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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 productions 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: 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

$$\mathrm{Ca(OH)_2(s \to aq) + CO_2(g \to aq) \to CaCO_3(aq \to s) + H_2O}. \qquad (1)$$

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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 ionic species (like chloride or sulfate), the carbonation typically facilitates corrosion, and hence, spalling of the concrete may occur. We refer to [Cha99] 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[1] 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, MB06b] (and analyzed by the author in [Mun06]) 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, LT03, 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 [Mun06]. 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 $\mathcal{O}(h)$ 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 [SMB05] 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[2]. 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 (2)-(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 section 7 and section 8 we

[1] With the terminology from [Mun06], we prepare the basic framework for the error analysis of the full semi-discrete P_Γ model.

[2] In this paper, an isoline 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_3 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 $u = u(x,t)$ ($x \in \Omega_1(t) =]0, s(t)[$, where $t \in S_T :=]0, T[$ 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]:

$$u_{1,t} - D_1 u_{1,xx} = P_1(Q_1 u_2 - u_1) \quad \text{in } \Omega_1(t) \tag{2}$$

$$u_{2,t} - D_2 u_{2,xx} = -P_2(Q_2 u_2 - u_1) \quad \text{in } \Omega_1(t) \tag{3}$$

$$u_{3,t} = S_{3,diss}(u_{3,eq} - u_3) \quad \text{at } \Gamma(t) \tag{4}$$

$$u_{\ell,t} - D_\ell u_{\ell,xx} = 0 \ (\ell \in \{4,5\}), \quad \text{in } \Omega_1(t), \tag{5}$$

initial conditions

$$u_i(0,x) = u_{i0}(x) \quad \text{in } \Omega_1(0) \ (i \in \{1,2,3,4,5\}), \tag{6}$$

and boundary conditions

$$u_i(t,0) = \lambda_i(t), t \in S_T \ (i \in \{1,2,4,5\}) \tag{7}$$

$$-D_1 u_{1,x}(s(t),t) = \eta_\Gamma(u(s(t),t) + s'(t)u_1(s(t),t) \tag{8}$$

$$-D_2 u_{2,x}(s(t),t) = s'(t)u_2(s(t),t) \tag{9}$$

$$-D_\ell u_{\ell,x}(s(t),t) = \eta_\Gamma(u(s(t),t) \ (\ell \in \{4,5\}). \tag{10}$$

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

$$s'(t) = \eta_\Gamma(u(s(t),t)), t \in S_T \quad s(0) = s_0 \tag{11}$$

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 (I) *Select*

$$D_i, P_j, Q_j, S_{3,diss} \in \mathbb{R}_+^* \quad (i \in \{1,2,4,5\}, j \in \{1,2\}), \tag{12}$$

$\lambda_i, u_{3,eq} : S_T \to \mathbb{R}_+^*, \ u_{i0} : \Omega_1(0) \to \mathbb{R}_+^* \quad (i \in \{1,2,3,4,5\})$ *are given functions*, (13)

[3]The underlying model represents a simplified case of a more general moving sharp-interface model, which was developed in [Mun06].

and

$$s_0 > 0, \tag{14}$$

$$s_0 \leq s(t) \leq L, \tag{15}$$

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

Under **Assumption (I)**, 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 $\Omega_1(t)$ 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 [Mun06] 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 [Mun06, 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 not 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 numerics 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, Nit80]) 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 fixing-front technique of Landau [Lan50] in order to freeze the boundaries of the moving phase and examined the transformed pde 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 [Vui90] are also related to this issue. In all these contributions, various $L^\infty-$, L^2-, 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 *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 Caboussat 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:*

$$\mathcal{I}_1 := \{1, 2, 4, 5\}, \quad \mathcal{I}_2 := \{3\}, \quad \mathcal{I} := \mathcal{I}_1 \cup \mathcal{I}_2. \tag{16}$$

(b) We denote $u'(t) := \frac{\partial u}{\partial t}(\cdot, t) = u_t(\cdot, t), u_y(y, t) := \frac{\partial u}{\partial y}(y, t)$ *for* $(y, t) \in \Omega \times S_T$*. Notice also that, sometimes, we omit to write explicitly the dependence of* u*,* $\bar{u}$*,* $\hat{u}$*, or the test function on the variables* t*,* y *and/or* x*. Also, we sometimes neglect to write the dependence of* s *on* t*. In particular,* $e(1)$*,* $u(1)$ *and* $u_{,y}(1)$ *replace* $e(1, t)$*,* $u(1, t)$ *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 $H = L^2(0, 1) = H_i$ $(i \in \mathcal{I}_1)$ and $\mathbb{H} = \prod_{i\in\mathcal{I}_1} H_i = H^{|\mathcal{I}_1|}$. The space H_i is equipped with the norm $|u|_{H_i} := \left(\int_a^b u^2(y)dy\right)^{\frac{1}{2}}$ and with the scalar product $(u, v)_{H_i} := \left(\int_a^b u(y)v(y)dy\right)^{\frac{1}{2}}$ for all $u, v \in H_i$. The product space $\mathbb{H}$ is normed by $|u|_{\mathbb{H}} = \left(\sum_{i\in\mathcal{I}_1\cup\mathcal{I}_2} |u_i|^2_{H_i}\right)^{\frac{1}{2}}$ for all $u \in \mathbb{H}$ and equipped with the standard scalar product.

Denote $V := \{v \in H^1(0, 1) : v(0) = 0\} := V_i$ $(i \in \mathcal{I}_1)$, $\mathbb{V} := \prod_{i\in\mathcal{I}_1} V_i := V^{|\mathcal{I}_1|}$. The space V_i is endowed with the norm $||u||_{V_i} = |u_{,y}|_{H_i}$.

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

The inequality

$$ab \le \xi a^p + c_\xi b^q, \tag{17}$$

where $\xi > 0$, $c_\xi := \frac{1}{q}\frac{1}{\sqrt[p]{(\xi p)^q}} > 0$, $\frac{1}{p} + \frac{1}{q} = 1$ with $p \in]1, \infty[$, 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

$$ab^\theta c^{1-\theta} \le \frac{\bar{\xi}}{2}a^2 + \xi c_{\bar{\xi}} b^2 + c_{\bar{\xi}} c_\xi c^2. \tag{18}$$

This holds for all $\theta \in [0,1]$ and $a, b, c \in \mathbb{R}_+$, where $c_{\bar{\xi}} := \frac{1}{2\bar{\xi}^2}$ and c_ξ is as in (17). We obtain (18) by applying first the arithmetic-geometric mean for the numbers a and $b^\theta c^{1-\theta}$ and then by using (17) in the second term for the numbers b^2 and c^2 with $\frac{1}{p} := \theta$ and $\frac{1}{q} := 1-\theta$. If in (18) ξ and $\bar{\xi}$ belong to a compact subset of $\mathbb{R}_+^*$, then it results that c_ξ and $c_{\bar{\xi}}$ are strictly positive and bounded above.

