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ERROR BOUNDS ON SEMI-DISCRETE FINITE ELEMENT APPROXIMATIONS OF A MOVING-BOUNDARY SYSTEM ARISING IN CONCRETE CORROSION

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Abstract. Finite element approximations of positive weak solutions to a one-phase unidimensional moving-boundary system with kinetic condition describing the penetration of a sharp-reaction interface in concrete are considered. *A priori* and *a posteriori* error estimates for the semi-discrete fields of active concentrations and for the position of the moving interface are obtained. The important feature of the system of partial differential equations is that the non-linear coupling occurs due to the presence of both the moving boundary and the non-linearities of localized sinks and sources by reaction.

Key Words. Reaction-diffusion system, moving-boundary problem, spatial semi-discretization, finite elements, *a priori* estimates, *a posteriori* estimates, concrete corrosion

1. Introduction

In real-world applications one frequently needs to determine both the *a priori unknown* domain, where the problem is stated, as well as the solution itself. Such settings are typically named *moving* or *free boundary* problems. A particularly important moving-boundary problem refers to the determination of the depth at which molecules of gaseous carbon dioxide succeed to penetrate concrete-based structures [8]. The process can be summarized as follows: 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

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

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 that affect the service life of concrete-based structures. In combination with the ingress of aggressive ionic species (like chloride [32] or sulfate [1]), the carbonation process typically facilitates corrosion, and hence, cracking and spalling of the concrete may occur [5, 8].

Conceptually different moving-boundary models for the carbonation penetration in concrete have been recently proposed in [2, 3, 21] and analyzed by the author in

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his PhD thesis [19]. This paper represents a preliminary study in what the error analysis of finite elements approximations for 1D two-phase moving-boundary systems with kinetic conditons is concerned. Our one-dimensional formulation refers to the slab $[0, L]$ ($L \in]0, \infty[$), away from corners or any other geometric singularity; see Fig. 1 for details. In this case, solving the moving-boundary model means the calculation of the involved mass concentrations and of the *a priori* unknown position of the moving interface, where the reaction is concentrated. Our main goal is to prove that the spatially semi-discrete solutions converge to the solution of the PDE system in question when the mesh size decreases to zero. *A priori* 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. An *a posteriori* error estimate is also obtained.

The paper is organized in the following fashion: We state the moving-boundary problem in section 2. Section 3 collects the technical preliminaries and section 4 presents the assumptions on which the error analysis relies. Along the lines of this section, we also formulate the functional framework and the concept of weak solution. The main results of this paper are announced in section 5 and proved in section 6 and section 7. Finally, a short summary and few conclusions and further remarks are given in section 8.

2. Statement of the problem

We denote by u_1 and u_2 the concentration of CO_2(g) and CO_2(aq), respectively, u_3 the $Ca(OH)_2$(aq) concentration, u_4 the $CaCO_3$(aq) concentration, and finally, u_5 represents the concentration of moisture produced by (1). The basic geometry is depicted in Fig. 1.

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 $T \in]0, \infty[$, $u = (u_1, u_2, \ldots, u_5)^t$) 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 system of mass-balance equations

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

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

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

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

initial conditions

$$u_i(0, x) = u_{i0}(x) \text{ in } \Omega_1(0) \ (i \in \{1, 2, 4, 5\}),\ u_3(0) = u_{30},\ \text{at } \Gamma(0), \tag{6}$$

and boundary conditions

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

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

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

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

In order to close the system, the couple (u, s) also needs to satisfy the non-local relation

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

To formulate (2)-(11), a set of parameters are employed. In Assumption (I), we summarize their range of application. The physical meaning of the parameters and their restrictions is explained in [19].

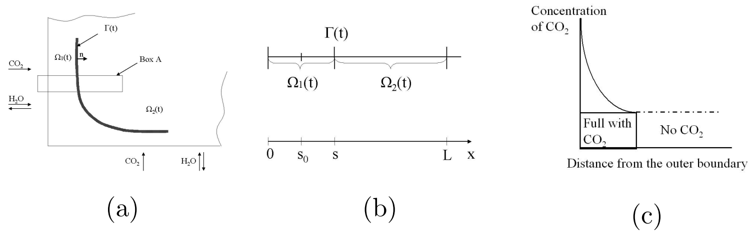

FIGURE 1. (a) Basic geometry for the model (2)-(11). The box A is the region which our model refers to. (b) Schematic 1D geometry. The reactants involved in (1) are spatially segregated at any time $t \in S_T$. $\Omega_2(t) :=]s(t), L[$ is the passive phase and the process is assumed to happen in $\Omega_1(t)$ (the active phase). (c) Definition of the interface position.

