).

A typical choice of \( \eta \) is the generalized mass-balance law, i.e.

\[
    \eta \left( u, A \right) := ku_1^p u_2^q, \quad p \geq 1, q \in \mathbb{R}, k > 0, \Lambda := \{ p, q, k \}, \tag{38}
\]

where \( u_0 \) is the positive solution of (4).

For the initial and boundary data we choose the following.
Assumption (III) Select
\[ \lambda \in W^{1,1}(S_T)^{\{2\}}, \lambda(t) \geq 0 \text{ a.e. } t \in S_T, \]  
(39)
\[ u_{3,eq} \in L^\infty(S_T), u_{3,eq}(t) \geq 0 \text{ a.e. } t \in S_T, \]  
(40)
\[ u_0 \in L^\infty(0,1)^{\{2\}}, u_0(y) + \lambda(0) \geq 0 \text{ a.e. } y \in [0,1], \]  
(41)
\[ u_0 \in L^\infty(0,s(t)), u_\infty(x) \geq 0 \text{ a.e. } x \in [0,s(t)]. \]  
(42)

Remark 5.1 Owing to (4), (38), (40) and (42), we see that Assumption (II) (A) is fulfilled with \( \eta_T \) chosen as in (38).

Definition 5.2 (Weak Solution to \( P_T^1 \)) We call the couple \((u,s)\) a local weak solution to problem \( P_T^1 \) if and only if there is a \( S_\delta := [0,\delta] \) with \( \delta \in [0,T] \) such that
\[ s_0 < s(\delta) \leq L_0, \]  
(43)
\[ s \in W^{1,\infty}(S_\delta), \]  
(44)
\[ u \in W^{1,1}(S_\delta; V; H) \cap [S_T \mapsto L^\infty(0,1)^{\{2\}}], \]  
(45)
\[ \begin{cases} 
\int \sum_{i \in \mathcal{I}_T} (a_i(u,s(t),\varphi_i) + a_i(s,u,\varphi_i) + c_i(s,u+\lambda,\varphi_i) = b_i(u+\lambda,s,\varphi_i) \\
+ h_i(s',u,\varphi_i) - s' \sum_{i \in \mathcal{I}_T} (\lambda_i(t),\varphi_i) \quad \text{for all } \varphi \in \mathcal{V}, \text{ a.e. } t \in S_\delta, \\
s'(t) = \eta_T(1,t) \text{ a.e. } t \in S_\delta, \\
u(0) = u_0 \in H, s(0) = s_0. 
\end{cases} \]  
(46)

We possess now all the ingredients which we need in order to state the existence and uniqueness of locally in time weak solutions to \( P_T^1 \).

Theorem 5.3 (Well-posedness of \( P_T^1 \)) Consider Assumptions (1)-(III) be fulfilled. In this case, the following assertions hold:
(a) There exists \( \delta \in [0,T] \) such that the problem \( P_T^1 \) admits a unique local solution on \( S_\delta \) in the sense of Definition 5.2.
(b) \( 0 \leq u_i(y,t) + \lambda_i(t) \leq k_i \text{ a.e. } y \in [0,1] \) for all \( t \in S_\delta \).
(c) \( s \in W^{1,\infty}(S_\delta) \)

Sketch of the proof of Theorem 5.3. If in the sharp-interface model \( P_T \), whose well-posedness was shown in [Mun08], the non-carbonated phase \( \zeta(t), L \) degenerates, then the techniques used to prove Theorem 5.4 in [Mun08] conclude the proof of Theorem 5.3. 

Definition 5.4 (Weak Solution to \( P_T^{1,\text{md}} \)) We call the couple \((u_h,s_h)\) a local weak solution to problem \( P_T^{1,\text{md}} \) if and only if there is a \( S_\delta := [0,\delta] \) with \( \delta \in [0,T] \) such that
\[ s_0 < s_h(\delta) \leq L_0, \]  
(47)
\[ s_h \in W^{1,1}(S_\delta), \]  
(48)
\begin{align} 
  u_h & \in [H^1(S_h, V_h) \cap L^{\infty}(S_h, H)]^{[2]} \\
  s_h \sum_{i \in J_n}(u_{h,i}(t), \varphi_{n_i}) + a(s_h u_h, \varphi_h) + \epsilon(s_h u_h, \varphi_h) + \mu_0(s_h, \varphi_h) + h(s_h u_h, \varphi_h) - \tau_n \sum_{i \in J_n}(\lambda_{i}u_{h,i}(t), \varphi_{n_i}) & \text{ for all } \varphi_h \in V_h, \text{ a.e. } t \in S_h, \\
  s_h(t) = & \begin{cases} 
    s_0(t) & \text{a.e. } t \in S_h, \\
  \end{cases} \\
  u_h(0) = & u_0 \in H, s_h(0) = s_0. 
\end{align}