The inequality

$$|a+b|^p \leq \begin{cases} (1+\xi)^{p-1}|a|^p + \left(1+\frac{1}{\xi}\right)^{p-1}|b|^p & \text{for } p \in [1,\infty[\\ |a|^p + |b|^p & \text{for } p \in]0,1[\end{cases} \tag{19}$$

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

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

$$|u_i|_\infty \leq \hat{c}|u_i|^{1-\theta}||u_i||^\theta \leq \hat{c}(\xi||u_i|| + c_\xi|u_i|) \quad \text{for all } u_i \in V_i,\ (i \in \mathcal{I}_1). \tag{20}$$

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 $J_n := \{0, \ldots, n\}$. For each $i \in J_n$, we denote $J_i :=]y_i, y_{i+1}[$. We take $y_0 = 0 < y_1 < y_2 < \ldots y_n < y_{n+1} = 1$ and set $h_j = y_{j+1} - y_j$ for all $j \in J_n$. Let h be the maximum mesh size, namely $h := \max_{i \in J_n} h_j$. Denote by $V_h := \{\psi \in C([0,1]) : \psi|_{[y_j, y_{j+1}]} \in \Pi_1, j \in J_n\}$, where Π_1 represents the set of polynomials of degree one.

Assume $u_0 \in \mathbb{V}$. In the sequel, u_{0h} denotes the Lagrange interpolant of $u_0 \in \mathbb{V}$ in $V_h^{|\mathcal{I}_1|}$, and respectively, for each $i \in \mathcal{I}_1$, u_{i0h} represents the interpolant of $u_{i0} \in V_i$ in V_h. Hence, we have $||u_{0,h}||_{\mathbb{V}} \leq ||u_0||_{\mathbb{V}}$. Set $\mathbb{V}_h := V_h^{|\mathcal{I}_1|}$.

If $u_{i0} \in H^2(0,1)$ for all $i \in \mathcal{I}_1$, then by classical interpolation results (see [Joh94] or Lemma 4.2 below) we obtain

$$|u_{i0} - u_{i0h}| \leq ch^2||u_0||_{H^2(0,1)}, \tag{21}$$

where c is a strictly positive constant independent of h.

Let us denote by I_h^i $(i \in \mathcal{I}_1)$ the interpolation operator

$$I_h^i : C([0,1]) \to V_h \text{ defined by } (I_h^i u)(y) := \sum_{j \in J_n} u_i(y,t)\psi_i(y),\ y \in [0,1].$$

Let P_h^i $(i \in \mathcal{I}_1)$ 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

$$|P_h^i u_i - u_i| \leq |I_h^i u_i - u_i| \leq ch^r||u_i||_{H^r \cap H^1} \text{ for all } v \in H^r \cap H^1, \tag{22}$$

where $H^r \cap H^1 := \{\varphi \in H^r(0,1) : \varphi(0) = \varphi(1) = 0\}$. For each $i \in \mathcal{I}_1$, let $R_h^i : H_0^1(0,1) \to V_h$ 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 $u_i \in H_0^1(0,1)$, where $a(u_i,\varphi) := (\nabla u_i, \nabla\varphi)$. The operator $\mathbb{R}_h := (R_h^1, R_h^2, R_h^4, R_h^5)^t$ is the elliptic (Ritz) operator. Note also that $\mathbb{R}_h u$ 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 $\theta \in \left[\frac{1}{2}, 1\right[$ and take $\varphi \in H^2(0,1)$. Let $\mathcal{R}_h$ denote Riesz's projection operator. Then there exists the strictly positive constants γ_1, γ_2 and γ_3 such that the Lagrange interpolant $\mathcal{R}_h\varphi$ of φ satisfies the following estimates:*

(i) $|\varphi - \mathcal{R}_h\varphi| \le \gamma_1 h^2 |\varphi|_{H^2(0,1)}$;

(ii) $||\varphi - \mathcal{R}_h\varphi|| \le \gamma_2 h |\varphi|_{H^2(0,1)}$;

(iii) $|\varphi(1) - \mathcal{R}_h(1)\varphi(1)| \le \gamma_3 h^{2-\theta} |\varphi|_{H^2(0,1)}$.

Proof. (i) and (ii) are classical results, see Theorem 5.5, p.65 in [LT03] (or [Joh94], e.g.). The proof of (iii) follows combining (i), (ii) and the multiplicative inequality (20). More precisely, we set $\gamma_3 := \hat{c}\gamma_1^{1-\theta}\gamma_2^{\theta}$, whereas $\hat{c} > 0$ is cf. (20) and $\theta \in \left[\frac{1}{2}, 1\right[$. ■

In sections 7 and 8, we use Lemma 4.2 with the choice $\mathcal{R}_h := R_h^i$ and $\varphi := \varphi_i \in V_i \cap H^2(0,1) = H^2 \cap H^1$ for $i \in \mathcal{I}_1$.

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

By the transformation

$$y = \frac{x}{s(t)}, \tag{23}$$

we map the moving domain $\Omega_1(t)$ 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 $u(x,t)$ in the original domain $\Omega_1(t)$, as $u(y,t)$. We also keep the same notation for the position of the interface, namely $s(t)$. Let $\varphi := (\varphi_1, \varphi_2, \varphi_4, \varphi_5)^t \in \mathbb{V}$ be an arbitrary test function and take $t \in S_T$. We let $a(\cdot)$ denote the transport part of the model, $b_f(\cdot)$ and $e(\cdot)$ comprise various volume and surface productions, and $h(\cdot)$ incorporate a non-local term, whose presence is due to the use of (23), viz.

$$a(s,u,\varphi) := \frac{1}{s}\sum_{i\in\mathcal{I}_1}(D_i u_{i,y}, \varphi_{i,y}), \tag{24}$$

$$b_f(u,s,\varphi) := s\sum_{i\in\mathcal{I}_1}(f_i(u), \varphi_i), \tag{25}$$

$$e(s',u,\varphi) := \sum_{i\in\mathcal{I}_1} g_i(s', u(1))\varphi_i(1), \tag{26}$$

$$h(s',u_y,\varphi) := \sum_{i\in\mathcal{I}_1} s'(y u_{i,y}, \varphi_i), \tag{27}$$

where the production terms f_i and g_i are given by

$$\begin{aligned} f_1(u) &:= P_1(Q_1u_2 - u_1), && (28)\\ f_2(u) &:= -P_2(Q_2u_2 - u_1), && (29)\\ f_4(u) &:= f_5(u) = 0, && (30)\\ g_1(s', u) &:= \eta_\Gamma(1, t) + s'(t)u_1(1, t), && (31)\\ g_2(s', u) &:= s'(t)u_2(1, t), && (32)\\ g_5(s', u) &:= \eta_\Gamma(1, t). && (33) \end{aligned}$$