Assumption (I). *Select*

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

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

and

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

$$s_0 \le s(t) \le L. \tag{15}$$

Remark 2.1. *1. We refer to the system (2)-(11) as problem P_Γ^1 and to its semidiscrete conterpart as problem $P_\Gamma^{1,\mathrm{sd}}$. P_Γ^1 consists of a weakly* coupled system *of semi-linear parabolic PDEs (2)-(10) to be simultaneously solved together with (11); (11) is the* kinetic condition *that drives the movement of the reaction interface $\Gamma(t)$. Certain analogies can be drawn between (11) and the kinetic laws by Visintin (*[33], *chapter V in* [34]*). Once the domain $\Omega_1(t)$ is determined, (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 significance (u_3 represents the concentration of* $\mathrm{Ca(OH)_2}$ *that waits to be reacted). The PDE system (2)-(11) represents a one-phase scenario of a more general moving sharp-interface model developed in* [19, 20]. *Employing the techniques from* [19], *it can be shown that locally in time positive weak solutions to (2)-(11) exist, are unique and depend continuously on data and parameters; see Theorem 4.3 in section 4.*

2. The system (2)-(11) refers to concrete carbonation [18, 19, 20, 22], *but contains structural features also present in models describing sulfate attack on concrete pipes* [1], *or redox fronts in geochemistry* [25]*(chapter 4) and* [26] *(chapters 3 and 4).*

3. The classical problem of ice melting (the so-called Stefan problem [7, 9]*) 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.* [23, 24]*) 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. Using a fixing-front technique by Landau* [13] *and a special scaling of the time variable, he "freezed"* *the boundaries of the moving phase and examined the transformed PDEs in fixed-domains. Developments of his technique, are reported, for instance, in* [27, 29, 28, 11, 16, 15, 12] *and* [35]. *In all these contributions, various* $L^\infty-$, L^2-, H^1- *and* H^2- *error estimates have been obtained for the scalar (both linear and quasi-linear scalar PDEs) provided that the standard Stefan conditions are imposed across the moving interface. Much less is known about how to deal with the case of coupled systems of PDEs when, additionally, non-standard boundary conditions (such as kinetic conditions) act across the moving boundary. This is the novelty brought in by this paper. At the technical level, we combine ideas from* [4, 6, 19] *and* [20]. *In* [6], *the authors are concerned with the error analysis of a viscous 1D Burgers equation, where the end of the moving domain is driven by a* linear kinetic condition. *In their setting, the main difficulty was to deal with the Burger's type non-linearity and with additional non-local terms typically arising when immobilizing the moving boundary. We rely on some of their arguments. The challenge here is to deal with both the strong coupling of the system and the non-linearity of the reaction rate.*

4. 2D situations cannot be treated in this framework due to the following reasons: (1) the kinetic law (11) is only valid for one-dimensional scenarios; (2) some of the imbeddings (e.g. $H^1(\Omega) \hookrightarrow L^\infty(\Omega)$*) work only in 1D, and (3) Landau-type transformations cannot be applied for multidimensional cases.*

3. Technical preliminaries

The error analysis requires some basic results concerning the approximation properties of first-order polynomials and of the functions spaces used. These results are elementary. We collect them in this section without proofs.

Notation 3.1. *(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* $(y,t) \in]a,b[\times S_T$. *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. *We often 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* $u_{,y}(1,t)$.

3.1. 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 means of $|u|_{\mathbb{H}} = \left(\sum_{i\in\mathcal{I}_1\cup\mathcal{I}_2} |u_i|^2_{H_i}\right)^{\frac{1}{2}}$ for all $u \in \mathbb{H}$ and is equipped with the standard scalar product. Sometimes, the following conflict of notations appear: For instance, we use in the same context $|u|_{H^2(0,1)}$ and $|u_1|_{H^2(0,1)}$. The first norm acts on the product space $H^2(0,1)^{|\mathcal{I}_1|}$, while the second one refers to $H^2(0,1)$.

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 $||u||_{V_i} = |u_{,y}|_{H_i}$.

The set $W_2^1(S_T,V,H) := \{u \in L^2(S_T,V)$ and $u_t \in L^2(S_T,V^*)\}$ forms a Banach space with the norm

$$||u||_{W_2^1} := ||u||_{L^2(S,V)} + ||u'||_{L^2(S,V^*)}.$$

The space $W_2^1(S_T, \mathbb{V}, \mathbb{H})$ is defined similarly. For more details on the mentioned function spaces, see [36].