A first result is the next theorem:

**Theorem 5.5 (Well-posedness of \(P_{t}^{Lsd}\))** Let Assumptions (I)-(III) be fulfilled. There exists \( \delta \in [0, \min\{\delta, \delta\}] \), which is independent of \( h \), such that problem \( P_{t}^{Lsd} \) has a unique weak solution

\[(u_h, s_h) \in [H^1(S_h, V_h) \cap L^{\infty}(S_h, H)]^{[2]} \times W^{1,4}(S_h), \]

in the sense of Definition 5.4 that continuously depends on data and model parameters.

The proof of Theorem 5.5 follows the lines of the proof of Theorem 3.1.5 from [Mun06]. Since here we intend to focus only on the error analysis, we omit it.

# 6 Main results

The next theorems contain the main results of this paper:

**Theorem 6.1 (A Priori Error Estimate)** Select \( u_0 \in V \cap [H^2(\Omega, 1)]^{[2]} \) and consider Assumptions (I)-(III). Then problems \( P_t^I \) and \( P_t^{Lsd} \) are uniquely solvable. Let \((u, s)\) and \((u_h, s_h)\) be the corresponding solutions. Then the following estimate holds: There exist a \( \delta_1 \in [0, \max\{\delta, \delta\}] \) and a strictly positive constant \( c \), which are independent of \( h \), such that

\[
\| u - u_h \|_{L^2(S_h, V_h) \cap L^{\infty}(S_h, V)} + \| s - s_h \|_{W^{1,4}(S_h)} \leq c h. 
\]

**Proof.** See section 7. \( \square \)

**Theorem 6.2 (A Posteriori Error Estimate)** Let \( u_0 \in V \cap [H^2(\Omega, 1)]^{[2]} \) and consider Assumptions (I)-(III). Then problems \( P_t^I \) and \( P_t^{Lsd} \) are uniquely solvable. Let \((u, s)\) and \((u_h, s_h)\) be the corresponding solutions. Then there exists \( \delta_2 \in [0, \max\{\delta, \delta\}] \) and strictly positive constants \( c \), \( \delta \in \{1, 2, \delta\} \) and \( c \), which are independent of \( h \) and \( u \), such that

\[
|u - u_h|^2 + c_1 \| s - s_h \|^2 + c_2 \int_0^t \| u - u_h \|^2 dt \leq c \sum_{i \in J_n} h_{i}^2 \left( \| R(u_n) \|_{L^{2}(S_h, L^{2}(\Omega, 1))} + h_{i}^2 \| u_n \|_{L^{2}(\Omega, 1)} \right), 
\]

whereas the residual \( R(u_h) \) is defined by

\[
R(u_h) = f_n(s_h, u_h) - u_{h,t} + s_{h} u_{h,y} + c_h(s_h, u_{h,1}). 
\]
In (52), the quantities \( f_\delta(s, u_h) \) and \( e_\delta(s', u_h(1)) \) are defined by
\[
\begin{align*}
f_\delta(s, u_h) & := s_h \sum_{i \in \Gamma_1} f_i(u_h), \\
e_\delta(s', u_h(1)) & := \sum_{i \in \Gamma_2} g_i(s', u_h).
\end{align*}
\]

Proof. See section 8. ■

Remark 6.3 What we have stated so far (cf. Theorem 6.1 and Theorem 6.2) are error estimates for \( u(y, t) \) with \( y \in [0, 1] \). This is precisely what one needs when using front-fixing methods to solve the moving-boundary problem (2)-(11). On the other hand, if one employs front-tracking methods for the same problem, error estimates obtained for the solution in the fixed-domain formulation are useless. In such a case, we need to go back to the initial formulation of the problem and get error estimates for the original unknowns, i.e. for \( u(x, t) \) with \( x \in [0, s(t)] \), see [KG87] for related ideas. Since the transformation (29) is affine and the solution \((u_h, s_h)\) of \( P_{\Gamma}^{1,\delta} \) is sufficiently regular (cf. Proposition 5.4.17 from [Mun06]), the inverse transformation \( x = y s_h(t) \) can be employed in order to make the estimates (31) and (32) available for the original problem (with moving boundaries).

Notation 6.4 For the sake of simplicity, we put \( \delta_1 = \delta_2 = \delta = \delta \) and \( \delta = \delta \).

In the remainder of this note, we concentrate on proving Theorem 6.1 and Theorem 6.2.