Set

$$\mathcal{K} := \prod_{i\in\mathcal{I}_1\cup\mathcal{I}_2} [0, k_i], \tag{34}$$

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

$$M_{\eta_\Gamma} := \max_{u\in\mathcal{K}}\{\eta_\Gamma(u, \Lambda)\}. \tag{35}$$

In (34), we set

$$\begin{cases} k_i &:= \max\{u_{i0}(y) + \lambda_i(t), \lambda_i(t) : y \in [0, 1], t \in \bar{S}_T\}, i = 1, 2, 4,\\ k_5 &:= \max\{u_{50}(y) + \lambda_5(t), \lambda_5(t), \kappa : y \in [0, 1], t \in \bar{S}_T\}, \end{cases} \tag{36}$$

where

$$\kappa := \frac{L_0}{D_5 - M_{\eta_\Gamma}LL_0}\left(M_{\eta_\Gamma} + \frac{L}{2}|\lambda_{5,t}| + 1\right). \tag{37}$$

The only assumptions that are needed to describe the reaction rate η_Γ are contained in the items (A) and (B) of the next **Assumption**:

Assumption (II) *Consider*

(A) Fix $\Lambda \in M_\Lambda$. Let $\eta_\Gamma(u, \Lambda) > 0$, if $u_1 > 0$ and $u_3 > 0$, and $\eta_\Gamma(u, \Lambda) = 0$, otherwise. Moreover, for any fixed $u_1 \in \mathbb{R}$ the reaction rate η_Γ is bounded.

(B) The reaction rate $\eta_\Gamma : \mathbb{R}^{|\mathcal{I}_1|} \times M_\Lambda \to \mathbb{R}_+$ is locally Lipschitz.

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

(C2) $P_1Q_1k_2 \leq P_1k_1$; $P_2k_1 \leq P_2Q_2k_2$;

(C3) $Q_2 > Q_1$.

A typical choice of η_Γ is the generalized mass-balance law, i.e.

$$\eta_\Gamma(u, \Lambda) := ku_1^pu_3^q, \quad p \geq 1, q \in \mathbb{R}, k > 0, \Lambda := \{p, q, k\}, \tag{38}$$

where u_3 is the positive solution of (4).

For the initial and boundary data we choose the following:

Assumption (III) *Select*

$$\lambda \in W^{1,2}(S_T)^{|\mathcal{I}_1|}, \lambda(t) \geq 0 \ \textit{a.e.}\ t \in \bar{S}_T, \tag{39}$$

$$u_{3,eq} \in L^\infty(S_T), u_{3,eq}(t) \geq 0 \ \textit{a.e.}\ t \in \bar{S}_T, \tag{40}$$

$$u_0 \in L^\infty(0,1)^{|\mathcal{I}_1|}, u_0(y) + \lambda(0) \geq 0 \ \textit{a.e.}\ y \in [0,1], \tag{41}$$

$$u_{30} \in L^\infty(0, s(t)), u_{30}(x) \geq 0 \ \textit{a.e.}\ x \in [0, s(t)]. \tag{42}$$

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

Definition 5.2 (Weak Solution to P_Γ^1) *We call the couple (u, s) a local weak solution to problem P_Γ^1 if and only if there is a $S_\delta :=]0, \delta[$ with $\delta \in]0, T]$ such that*

$$s_0 < s(\delta) \leq L_0, \tag{43}$$

$$s \in W^{1,4}(S_\delta), \tag{44}$$

$$u \in W_2^1(S_\delta; \mathbb{V}, \mathbb{H}) \cap [\bar{S}_\delta \mapsto L^\infty(0,1)]^{|\mathcal{I}_1|}, \tag{45}$$

$$\begin{cases} s\sum_{i\in\mathcal{I}_1}(u_{i,t}(t), \varphi_i) + a(s, u, \varphi) + e(s', u + \lambda, \varphi) = b_f(u + \lambda, s, \varphi) \\ +h(s', u_{,y}, \varphi) - s\sum_{i\in\mathcal{I}_1}(\lambda_{i,t}(t), \varphi_i) \qquad \textit{for all } \varphi \in \mathbb{V}, \ \textit{a.e.}\ t \in S_\delta, \\ s'(t) = \eta_\Gamma(1, t) \ \textit{a.e.}\ t \in S_\delta, \\ u(0) = u_0 \in \mathbb{H}, s(0) = s_0. \end{cases} \tag{46}$$

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_Γ^1.

Theorem 5.3 (Well-posedness of P_Γ^1) *Consider* **Assumptions (I)-(III)** *be fulfilled. In this case, the following assertions hold:*
(a) There exists a $\delta \in]0, T[$ such that the problem P_Γ^1 admits a unique local solution on S_δ in the sense of Definition 5.2;
(b) $0 \leq u_i(y, t) + \lambda_i(t) \leq k_i$ a.e. $y \in [0, 1]$ $(i \in \mathcal{I}_1)$ 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_Γ, whose well-posedness was shown in [Mun06], the non-carbonated phase $]s(t), L[$ degenerates, then the techniques used to prove Theorem 3.4.6 in [Mun06] conclude the proof of Theorem 5.3. ■

Let us now turn the attention to the semi-discrete FEM approximation. Denote by η_Γ^h the approximation of the reaction rate η_Γ and let $s_h \in W^{1,4}(S_\delta)$ be an approximation of $s \in W^{1,4}(S_\delta)$. The connection between the quantities s_h and η_Γ^h is given by $s_h' = \eta_\Gamma^h(u_h(s_h(t), t))$, where $s_h(0) = s(0)$ and $u_h := (u_{1h}, u_{2h}, u_{4h}, u_{5h})^t \in \mathbb{V}_h$ represents an approximation of $u := (u_1, u_2, u_4, u_5)^t \in \mathbb{V}$. Furthermore, set $v_h := (v_{1h}, v_{2h}, v_{4h}, v_{5h})^t \in \mathbb{V}_h$. The precise definition of the space $\mathbb{V}_h$ is given in section 4.