(ii) We list a few elementary inequalities that we extensively use in the sequel. We have

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

where $\xi > 0$, $c_\xi := \frac{1}{q}\frac{1}{\sqrt[p]{(\xi p)^q}} > 0$, $\frac{1}{p} + \frac{1}{q} = 1$, $p \in]1, \infty[$ and $a, b \in \mathbb{R}_+$. (17) is the inequality of Young. We also make use of the following generalization[1] of (17)

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

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 taken as in (17).

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

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

(20) is the so-called interpolation inequality [36].

3.2. Useful basic facts from approximation theory. In section 4, we employ a piecewise-linear finite element discretization of the interval $[0, 1]$. For each $i \in J_n := \{0, \ldots, n\}$, we denote $J_i :=]y_i, y_{i+1}[$, 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 $h := \max_{i \in J_n} h_j$. We introduce the space

$$V_h := \{\psi \in C([0, 1]) : \psi|_{[y_j, y_{j+1}]} \in \Pi_1, j \in J_n\},$$

where Π_1 represents the set of polynomials of degree one. In the sequel, u_{0h} is 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 [10] or Lemma 3.2 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

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

and P_h^i ($i \in \mathcal{I}_1$) the orthogonal projection

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

[1] 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 from above.

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

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

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; $\mathbb{R}_h u$ is the finite element approximation of the solution of the corresponding elliptic problem in terms of u. Finally, we recall the following classical interpolation result:

Lemma 3.2. *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 [14] (or [10], e.g.). The proof of (iii) follows combining (i), (ii) and the interpolation 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 $\theta \in \left[\frac{1}{2}, 1\right[$. □

Remark 3.3. *In sections 6 and 7, we use Lemma 3.2 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 $i \in \mathcal{I}_1$.*

4. Fixed-domain formulation. Further notations and assumptions. Auxiliary results

By the Landau transformation [13]

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

we map the moving domain $\Omega_1(t)$ into $]0,1[$. We perform (23) for (2)-(11), but keep (4) unchanged. The calculations are obvious, and therefore, we omit to write down the classical formulation of the transformed system and only give its weak form in (46). The concentrations vector acting in the fixed-domain is denoted by $u(y,t)$ and corresponds to the concentrations vector $u(x,t)$ that is acting in the original domain $\Omega_1(t)$. We keep the same notation $s(t)$ for the position of the interface in both the moving-domain and fixed-domain formulations.

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.

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

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

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

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

The production terms f_i and g_i are given by

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

We define

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

and

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

for fixed $\Lambda \in M_\Lambda$. In (34), we set

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

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 assumptions that are needed to describe the reaction rate η_Γ are contained in the items (A) and (B) below:
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) $P_1Q_1k_2 \leq P_1k_1$; $P_2k_1 \leq P_2Q_2k_2$.

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 strictly positive solution of (4).

For the initial and boundary data, we assume:
Assumption (III). *Select*

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

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

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

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

Remark 4.1. *Owing to (4), (38), (40) and (42), we see that* **Assumption (II)** *(A) is fulfilled with η_Γ chosen as in (38). Relations (36), (37), (C1) and (C2) are of technical nature. Their are needed to ensure the positivity and L^∞- estimates for the involved concentrations. The reader is referred to* [19] *for their physical interpretation.*

Definition 4.2 (Weak Solution to P^1_Γ)**.** *We call the couple (u, s) a weak solution to problem P^1_Γ if and only if there is a $S_\delta :=]0, \delta[$ with $\delta \in]0, T]$ such that*

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

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

$$u \in W^1_2(S_\delta; \mathbb{V}, \mathbb{H}) \cap [\bar{S}_\delta \mapsto L^\infty(0,1)]^{|\mathcal{I}_1|}, \tag{45}$$

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

We possess now all the ingredients that we need in order to state the existence and uniqueness of locally in time weak solutions in the sense of Definition 4.2.

Theorem 4.3. *Consider* **Assumptions (I)-(III)** *be fulfilled. In this case, the following assertions hold:*
(a) There exists a $\delta \in]0, T[$ such that there is a unique weak solution on S_δ in the sense of Definition 4.2;
(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) $s \in W^{1,\infty}(S_\delta)$.