7 Proof of Theorem 6.1

The role of Theorem 6.3 and Theorem 6.5 is to ensure the existence of local in time solutions to \( P_{\Gamma} \) and \( P_{\Gamma}^{1,\delta} \), respectively. Let us denote by \( S_\delta = [0, \delta] \) (with \( \delta \) chosen as in Notation 6.4) the common time interval on which the continuous and discrete solutions exist and let \( e := u - u_h \) and \( \sigma := s - s_h \) be the errors of approximation. Also, define \( e_i := u_i - u_{ih} \) and \( e^i := (e_1, e_2, e_3, e_4)^t \). For each test function \( w_{ih} \in V_h \) (\( i \in \Gamma_1 \)), we subtract the variational formulation in terms of \( u_h \) from that one in terms of \( u \) and obtain the following equality
\[
\begin{align*}
\left( (u + \lambda), w_h \right) & - \left( (u_h + \lambda), w_h \right) + \frac{1}{\delta^3} \sum_{i \in \Gamma_1} \langle D_i u_{ih}, u_{ih} \rangle \\
& = \frac{1}{\delta^3} \sum_{i \in \Gamma_1} \langle D_i u_{ih}, u_{ih} \rangle + \frac{1}{\delta} \left[ \left( e + s'(u_{ih}(1) + \lambda) \right) w_{ih}(1) \\
& - \frac{1}{\delta} \left[ \left. \left[ e_i + s'(u_{ih}(1) + \lambda) \right] w_{ih}(1) \right| \right] + \frac{s'}{\delta} (u_{ih}(1) + \lambda) w_{ih}(1) \\
& - \frac{s}{\delta^2} (u_{ih}(1) + \lambda) w_{ih}(1) - \frac{1}{s} \left[ w_{ih}(1) + \frac{1}{s} w_{ih}(1) \right] \\
& = (P_1 (Q_2 (u_2 + \lambda) - (u_1 + \lambda)), u_{ih}) \\
& - (P_2 (Q_1 (u_{ih} + \lambda_2) - (u_{ih} + \lambda_1)), u_{ih}) \\
& - (P_3 (Q_2 (u_2 + \lambda_3) - (u_1 + \lambda_1)), u_{ih})
\end{align*}
\]
\begin{align}
&+ \langle P_2(Q_2(u_{2h} + \lambda_2) - (u_{1h} + \lambda_1)), u_{2h} \rangle \\
&+ \frac{s'}{s} \sum_{i \in T_i} (g_{i, u_{2h}}, w_{i, h}) - \frac{s'}{s} \sum_{i \in T_i} (g_{i, u_{1h}}, w_{i, h}) \rangle. \tag{51}
\end{align}

Grouping some of the terms in (51), we obtain

\begin{align}
\langle c, u_h \rangle + \frac{1}{s} \sum_{i \in T_i} (D_i(u_i - u_{ih}, y), u_{ih, y}) = \left( \frac{1}{s_h} - \frac{1}{s} \right) \sum_{i \in T_i} (D_i u_{ih, y}, u_{ih, y}) \\
- \left( \frac{s'}{s} \langle u_{1h}(1) + \lambda_1 \rangle \right) - \frac{s'}{s} \langle u_{1h}(1) + \lambda_1 \rangle + \frac{\nu}{s} - \frac{\nu h}{s} \right) w_{1h}(1) \\
- \left( \frac{s'}{s} \langle u_{2h}(1) + \lambda_2 \rangle \right) - \frac{s'}{s} \langle u_{2h}(1) + \lambda_2 \rangle + \frac{\nu}{s} - \frac{\nu h}{s} \right) w_{2h}(1) \\
+ P_1 Q_1(e_2, u_{1h}) - P_1(e_1, u_{1h}) - P_3 Q_3(e_2, u_{2h}) + P_3(e_1, u_{2h}) \\
+ \frac{s'}{s} \sum_{i \in T_i} (g_{i, e_{ih}}, u_{ih}) + \left( \frac{s'}{s} - \frac{s'}{s} \right) \sum_{i \in T_i} (g_{i, u_{ih}}, u_{ih}) \rangle. \tag{55}
\end{align}