Definition 5.4 (Weak Solution to $P_\Gamma^{1,\mathrm{sd}}$) *We call the couple (u_h, s_h) a local weak solution to problem $P_\Gamma^{1,\mathrm{sd}}$ if and only if there is a $S_{\hat{\delta}} :=]0, \hat{\delta}[$ with $\hat{\delta} \in]0, \delta]$ such that*

$$s_0 < s_h(\hat{\delta}) \leq L_0, \tag{47}$$

$$s_h \in W^{1,4}(S_{\hat{\delta}}), \tag{48}$$

$$u_h \in \left[H^1(S_{\hat{\delta}}, V_h) \cap L^\infty(S_{\hat{\delta}}, H)\right]^{|\mathcal{I}_1|} \tag{49}$$

$$\begin{cases} s_h \sum_{i\in\mathcal{I}_1}(u_{ih,t}(t), \varphi_{ih}) + a(s_h, u_h, \varphi_h) + e(s_h', u_h + \lambda, \varphi_h) = b_f(u_h + \lambda, s_h, \varphi_h) \\ +h(s_h', u_{h,y}, \varphi_h) - s_h \sum_{i\in\mathcal{I}_1}(\lambda_{i,t}(t), \varphi_{ih}) \qquad \text{for all } \varphi_h \in \mathbb{V}_h, \text{ a.e. } t \in S_{\hat{\delta}}, \\ s_h'(t) = \eta_\Gamma^h(1,t) \text{ a.e. } t \in S_{\hat{\delta}}, \\ u_h(0) = u_0 \in \mathbb{H}, s_h(0) = s_0. \end{cases} \tag{50}$$

A first result is the next theorem:

Theorem 5.5 (Well-posedness of $P_\Gamma^{1,\mathrm{sd}}$) *Let* **Assumptions (I)-(III)** *be fulfilled. There exists $\bar{\delta} \in]0, \min\{\delta, \hat{\delta}\}]$, which is independent of h, such that problem $P_\Gamma^{1,\mathrm{sd}}$ has a unique weak solution*

$$(u_h, s_h) \in \left[H^1(S_{\bar{\delta}}, V_h) \cap L^\infty(S_{\bar{\delta}}, H)\right]^{|\mathcal{I}_1|} \times W^{1,4}(S_{\bar{\delta}}),$$

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 3.4.6 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 $u_0 \in \mathbb{V} \cap \left[H^2(0,1)\right]^{|\mathcal{I}_1|}$ and consider* **Assumptions (I)-(III)**. *Then problems P_Γ^1 and $P_\Gamma^{1,\mathrm{sd}}$ are uniquely solvable. Let (u, s) and (u_h, s_h) be the corresponding solutions. Then the following estimate holds: There exist a $\delta_1 \in]0, \max\{\delta, \bar{\delta}\}]$ and a strictly positive constant c, which are independent of h, such that*

$$||u - u_h||_{L^\infty(S_{\delta_1}, \mathbb{H}) \cap L^2(S_{\delta_1}, \mathbb{V})} + ||s - s_h||_{W^{1,4}(S_{\delta_1})} \leq ch. \tag{51}$$

Proof. See section 7. ■

Theorem 6.2 (*A Posteriori* Error Estimate) *Let $u_0 \in \mathbb{V} \cap \left[H^2(0,1)\right]^{|\mathcal{I}_1|}$ and consider* **Assumptions (I)-(III)**. *Then problems P_Γ^1 and $P_\Gamma^{1,\mathrm{sd}}$ are uniquely solvable. Let (u, s) and (u_h, s_h) be the corresponding solutions. There exist $\delta_2 \in]0, \max\{\delta, \bar{\delta}\}]$ and strictly positive constants c_i ($i \in \{1, 2, 3\}$) and c, which are independent of h and u, such that*

$$\begin{aligned} &|u - u_h|_{\mathbb{H}}^2 + c_1|s - s_h|^2 + c_2 \int_0^t ||u - u_h||_{\mathbb{V}}^2 d\tau \\ &\leq c \sum_{i\in J_n} h_i^2 \{||R(u_h)||_{L^2(S_{\delta_2}; L^2(\mathcal{J}_i))}^2 + h_i^2 ||u_0||_{H^2(\mathcal{J}_i)}^2\}, \end{aligned} \tag{52}$$

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

$$R(u_h) = f_h(s_h, u_h) - u_{h,t} + \frac{s_h'}{s_h} y u_{h,y} + e_h(s_h', u_h(1)). \tag{53}$$

In (53), the quantities $f_h(s_h, u_h)$ and $e_h(s'_h, u_h(1))$ are defined by

$$\begin{aligned} f_h(s_h, u_h) &:= s_h \sum_{i\in\mathcal{I}_1} f_i(u_h), \\ e_h(s'_h, u_h(1)) &:= \sum_{i\in\mathcal{I}_1} g_i(s'_h, u_h). \end{aligned}$$

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 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 (23) is affine and the solution (u_h, s_h) of $P_\Gamma^{1,\mathrm{sd}}$ is sufficiently regular (cf. Proposition 3.4.17 from [Mun06]), the inverse transformation $x = ys_h(t)$ can be employed in order to make the estimates (51) and (52) available for the original problem (with moving boundaries).*

Notation 6.4 *For the sake of simplicity, we put $\delta_1 = \delta_2 = \bar{\delta} = \hat{\delta}$ and $\delta = \hat{\delta}$.*

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 5.3 and Theorem 5.5 is to ensure the existence of local in time solutions to P_Γ^1 and $P_\Gamma^{1,\mathrm{sd}}$, respectively. Let us denote by $S_\delta =]0, \delta[$ (with δ 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 $e := (e_1, e_2, e_4, e_5)^t$. For each test function $w_{ih} \in V_h$ $(i \in \mathcal{I}_1)$, we subtract the variational formulation in terms of u_h from that one in terms of u and obtain the following equality:

$$\begin{aligned} ((u+\lambda)_{,t}, w_h) &- ((u_h+\lambda)_{,t}, w_h) + \frac{1}{s^2}\sum_{i\in\mathcal{I}_1}(D_i u_{i,y}, w_{ih,y}) \\ &- \frac{1}{s_h^2}\sum_{i\in\mathcal{I}_1}(D_i u_{ih,y}, w_{ih,y}) + \frac{1}{s}\left[\eta_\Gamma + s'(u_1(1)+\lambda_1)\right] w_{1h}(1) \\ &- \frac{1}{s_h}\left[\eta_\Gamma^h + s'_h(u_{1h}(1)+\lambda_1)\right] w_{1h}(1) + \frac{s'}{s}(u_2(1)+\lambda_2) w_{2h}(1) \\ &- \frac{s'_h}{s_h}(u_{2h}(1)+\lambda_2) w_{2h}(1) - \frac{1}{s}\eta_\Gamma w_{5h}(1) + \frac{1}{s_h}\eta_\Gamma^h w_{5h}(1) \\ &= (P_1(Q_1(u_2+\lambda_2) - (u_1+\lambda_1)), w_{1h}) \\ &- (P_1(Q_1(u_{2h}+\lambda_2) - (u_{1h}+\lambda_1)), w_{1h}) \\ &- (P_2(Q_2(u_2+\lambda_2) - (u_1+\lambda_1)), w_{2h}) \end{aligned}$$

$$
\begin{aligned}
&+ \quad (P_2(Q_2(u_{2h}+\lambda_2)-(u_{1h}+\lambda_1)),w_{2h}) \\
&+ \quad \frac{s'}{s}\sum_{i\in\mathcal{I}_1}(yu_{i,y},w_{ih}) - \frac{s'_h}{s_h}\sum_{i\in\mathcal{I}_1}(yu_{ih,y},w_{ih}). \qquad (54)
\end{aligned}
$$

Grouping some of the terms in (54), we obtain

$$
\begin{aligned}
(e_{,t},w_h) \quad &+ \quad \frac{1}{s^2}\sum_{i\in\mathcal{I}_1}(D_i(u_i-u_{ih})_{,y},w_{ih,y}) = \left(\frac{1}{s_h^2}-\frac{1}{s^2}\right)\sum_{i\in\mathcal{I}_1}(D_iu_{ih,y},w_{ih,y}) \\
&- \quad \left(\frac{s'}{s}(u_1(1)+\lambda_1)-\frac{s'_h}{s_h}(u_{1h}(1)+\lambda_1)+\frac{\eta_\Gamma}{s}-\frac{\eta_\Gamma^h}{s_h}\right)w_{1h}(1) \\
&- \quad \left(\frac{s'}{s}(u_2(1)+\lambda_2)-\frac{s'_h}{s_h}(u_{2h}(1)+\lambda_2)\right)w_{2h}(1)-\left(\frac{\eta_\Gamma}{s}-\frac{\eta_\Gamma^h}{s_h}\right)w_{5h}(1) \\
&+ \quad P_1Q_1(e_2,w_{1h})-P_1(e_1,w_{1h})-P_2Q_2(e_2,w_{2h})+P_2(e_1,w_{2h}) \\
&+ \quad \frac{s'}{s}\sum_{i\in\mathcal{I}_1}(ye_{i,y},w_{ih})+\left(\frac{s'}{s}-\frac{s'_h}{s_h}\right)\sum_{i\in\mathcal{I}_1}(yu_{ih,y},w_{ih}). \qquad (55)
\end{aligned}
$$

Therefore, we may write

$$
(e_{,t},w_h)+\frac{\min_{i\in\mathcal{I}_1}D_i}{s(t)}(e_{,y},w_{h,y}) \le \sum_{\ell=1}^{5} I_\ell, \qquad (56)
$$

where the terms I_ℓ are given by

$$
\begin{aligned}
I_1 &:= \left(\frac{1}{s_h^2}-\frac{1}{s^2}\right)\sum_{i\in\mathcal{I}_1}(D_iu_{ih,y},w_{ih,y}), \\
I_2 &:= |\left(\frac{\eta_\Gamma}{s}-\frac{\eta_\Gamma^h}{s_h}\right)||w_{1h}(1)+w_{5h}(1)|, \\
I_3 &:= \sum_{i=1}^{2}|\left(\frac{s'}{s}(u_i(1)+\lambda_i)-\frac{s'_h}{s_h}(u_{ih}(1)+\lambda_i)|\right)|w_{ih}(1)| \\
I_4 &:= P_1Q_1(e_2,w_{1h})-P_1(e_1,w_{1h})-P_2Q_2(e_2,w_{2h})+P_2(e_1,w_{2h}) \\
I_5 &:= \frac{s'}{s}\sum_{i\in\mathcal{I}_1}(ye_{i,y},w_{ih})+\left(\frac{s'}{s}-\frac{s'_h}{s_h}\right)\sum_{i\in\mathcal{I}_1}(yu_{ih,y},w_{ih}).
\end{aligned}
$$

Set $d := \min_{i\in\mathcal{I}_1} D_i$. For any $v_h \in \mathbb{V}_h$, the following estimate holds:

$$
\begin{aligned}
\frac{1}{2}\frac{d}{dt}|e|^2+\frac{d}{s^2}||e||^2 \le &= (e_{,t},u-u_h) \\
+\frac{d}{s^2}(e_{,y},(u-u_h)_{,y}) = (e_{,t},u-v_h)+\frac{d}{s^2}&(e_{,y},(u-v_h)_{,y}) \\
+(e_{,t},v_h-u_h)+\frac{d}{s^2}&(e_{,y},(v_h-u_h)_{,y}). \qquad (57)
\end{aligned}
$$

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

$$
\frac{1}{2}\frac{d}{dt}|e|^2 \quad + \quad \frac{d}{s^2}||e||^2 \le (e_{,t},u-v_h)+\frac{d}{s^2}(e_{,y},(u-v_h)_{,y})
$$

$$
\begin{aligned}
&+ \quad \left(\frac{1}{s_h^2}-\frac{1}{s^2}\right)\sum_{i\in\mathcal{I}_1}(D_i(u_{ih})_{,y},(v_{ih}-u_{ih})_{,y})\\
&+ \quad \left(\frac{\eta_\Gamma}{s}-\frac{\eta_\Gamma^h}{s_h}\right)|\,(v_{1h}(1)-u_{1h}(1)+v_{5h}(1)-u_{5h}(1))\,|\\
&+ \quad P_1Q_1(e_2,v_{1h}-u_{1h})-P_1(e_1,v_{1h}-u_{1h})\\
&- \quad P_2Q_2(e_2,v_{2h}-u_{2h})+P_2(e_1,v_{2h}-u_{2h})\\
&+ \quad \frac{s'}{s}\sum_{i\in\mathcal{I}_1}(ye_{i,y},v_{ih}-u_{ih})\\
&+ \quad \left(\frac{s'}{s}-\frac{s'_h}{s_h}\right)\sum_{i\in\mathcal{I}_1}(yu_{ih,y},v_{ih}-u_{ih}). \qquad (58)
\end{aligned}
$$

In order to simplify the writing of some of the inequalities, we introduce the strictly positive constants c_ℓ ($\ell\in\{1,\dots,7\}$), whose precise expression is not explicitly written but can be easily derived. However, it is worth mentioning that for each $\ell\in\{1,\dots,7\}$ 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 $c_1=c_1(\Lambda,s_0)>0$ such that*

$$
\frac{\eta_\Gamma^h}{s_h}-\frac{\eta_\Gamma}{s}\le|s-s_h|\frac{\eta_\Gamma}{ss_h}+\frac{1}{s_h}|\left(\frac{\eta_\Gamma}{s}-\frac{\eta_\Gamma^h}{s_h}\right)|\le c_1(|s-s_h|+|s'-s'_h|).
$$