Therefore, we may write

\begin{align}
\langle c, u_h \rangle + \frac{\min_{i \in T_i} D_i}{s(t)} \langle c, u_{ih}, y \rangle \leq \sum_{i=1}^{s} I_i, \tag{56}
\end{align}

where the terms I_i are given by

\begin{align}
I_1 := \left( \frac{1}{s_h} - \frac{1}{s} \right) \sum_{i \in T_i} (D_i u_{ih, y}, u_{ih, y}), \\
I_2 := \left( \frac{\nu}{s} - \frac{\nu h}{s} \right) \langle w_{1h}(1) + w_{2h}(1) \rangle, \\
I_3 := \sum_{i=1}^{s} \left( \frac{s'}{s} \langle u_{1h}(1) + \lambda_1 \rangle \right) \langle u_{1h}(1) \rangle \\
I_4 := P_1 Q_1(e_2, u_{1h}) - P_1(e_1, u_{1h}) - P_3 Q_3(e_2, u_{2h}) + P_3(e_1, u_{2h}) \\
I_5 := \frac{s'}{s} \sum_{i \in T_i} (g_{i, e_{ih}}, u_{ih}) + \left( \frac{s'}{s} - \frac{s'}{s} \right) \sum_{i \in T_i} (g_{i, u_{ih}}, u_{ih}) \rangle.
\end{align}

Set \( d := \min_{i \in T_i} D_i \). For any \( u_h \in V_h \), the following estimate holds

\begin{align}
\frac{1}{2} \frac{d}{dt} |c|^2 + \frac{d}{s^2} |c|^2 \leq \langle c, c - u_h \rangle + \frac{d}{s^2} \langle c, c - u_h \rangle \langle c, c - u_h \rangle \rangle. \tag{57}
\end{align}

Note that \( u_h = u_h - u_h \in V_h \) decomposes into \( u_h = (u_h - u) + e \). Now, choosing the test function \( u_h := u_h - u_h \) in (56), we obtain

\begin{align}
\frac{1}{2} \frac{d}{dt} |c|^2 + \frac{d}{s^2} |c|^2 \leq \langle c, c - u_h \rangle + \frac{d}{s^3} \langle c, c - u_h \rangle \rangle. \tag{57}
\end{align}
+ \left( \frac{1}{s_h^3} - \frac{1}{s^3} \right) \sum_{i \in I_s} (D_i(u_{ih}, y_i) (v_{ih} - u_{ih}))_y \\
+ \left( \frac{v_{ih}}{s} - \frac{v_{ih}}{s_h} \right) \left( |v_{ih}(1) - u_{ih}(1) + u_{ih}(1) - u_{ih}(1)| \right) \\
+ P_1 C_3 (\varepsilon_3, v_{ih} - u_{ih}) - P_1 (e_1, v_{ih} - u_{ih}) \\
- P_2 C_3 (\varepsilon_3, v_{ih} - u_{ih}) + P_2 (e_1, v_{ih} - u_{ih}) \\
+ \sum_{i \in I_s} s^2 \langle y e_{i,y}, u_{ih} - u_{ih} \rangle \\
+ \left( \frac{s^2}{s} - \frac{s_h^2}{s_h} \right) \sum_{i \in I_s} s^2 \langle y (u_{ih,y} - u_{ih}) \rangle 
(58)

In order to simplify the writing of some of the inequalities, we introduce the strictly positive constants \( c_\ell [\ell \in \{1, \ldots, 7\}] \), whose precise expression is not explicitly written but can be easily derived. However, it is worth mentioning that for each \( \ell \in \{1, \ldots, 7\} \) we have \( c_\ell < \infty \). Before estimating the right-hand side of (56), let us point out a few technical facts, which we list in the next Remark. They are useful for following the estimates. Their proofs are straightforward (use of the integration by parts and the inequality between the geometric and arithmetic means).

**Remark 7.1**

1. There exists a constant \( c_1 = c_1(A, s_0) > 0 \) such that

\[
\frac{v_{ih}}{s} - \frac{v_{ih}}{s_h} \leq |s - s_h| \left( \frac{v_{ih}}{s} - \frac{v_{ih}}{s_h} \right) \leq c_1 (|s - s_h| + |s' - s'_h|)
\]

2. For each \( i \in \{1, 2\} \), there exists a constant \( c_2 = c_2(A, s_0) > 0 \) such that

\[
\frac{s^2}{s_h} (\varepsilon_1 (1) + \lambda_i) - \frac{s^2}{s} (\varepsilon_1 (1) + \lambda_i) - \frac{s_h}{s} c_2 (1) (\varepsilon_1 (1) + \lambda_i) \left( \frac{s^2}{s_h} - \frac{s^2}{s} \right) \leq c_2 (|\varepsilon_1 (1)| + |s - s_h| + |s' - s'_h|)
\]

3. For each \( i \in I_s \), we have

\[
\langle y e_{i,y}, v_{ih} - u_{ih} \rangle = \langle y e_{i,y}, e_i \rangle + \langle y e_{i,y}, u_{ih} - u_i \rangle \leq \frac{1}{2} |\varepsilon_1 (1)|^2 + |\varepsilon_i (1)| |v_{ih} - u_{ih}|
\]