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

$$
\begin{aligned}
\frac{s'_h}{s_h}(u_{ih}(1)+\lambda_i)-\frac{s'}{s}(u_i(1)+\lambda_i) &= -\frac{s'_h}{s_h}e_i(1)+(u_i(1)+\lambda_i)\left(\frac{s'_h}{s_h}-\frac{s'}{s}\right)\\
&\le c_2(|e_i(1)|+|s-s_h|+|s'-s'_h|).
\end{aligned}
$$

(3) For each $i\in\mathcal{I}_1$, we have

$$
(ye_{i,y},v_{ih}-u_{ih})=(ye_{i,y},e_i)+(ye_{i,y},v_{ih}-u_i)\le\frac{1}{2}|e_i(1)|^2+||e_i|||v_{ih}-u_i|.
$$

(4) It holds

$$
(yu_{ih,y},v_{ih}-u_{ih})\le|u_{ih}||v_{ih}-u_{ih}|+|u_{ih}|||v_{ih}-u_{ih}||.
$$

(5) It holds

$$
(u_{ih,y},(v_{ih}-u_{ih})_{,y})\le||u_{ih}||||u_{ih}-v_{ih}||.
$$

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

$$
\begin{aligned}
\frac{1}{2}\frac{d}{dt}|e|^2 \quad &+ \quad \frac{d}{s^2}||e||^2\le|e_{,t}||u-v_h|+\frac{d}{s^2}||e||||u-v_h||\\
&+ \quad |s-s_h|\frac{s+s_h}{s^2s_h^2}\sum_{i\in\mathcal{I}_1}|(D_iu_{ih,y},(u_h-v_h)_{,y})dy
\end{aligned}
$$

$$
\begin{aligned}
&+ \quad c_1(|s-s_h|+|s'-s'_h|)|v_h(1)-u(1)+e(1)| \\
&+ \quad c_2(|e(1)|+|s-s_h|+|s'-s'_h|)|v_h(1)-u(1)+e(1)| \\
&+ \quad P_1Q_1|e_2|\left(|v_{1h}-u_1|+|e_1|\right)+P_1|e_1|\left(|v_{1h}-u_1|+|e_1|\right) \\
&+ \quad P_2Q_2|e_2|\left(|v_{2h}-u_2|+|e_2|\right)+P_2|e_1|\left(|v_{2h}-u_2|+|e_2|\right) \\
&+ \quad \frac{s'}{2s}\sum_{i\in\mathcal{I}_1}[(|e_i(1)|^2-|e_i|^2)+||e_i|||v_{ih}-u_{ih}|] \\
&+ \quad c_3(|s-s_h|+|s'-s'_h|)\sum_{i\in\mathcal{I}_1}(|u_{ih}||v_{ih}-u_{ih}| \\
&+ \quad |u_{ih}|||v_{ih}-u_{ih}||). \qquad (59)
\end{aligned}
$$

After some elementary manipulations, we directly gain the estimate:

$$
\begin{aligned}
\frac{d}{dt}|e|^2+\frac{d}{s^2}||e||^2 &\leq |e_{,t}||u-v_h|+\frac{d}{s^2}||e||||u-v_h|| \\
+c_3|s-s_h|||u_h||(||v_h-u||+||e||)+c_1(|s-s_h|+|s'-s'_h|)\hat{c}||e||^{\theta}|e|^{1-\theta} & \\
+c_4(|s-s_h|+|s'-s'_h|)\hat{c}||v_h-u||^{\theta}|v_h-u|^{1-\theta} & \\
+c_2|e(1)|^2+c_2(|s-s_h|+|s'-s'_h|)\hat{c}||e||^{\theta}|e|^{1-\theta} & \\
+\frac{P_1Q_1}{2}\left(2|e_2|^2+|v_{1h}-u_1|^2+|e_1|^2\right)+\frac{P_1}{2}\left(2|e_1|^2+|v_{1h}-u_1|^2\right) & \\
+\frac{P_2Q_2}{2}\left(2|e_2|^2+|v_{2h}-u_2|^2\right)+\frac{P_2}{2}\left(2|e_1|^2+|v_{2h}-u_2|^2\right) & \\
+\frac{s'}{2s}\hat{c}||e||^{2\theta}|e|^{2(1-\theta)}+\frac{s'}{s}||e|||v_h-u| & \\
+c_3(|s-s_h|+|s'-s'_h|)|v_h-u|+c_5(||v_h-u||+||e||). \qquad (60) &
\end{aligned}
$$

We set $v_h=\mathbb{R}_h u$ and rearrange some of the terms in (60). Afterwards we use Lemma 4.2 to obtain the next estimate. It therefore yields

$$
\begin{aligned}
\frac{d}{dt}|e|^2+\frac{d}{s^2}||e||^2 &\leq |e_{,t}|\gamma_1 h^2|u|_{H^2(0,1)}+\frac{d}{s^2}||e||\gamma_2 h|u|_{H^2(0,1)} \\
+c_3|s-s_h|||u_h||\left(\gamma_2 h|u|_{H^2(0,1)}+||e||\right) & \\
+(c_1+c_2)(|s-s_h|+|s'-s'_h|)\hat{c}||e||^{\theta}|e|^{1-\theta} & \\
+c_4(|s-s_h|+|s'-s'_h|)c\gamma_2^{\theta}h^{\theta}\gamma_1^{1-\theta}h^{2(1-\theta)}|u|_{H^2(0,1)}+c_6\left(|e_1|^2+|e_2|^2\right) & \\
+c_7\gamma_1^2h^4\left(|u_1|^2_{H^2(0,1)}+|u_2|^2_{H^2(0,1)}\right)+\frac{s'}{2s}\hat{c}||e||^{2\theta}|e|^{2(1-\theta)} & \\
+\frac{\xi}{2}\frac{||e||^2}{s^2}+\frac{s'}{2\xi}\gamma_1^2h^4|u|^2_{H^2(0,1)} & \\
+c_5\left(\gamma_2 h|u|_{H^2(0,1)}+||e||\right)(|s-s_h|+|s'-s'_h|). \qquad (61) &
\end{aligned}
$$

Since $s'(t)-s'_h(t)\leq c(u(1,t)-u_h(1,t))=\int_0^1 e_y(\zeta,t)d\zeta$, we obtain

$$
|\sigma|=|s'-s'_h|\leq||e||. \qquad (62)
$$

Now, using Young's inequality (see also (46) in [CR05]), we derive

$$
\frac{d|\sigma|^2}{dt}=\frac{d}{dt}(|s-s_h|^2)\leq||e||^2+|s-s_h|^2. \qquad (63)
$$

Inequality (61) 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 $|e|^2 + c|s - s_h|^2$) or [Mun06] (use $\int_{S_\delta} |s(\tau) - s_h(\tau)|^2 d\tau \leq \delta^2 \int_{S_\delta} |s'(\tau) - s'_h(\tau)|^2 d\tau$ and then apply Gronwall's inequality for the quantity $|e|^2$).