4. It holds

\[
\langle y u_{ih,y}, v_{ih} - u_{ih} \rangle \leq |u_{ih}||v_{ih} - u_{ih}| + |u_{ih}||v_{ih} - u_{ih}|
\]

5. It holds

\[
\langle u_{ih,y}, (v_{ih} - u_{ih})_y \rangle \leq |u_{ih}||v_{ih} - u_{ih}|
\]

By Remark 7.1, (57) and (58), we have

\[
\frac{1}{2} \frac{d}{dt} |\varepsilon|^2 + \frac{1}{s^2} ||\varepsilon||^2 \leq |\varepsilon| ||u - v_{ih}|| + s \frac{1}{s} ||\varepsilon|| ||u - v_{ih}|| \\
+ \left| s - s_h \right| \frac{s + s_h}{s s_h} \sum_{i \in I_s} \langle D_i u_{ih,y}, (u_{ih} - v_{ih})_y \rangle dy
\]
\begin{align}
&+ c_3(|s - s_h| + |s' - s'_h|)|\nu_n(1) - u(1)| + \varepsilon(1)| \\
&+ c_3(|\varepsilon(1)| + |s - s_h| + |s' - s'_h|)|\nu_n(1) - u(1)| + \varepsilon(1)| \\
&+ P_1 Q_2 |\varepsilon(1)| (|\nu_{n1} - u_1| + |\varepsilon|) + P_1 |\nu_{n1} - u_1| + |\varepsilon| \\
&+ P_2 Q_2 |\varepsilon(1)| (|\nu_{n1} - u_1| + |\varepsilon|) + P_2 |\nu_{n1} - u_1| + |\varepsilon| \\
&+ \frac{s'}{2s} \sum_{\ell \in I_1} [(|\varepsilon_{\ell}(1)|^3 - |e_{\ell}|^3) + \delta_1(1)|\nu_{n1} - u_{n1}|| \\
&+ c_3(|s - s_h| + |s' - s'_h|) \sum_{\ell \in I_1} (|\nu_{n1}| \nu_{n1} - u_{n1}|| \\
&+ |u_{n1}| ||v_{n1} - u_{n1}||. \tag{59}
\end{align}

After some elementary manipulations, we directly gain the estimate
\begin{align}
&\frac{d}{dt} |e|^2 + \frac{d}{dt} ||e||^2 \leq |\varepsilon_d| |u - u_h| + \frac{d}{dt} ||e||^2 (|u - u_h|| \\
&+ c_3 |s - s_h| ||\nu_n(1)| \nu_{n1} - u_1| + |\varepsilon| ) + c_3 (|s - s_h| + |s' - s'_h|) |\varepsilon||^2 |e| |e|^{1-\theta} \\
&+ c_4 (|s - s_h| + |s' - s'_h|) |\varepsilon||^2 |\nu_n - u_1|^{1-\theta} + c_4 (|s - s_h| + |s' - s'_h|) |\varepsilon||^2 |e|^{1-\theta} \\
&+ P_1 Q_1 (2 |\varepsilon_{\ell}|^3 + |\nu_{n1} - u_1|^3 + |\varepsilon||^3) + P_1 (2 |\varepsilon_{\ell}|^3 + |\nu_{n1} - u_1|^3) \\
&+ P_2 Q_2 (2 |\varepsilon_{\ell}|^3 + |\nu_{n1} - u_1|^3) + P_2 (2 |\varepsilon_{\ell}|^3 + |\nu_{n1} - u_1|^3) \\
&+ \frac{s'}{2s} |\varepsilon||^2 |e||^2 |e|^{1-\theta} + \frac{s'}{s} ||e||^2 |\nu_n - u_1| + c_5 (|\varepsilon||^2 + ||e||). \tag{60}
\end{align}

We set \( u_h = \Pi_h u \) and rearrange some of the terms in (60). Afterwards we use Lemma 4.2 to obtain the next estimate. It therefore yields
\begin{align}
&\frac{d}{dt} |e|^2 + \frac{d}{dt} ||e||^2 \leq |\varepsilon_d| \gamma_1 \gamma_1^2 |u| |u|_{H^2(\Omega, 1)} + \frac{d}{dt} ||e||^2 |\gamma_2\varepsilon| |u| |H^2(\Omega, 1) \\
&+ c_3 |s - s_h| ||\nu_n(1)| \nu_{n1} - u_1| + |\varepsilon| ||\varepsilon| |e| |e|^{1-\theta} \\
&+ c_4 (|s - s_h| + |s' - s'_h|) |\gamma_2\varepsilon| |u| |H^2(\Omega, 1) + c_4 (|s - s_h| + |s' - s'_h|) |\gamma_2\varepsilon| |u| |H^2(\Omega, 1) \\
&+ c_4 (|s - s_h| + |s' - s'_h|) |\gamma_2\varepsilon| |u| |H^2(\Omega, 1) + c_4 (|s - s_h| + |s' - s'_h|) |\gamma_2\varepsilon| |u| |H^2(\Omega, 1) \\
&+ \frac{s'}{2s} |\varepsilon||^2 |e||^2 |e|^{1-\theta} + \frac{s'}{2s} |\gamma_2\varepsilon| |u||H^2(\Omega, 1) \\
&+ c_5 (|\gamma_2\varepsilon| |u| |H^2(\Omega, 1) + ||e||) (|s - s_h| + |s' - s'_h|). \tag{61}
\end{align}