8 Proof of Theorem 6.2

For all $v \in \mathbb{V}$, we can write

$$\begin{aligned}(e_{,t}, v) \quad &+ \quad \frac{d}{L_0^2}(e_{,y}, v_{,y}) \leq (u_{,t}, v) + \frac{1}{s^2}\sum_{i\in\mathcal{I}_1} D_i(u_{iy}, v_{iy}) \\ &- \quad \left[(u_{h,t}, v) + \frac{1}{s^2}\sum_{i\in\mathcal{I}_1} D_i(u_{ihy}, v_{ihy})\right] \leq -e(s', u, v) + b_f(s, u, v) \\ &+ \quad h(s', u_{,y}, v) - \left[(u_{h,t}, v) + \frac{1}{s^2}\sum_{i\in\mathcal{I}_1} D_i(u_{ihy}, v_{ihy})\right]. \end{aligned} \tag{64}$$

By (64), we obtain

$$\begin{aligned}(e_{,t}, v) \quad &+ \quad \frac{d}{L_0^2}(e_{,y}, v_{,y}) \leq b_f(s, u, v) + h(s', u_{,y}, v) - e(s', u, v) \\ &- \quad \left[(u_{h,t}, v) + \frac{1}{s_h^2}\sum_{i\in\mathcal{I}_1} D_i(u_{ihy}, v_{iy}) + \left(\frac{1}{s^2} - \frac{1}{s_h^2}\right)\sum_{i\in\mathcal{I}_1}(D_i u_{ihy}, v_{,y})\right] \\ &= \quad b_f(s, u, v) + h(s', u_{,y}, v) - e(s', u, v) - b_f(s_h, u_h, v) \\ &- \quad h(s'_h, u_{h,y}, v) + e(s'_h, u_h, v) - \left(\frac{1}{s^2} - \frac{1}{s_h^2}\right)\sum_{i\in\mathcal{I}_1}(D_i u_{ihy}, v_{,y}) \\ &+ \quad \int_0^1 R(u_h) v dy - \frac{1}{s_h^2}\sum_{i\in\mathcal{I}_1}\int_0^1 D_i(u_{ih,y}, v_{i,y}) dy, \end{aligned} \tag{65}$$

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

$$\int_0^1 R(u_h) v dy - \frac{1}{s_h^2}\sum_{i\in\mathcal{I}_1}\int_0^1 D_i(u_{ih,y}, v_{i,y}) dy$$

can be estimated from above by

$$\sum_{i\in J_n}\int_{y_i}^{y_{i+1}} R(u_h) v dy - \frac{1}{s_h^2}\sum_{i\in J_n}\sum_{\ell\in\mathcal{I}_1}\max_{\ell\in\mathcal{I}_1} D_\ell \left[u_{\ell h,y}(y_{i+1} v(y_{i+1}) - u_{\ell h,y}(y_i) v(y_i)\right]. \tag{66}$$

Owing to $P_\Gamma^{1,\mathrm{sd}}$, we note that relation (66) vanishes when selecting as test function $v = v_h$. We rely on this observation to add (66) (in which we take $v := v_h$) to (65). Selecting in the result $v = e \in \mathbb{V}$ and $v_h := R_h e \in \mathbb{V}_h$, we obtain the following inequality:

$$(e_{,t}, e) \quad + \quad \frac{d}{L_0^2}||e||^2 \leq b_f(s, u, e) - b_f(s_h, u_h, e) + e(s'_h, u_h, e)$$

$$
\begin{aligned}
&- \quad e(s',u,e) + h(s',u_{,y},e) - h(s'_h,u_{h,y},e) - \left(\frac{1}{s^2} - \frac{1}{s_h^2}\right) \sum_{i\in\mathcal{I}_1} (D_i u_{ihy}, v_{,y}) \\
&+ \quad \sum_{i\in J_n} \int_{y_i}^{y_{i+1}} (e - \mathbb{R}e) dy \\
&- \quad \frac{1}{s_h^2} \sum_{i\in J_n} \sum_{\ell\in\mathcal{I}_1} \max_{\ell\in\mathcal{I}_1} D_\ell \left[u_{\ell h,y} y_{i+1}(e - \mathbb{R}_h e)(y_{i+1}) - u_{jh,y}(y_i)(e - \mathbb{R}_h e)(y_i)\right] \\
&= \quad \sum_{\ell=1}^{5} I_\ell, \qquad (67)
\end{aligned}
$$

where we have

$$
\begin{aligned}
I_1 &:= b_f(s,u,e) - b_f(s_h,u_h,e), \\
I_2 &:= e(s'_h,u_h,e) - e(s',u,e), \\
I_3 &:= h(s',u_{,y},e) - h(s'_h,u_{h,y},e), \\
I_4 &:= -\left(\frac{1}{s^2} - \frac{1}{s_h^2}\right) \sum_{i\in\mathcal{I}_1} (D_i u_{ihy}, e_{,y}), \\
I_5 &:= \sum_{i\in J_n} \int_{y_i}^{y_{i+1}} (e - \mathbb{R}_h e) dy \\
&\quad - \frac{1}{s_h^2} \sum_{i\in J_n} \sum_{\ell\in\mathcal{I}_1} \max_{\ell\in\mathcal{I}_1} D_\ell \left[u_{\ell h,y} y_{i+1}(e - \mathbb{R}_h e)(y_{i+1}) - u_{jh,y}(y_i)(e - \mathbb{R}_h e)(y_i)\right]. \qquad (68)
\end{aligned}
$$

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

$$
|I_1| \le \frac{P_1 Q_1 + P_2}{2} \left(|e_1|^2 + |e_2|^2\right), \qquad (69)
$$

$$
\begin{aligned}
|I_2| &\le |s - s_h|^2 + |s' - s'_h|^2 + c_\xi \left(\hat{c}^2(\bar{c} + \bar{c}^2)\right)^{\frac{1}{1-\theta}} s^{\frac{2\theta}{1-\theta}} |e|^2 \\
&+ \xi \frac{||e||^2}{s^2}, \qquad (70) \\
|I_3| &\le \frac{s'_h}{2s_h} \sum_{i\in\mathcal{I}_1} (|e_i(1)|^2 - |e_i|^2) \\
&+ \frac{1}{s s_h} \left(s_h(s' - s'_h) + s'_h(s_h - s)\right) \left(||e||^2 + |e|^2\right). \qquad (71)
\end{aligned}
$$