Since \( s'(t) - s'_h(t) \leq c(\varepsilon(1, t) - u_h(1, t)) = \int_0^t \varepsilon_h(\zeta, t) d\zeta \), we obtain
\begin{align}
|\sigma| = |s' - s'_h| \leq ||\varepsilon||. \tag{62}
\end{align}

Now, using Young's inequality (see also (46) in [CR05]), we derive
\begin{align}
\frac{d}{dt} |\sigma|^2 = \frac{d}{dt} (|s - s_h|^2) \leq ||\varepsilon||^2 + |s - s_h|^2. \tag{63}
\end{align}
Inequality (51) can be conveniently arranged such that the proof can be completed by Gronwall argument. Similar ideas have been employed, e.g., in [CR05] (apply Gronwall's inequality for the quantity $|z|^2 + q|z - s_0|^2$ or [Mau06] (use $\int_{s_0}^{s_1} |s(r) - s_0(r)|^2 dr \leq s^3 \int_{s_0}^{s_1} |s'(r) - s'(r)|^2 dr$ and then apply Gronwall's inequality for the quantity $|z|^2$).

8 Proof of Theorem 6.2

For all $v \in V$, we can write

$$
\langle c_v, v \rangle + \frac{d}{ds} \langle e_v, v, v \rangle \leq \langle u, v \rangle + \frac{1}{s^3} \sum_{s \in E_s} D_s(u_{s_{0}}, v_{s_{0}}) - \left( \frac{1}{s^3} + \frac{1}{s^3} \sum_{s \in E_s} D_s(u_{s_{0}}, v_{s_{0}}) \right) \leq -c(s', u, v) + by(s, u, v) $$

$$+ h(s', u, v, v) - \left[ (u_{s_{0}}, v) + \frac{1}{s^3} \sum_{s \in E_s} D_s(u_{s_{0}}, v_{s_{0}}) \right].
$$

(64)

By (64), we obtain

$$
\langle e_v, v \rangle + \frac{d}{ds} \langle e_v, v, v \rangle \leq b(y, u, v) + h(s', u, v, v) - e(s', u, v) + \langle u_{s_{0}}, v \rangle + \frac{1}{s^3} \sum_{s \in E_s} D_s(u_{s_{0}}, v_{s_{0}}) - \left( \frac{1}{s^3} + \frac{1}{s^3} \sum_{s \in E_s} D_s(u_{s_{0}}, v_{s_{0}}) \right) $$

$$= b(y, u, v) + h(s', u, v, v) - e(s', u, v) + \langle u_{s_{0}}, v \rangle + \frac{1}{s^3} \sum_{s \in E_s} D_s(u_{s_{0}}, v_{s_{0}}) $$

$$+ \int_0^1 R(u_{s}) dy - \frac{1}{s^3} \sum_{s \in E_s} \int_0^1 D_s(u_{s_{0}}, v_{s_{0}}) dy,
$$

(65)

where the residual $R(u_{s})$ is defined by (53). Since for all $y \in (0, 1)$ we have that $u_{s_{0}, 0} = 0$, the term

$$
\int_0^1 R(u_{s}) dy - \frac{1}{s^3} \sum_{s \in E_s} \int_0^1 D_s(u_{s_{0}}, v_{s_{0}}) dy
$$

can be estimated from above by

$$
\sum_{s \in E_s} \int_0^{y_{s} + 1} R(u_{s}) dy - \frac{1}{s^3} \sum_{s \in E_s} \max_{t \in E_t} D_t(u_{s_{0}, y_{s} + 1}, v_{s_{0}, y_{s} + 1}) - u_{s_{0}, y_{s} + 1} v_{s_{0}, y_{s} + 1}.
$$

(66)