In (70), the constant $\bar{c}$ only depends on s_0 and L. In order to estimate $|I_4|$, we proceed as follows:

$$
\begin{aligned}
|I_4| &= -\left(\frac{1}{s^2} - \frac{1}{s_h}\right)^2 \sum_{i\in\mathcal{I}_1} (D_i u_{ih,y}, e_{,y}) \\
&\le |s - s_h| \frac{s + s_h}{s_h^2 s} \sum_{i\in\mathcal{I}_1} \left(|D_i u_{ih}(1) e(1)| + |D_i u_{ih}|||e||\right)
\end{aligned}
$$

$$\leq \hat{c}|s-s_h|||e||^{\theta}|e|^{1-\theta}\frac{s+s_h}{s_h^2 s}\sum_{i\in\mathcal{I}_1} D_i|u_{ih}(1)| + |s-s_h|\frac{||e||}{s_h}\frac{s+s_h}{ss_h}\sum_{i\in\mathcal{I}_1}|D_i u_{ih}|$$

$$\leq \bar{\xi}|s-s_h|^2 + c_{\bar{\xi}}\xi\frac{||e||^2}{s_h^2} + c_\xi c_{\bar{\xi}}\left(\hat{c}\frac{(s+s_h)\sum_{i\in\mathcal{I}_1} D_i|u_h(1)|}{s_h^{2-\theta}s}\right)^{\frac{2}{1-\theta}}|e|^2. \quad (72)$$

To bound above $|I_5|$, we firstly note that since $\mathbb{R}_h e$ is the Lagrange interpolant of e, then we have that $(e-\mathbb{R}_h)e(y_i)=0$ for all $i\in J_n\cup\{n+1\}$. Additionally, we easily see that

$$\int_{y_i}^{y_{i+1}} R(u_n)(e-R_h e)dy \leq ||R(u_h)||_{L^2(\mathcal{J}_i)}h_i^2||e||_{H^1(\mathcal{J}_i)}.$$

Owing to the latter inequality and the embedding $H^1(\mathcal{J}_i)\hookrightarrow H^1(0,1)$ $(\forall i\in J_n)$, we deduce the following bound on $|I_5|$:

$$\begin{aligned}
|I_5| &\leq \sum_{i\in J_n}\int_{y_i}^{y_{i+1}} R(u_h)(e-\mathbb{R}_h e)dy \\
&\leq \sum_{i\in J_n}||R(u_h)||_{L^2(\mathcal{J}_i)}h_i^2||e||_{H^1(\mathcal{J}_i)} \\
&\leq c\left(\sum_{i\in J_n}||R(u_h)||_{L^2(\mathcal{J}_i)}h_i^2\right)^{\frac{1}{2}}||e||_{H^1(0,1)} \\
&\leq \xi\frac{||e||^2}{s^2} + c_\xi c^2 s^2\sum_{i\in J_n}||R(u_h)||_{L^2(\mathcal{J}_i)}h_i^2|e|^2, \qquad (73)
\end{aligned}$$

where c only depends on $|J_n|$. Set $C_c := \hat{c}^2(\bar{c}+\bar{c}^2)$. Combining (69)-(73), we obtain

$$\begin{aligned}
\frac{1}{2}\frac{d}{dt}|e|^2 + \frac{d}{L_0^2}||e||^2 \leq \frac{P_1Q_1+P_2}{2}\left(|e_1|^2+|e_2|^2\right) \\
+|s-s_h|^2 + |s'-s_h'|^2 + \xi\frac{||e||^2}{s^2} + c_\xi(C_c)^{\frac{1}{1-\theta}}|s|^{\frac{2\theta}{1-\theta}}|e|^2 \\
+\left(\frac{1}{s}|s'-s_h'| + \frac{s_h'}{ss_h}|s-s_h|\right)||e||^2 + \xi\frac{||e||^2}{s^2} \\
+\left(c_\xi\hat{c}^{\frac{2}{1-\theta}}|s|^{\frac{2\theta}{1-\theta}} + \frac{1}{s}|s'-s_h'| + \frac{s_h'}{ss_h}|s-s_h|\right)|e|^2 \\
+\xi\frac{||e||^2}{s^2}(s-s_h)\frac{s+s_h}{s_h^2 s}\max_{\ell\in\mathcal{I}_1}D_\ell + \frac{1}{\xi}|s-s_h|\frac{s+s_h}{2s_h^2 s}\max_{\ell\in\mathcal{I}_1}||u||^2 \\
+\xi\frac{||e||^2}{s^2} + c_\xi c^2 s^2\sum_{i\in J_n}||R(u_h)||_{L^2(\mathcal{J}_i)}h_i^2. \qquad (74)
\end{aligned}$$

This finally yields

$$\begin{aligned}
\frac{1}{2}\frac{d}{dt}|e|^2 + \frac{d}{s^2}||e||^2 \leq \mathcal{A}_1\left(|s-s_h|^2+|s'-s_h'|^2\right) + \mathcal{A}_2\frac{||e||^2}{s^2} \\
+ \mathcal{A}_3|e|^2 + \mathcal{A}_4\sum_{i\in J_n}||\mathcal{R}(u_h)||_{L^2(J_i)}h_i^2, \qquad (75)
\end{aligned}$$

where $M(s,s',s_h,s_h') := \frac{1}{s}|s'-s_h'| + \frac{s_h'}{ss_h}|s-s_h|$ and $\mathcal{A}_i$ $(i \in \{1,2,3,4\})$ are uniformly bounded positive coefficients defined by

$$\begin{aligned}
\mathcal{A}_1 &:= 1,\\
\mathcal{A}_2 &:= 3\xi + c_{\bar{\xi}}\xi,\\
\mathcal{A}_3 &:= M(s,s',s_h,s_h') + \frac{P_1Q_1+P_2}{2} + \left(c_\xi C_c^{\frac{1}{1-\theta}} + c_\xi \hat{c}^{\frac{2}{1-\theta}}\right)|s|^{\frac{2\theta}{1-\theta}}\\
&+ c_\xi c_{\bar{\xi}} \hat{c}^{\frac{2}{1-\theta}} \left(\frac{(s+s_h)\sum_{i\in\mathcal{I}_1} D_i}{ss_h^{2-\theta}}|u_h(1)|\right)^{\frac{2}{1-\theta}},\\
\mathcal{A}_4 &:= c_\xi c^2 L^2. \qquad (76)
\end{aligned}$$

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 *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 *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 *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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