Owing to $P_{t_{n_{0}}}^1$, we note that relation (66) vanishes when selecting as test function $v = u_{s_{0}}$. We rely on this observation to add (66) (in which we take $v = u_{s_{0}}$) to (58). Selecting in the result $v = e \in V$ and $u_{s_{0}} := R_{s_{0}} e \in V_{s_{0}}$, we obtain the following inequality

$$
\langle e_v, e \rangle + \frac{d}{ds} ||e||^2 \leq b(y, u, e) + h(s', u, e) + c(s', u, e)
$$

\[15\]
\[- e(s', u, \varepsilon) + h(s', u, \varepsilon) - h(s_n, u_{n, h}, \varepsilon) - \left(\frac{1}{s^3} - \frac{1}{s_h^3}\right) \sum_{i \in T_s} \langle D_i u_{i+h}, u_h \rangle \]
\[+ \sum_{i \in L_s} \int_{y_i}^{y_i+1} (e - \Pi_h e) dy \]
\[- \frac{1}{s^3} \sum_{i \in J_n} \max_{i \in T_s} D_i \left[ u_{i+h} (y_{i+1}) (e - \Pi_h e)(y_{i+1}) - u_{i+h} (y_i) (e - \Pi_h e)(y_i) \right] \]
\[= \sum_{f=1}^{5} I_f, \quad (67)\]

where we have
\[I_1 := b_f(s', u, \varepsilon) - b_f(s_n, u_{n, h}, \varepsilon), \]
\[I_2 := e(s', u, \varepsilon) - e(s', u, \varepsilon), \]
\[I_3 := h(s', u, \varepsilon) - h(s', u_{n, h}, \varepsilon), \]
\[I_4 := - \left(\frac{1}{s^3} - \frac{1}{s_h^3}\right) \sum_{i \in T_s} \langle D_i u_{i+h}, e_h \rangle, \]
\[I_5 := \sum_{i \in L_s} \int_{y_i}^{y_i+1} (e - \Pi_h e) dy \]
\[= \frac{1}{s^3} \sum_{i \in J_n} \max_{i \in T_s} D_i \left[ u_{i+h} (y_{i+1}) (e - \Pi_h e)(y_{i+1}) - u_{i+h} (y_i) (e - \Pi_h e)(y_i) \right]. \quad (68)\]

Simple manipulations of the multiplicative inequality (20) together with Cauchy-Schwarz's and Young's inequalities (17) and (18) lead to the following bounds. We obtain
\[|I_1| \leq \frac{F_1 Q_1 + F_2}{2} (|e_1|^3 + |e_2|^3), \quad (69)\]
\[|I_2| \leq |s - s_n|^3 + |s' - s_n'|^3 + \frac{1}{s^3} \left( \frac{|e|^3}{|e_h|^3} \right) \sum_{i \in T_s} \langle e_h, e \rangle \]
\[+ \frac{\epsilon^2}{s^3} \sum_{i \in T_s} |e_h|^3, \quad (70)\]
\[|I_3| \leq \frac{s_{h'}^2}{s_h^3} \sum_{i \in T_s} (|e_1|^3 - |e_2|^3) \]
\[+ \frac{1}{s_{h'}^3} (s_n (s' - s_n') + s_n' (s_n - s_n')) (|e|^3 + |e|^2) . \quad (71)\]

In (70), the constant \(\epsilon\) only depends on \(s_0\) and \(L\). In order to estimate \(|I_4|\), we proceed as follows
\[|I_4| = - \left(\frac{1}{s^3} - \frac{1}{s_h^3}\right) \sum_{i \in T_s} \langle D_i u_{i+h}, e_h \rangle \]
\[\leq |s - s_n| \frac{s + s_n}{s_h} \sum_{i \in T_s} (|D_i u_{i+h}| (1) |e_1| + |D_i u_{i+h}| |e_2|) \]

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\begin{align*}
\leq c |s - s_h| \|e\|^2 + \frac{c}{s_h} \sum_{i \in I_0} D_i |u_{i0}(1)| + |s - s_h| \frac{\|e\|}{s_h} \sum_{i \in I_0} |D_i u_{i0}| \\
\leq \xi |s - s_h|^3 + c \varepsilon \frac{\|e\|^2}{s_h^3} + c \varepsilon \left( \frac{c}{s_h^2} \sum_{i \in I_0} D_i |u_{i0}(1)| \right) \frac{\|e\|^2}{s_h^2}.
\end{align*}

(72)

To bound above \(|J_0|\), we firstly note that since \(R_h e\) is the Lagrange interpolant of \(e\), then we have that \((e - R_h e)(y_i) = 0\) for all \(i \in J_0 \cup \{n + 1\}\). Additionally, we easily see that

\[
\int_{y_0}^{y_{n+1}} R(u_h)(e - R_h e) dy \leq \|R(u_h)\|_{L^2(J_0)^2} \|e\|_{H^1(J_0)}.
\]

Owing to the latter inequality and the embedding \(H^1(J_0) \to H^1(0,1) (\forall \in J_0)\), we deduce the following bound on \(|J_0|\):

\[|J_0| \leq \sum_{i \in J_0} \int_{y_0}^{y_i} R(u_h)(e - R_h e) dy \]

\[\leq \sum_{i \in J_0} \|R(u_h)\|_{L^2(J_0)^2} \|e\|_{H^1(J_0)} \]

\[\leq c \left( \sum_{i \in J_0} \|R(u_h)\|_{L^2(J_0)^2} \right)^{1 \over 2} \|e\|_{H^1(J_0)} \]

\[\leq \xi \frac{\|e\|^2}{s_h} + c \varepsilon s^3 \sum_{i \in J_0} \|R(u_h)\|_{L^2(J_0)^2} |s - s_h|^3.
\]

(73)

where \(c\) only depends on \(|J_0|\). Set \(C_\varepsilon := \varepsilon^2 (\varepsilon + \varepsilon^3)\). Combining (69)-(73), we obtain

\[\frac{1}{2} \frac{d}{dt} \|e\|^2 + \frac{d}{dt} \|e\|^2 \leq \frac{P_1 Q_1}{2} (\|e\|^2 + |s - s_h|^2) + \xi |s - s_h|^3 + |s' - s_h'|^2 + \xi \frac{\|e\|^2}{s^3} + c (C_\varepsilon) \frac{s^3}{s_h^2} |s - s_h| \frac{\|e\|^2}{s^3}
\]

\[+ \left( \frac{1}{s} |s' - s_h'| + \frac{s - s_h}{s_h^2} \right) \|e\|^2 + \xi \frac{\|e\|^2}{s^3} + c \varepsilon \left( \frac{\|e\|^2}{s^3} + \frac{1}{s} |s' - s_h'| + \frac{s^3}{s_h^2} \right) \|e\|^2
\]

\[+ \xi \frac{\|e\|^2}{s^3} + c \varepsilon s^3 \sum_{i \in J_0} \|R(u_h)\|_{L^2(J_0)^2} |s - s_h|^3.
\]

(74)

This finally yields

\[\frac{1}{2} \frac{d}{dt} \|e\|^2 + \frac{d}{dt} \|e\|^2 \leq A_1 (|s - s_h|^3 + |s' - s_h'|^3) + A_2 \frac{\|e\|^2}{s^3}
\]

\[+ A_3 |s - s_h|^3 + A_4 \sum_{i \in J_0} \|R(u_h)\|_{L^2(J_0)^2} |s - s_h|^3,
\]

(75)
where \( M(s, s', s_n, s_b) := \frac{1}{2}s' - s_n' + \frac{s_b}{s_n} s - s_n \) and \( A_i \ (i \in \{1, 2, 3, 4\}) \) are uniformly bounded positive constants defined by

\[ A_1 := 1, \]
\[ A_2 := 3\xi + c\eta, \]
\[ A_3 := M(s, s', s_n, s_b') + \frac{F_1 + F_2}{2} + \left( c\xi \xi \frac{1}{2} + c\xi^{\frac{1}{2}} \right) |s|^{1/2} \]
\[ + c\xi \xi \frac{1}{2} \left( \frac{1 + s_n}{ss_n} + |\mathbf{D}| \right) |t|^{1/2}, \]
\[ A_4 := c\xi \xi \frac{1}{2}. \] (76)

It is worth noting that the right-hand side of (75) depends on \( u_h \) but is independent of \( u \), and hence, (75) keeps the \textit{a posteriori} character.

Applying conveniently Gronwall's inequality, we conclude the proof of Theorem 6.2.

9 Conclusion

The problem discussed in this note represents a simplification to a one-phase setting of a more complex problem posed in two-phase moving domains, which arises when modeling the progress of the concrete carbonation via moving reaction interfaces. Our results can be summarized as follows:

- By means of the \textit{a priori} estimate (51), we showed that the approximation by piecewise linear finite elements for the semi-discretization in space converges to the solution of the initial problem when the discretization grid becomes finer. (51) also shows an order of convergence of \( \mathcal{O}(h) \) for our semi-discretization method.
- The \textit{a posteriori} error estimate (52) can be employed in order to calculate in an adaptive manner the 1D penetration of a sharp carbonation front in concrete.

We expect that the way we proceeded to obtain the error estimates may be applied to deal with a wealth of 1D scenarios, in which several moving phases and internal fixed or moving boundaries occur.

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