The techniques developed to prove Theorem 3.4.6 in [19] can be applied to prove Theorem 4.3. Now, we turn the attention to the semi-discrete FEM approximation. We denote by η^h_Γ 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^h_Γ is given by $s'_h = \eta^h_\Gamma(u_h(s_h(t), t))$, 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 $v_h := (v_{1h}, v_{2h}, v_{4h}, v_{5h})^t \in \mathbb{V}_h$.

Definition 4.4 (Weak Solution to $P^{1,\mathrm{sd}}_\Gamma$)**.** *We call the couple (u_h, s_h) a weak solution to problem $P^{1,\mathrm{sd}}_\Gamma$ if and only if there is a $S_{\hat\delta} :=]0, \hat\delta[$ with $\hat\delta \in]0, \delta]$ such that*

$$s_0 < s_h(\hat\delta) \leq L_0, \tag{46}$$

$$s_h \in W^{1,4}(S_{\hat\delta}), \tag{47}$$

$$u_h \in \left[H^1(S_{\hat\delta}, V_h) \cap L^\infty(S_{\hat\delta}, H)\right]^{|\mathcal{I}_1|} \tag{48}$$

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

A first result is the next theorem:

Theorem 4.5. *Let* **Assumptions (I)-(III)** *be fulfilled. There exists $\bar\delta \in]0, \min\{\delta, \hat\delta\}]$, which is independent of h, such that there is a unique positive 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 4.4.

The proof of Theorem 4.5 follows the lines of the proof of Theorem 3.4.6 from [19]. Since here we focus only on the error analysis, we omit it. The positivity and boundedness of the vector of concentrations u_h will play an essential role in obtaining the error estimates.

5. Main results

The next theorems contain the main results:

Theorem 5.1 (*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^1_Γ *and* $P^{1,\mathrm{sd}}_\Gamma$ *are uniquely solvable. Let* (u,s) *and* (u_h,s_h) *be the corresponding solutions. Then the following estimate holds: There exist* $\delta_1 \in]0, \max\{\delta,\bar{\delta}\}]$ *and the strictly positive constants* c_i $(i \in \{1,2,3\})$*, which are independent of* h*, such that*

$$||u-u_h||_{L^2(S_{\delta_1},\mathbb{V})} \le c_1\left(h^2 + |s-s_h|_{W^{1,4}(S_{\delta_1})}\right), \tag{49}$$

$$|s'-s'_h|_{L^2(S_{\delta_1})} \le c_2 h, \tag{50}$$

and

$$||u-u_h||_{L^\infty(S_{\delta_1},\mathbb{H})\cap L^2(S_{\delta_1},\mathbb{V})} + ||s-s_h||_{W^{1,4}(S_{\delta_1})} \le c_3 h. \tag{51}$$

Proof. See section 6. □

Theorem 5.2 (*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^1_Γ *and* $P^{1,\mathrm{sd}}_\Gamma$ *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*

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

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 7. □

Remark 5.3. *(i) What we have stated so far (in Theorem 5.1 and Theorem 5.2) are error estimates for* $u(y,t)$ *with* $y \in [0,1]$*. They may be useful when employing front-fixing methods to solve (2)-(11). On the other hand, if one employs front-tracking methods, error estimates obtained for the solution in the fixed-domain formulation are useless. In such case, we need to transform back to the initial formulation of (2)-(11) and obtain error estimates for the original unknowns, i.e. for* $u(x,t)$ *with* $x \in [0, s(t)]$*. Related ideas are reported in* [12]*. Since (23) is affine and the solution* (u_h,s_h) *is actually sufficiently regular (cf. Proposition 3.4.17 from* [19]*), the inverse transformation* $x = ys_h(t)$ *can indeed be employed in order to make the estimates (51) and (52) available for the original setting with moving boundaries.*

(ii) If additional constraints on the model parameters are fulfilled (see Theorem 3.4.16 in [19]*, e.g.), then local weak solutions as in Definition 4.2 can be extended*

globally in time. Now, the relevant question is: Can the local semi-discrete weak solution (cf. Definition 4.4) be extended globally in time? We expect that the techniques employed in [17] *for the case of a Stefan-like problem arising in subsurface contaminant transport with remediation can provide a positive answer to this question. In this paper, we restrict our attention to the case*

$$\delta_1 = \delta_2 = \bar{\delta} = \hat{\delta} = \delta \tag{54}$$

and only focus on the behavior of locally in time weak solutions satisfying Definition 4.4.

6. Proof of Theorem 5.1

We denote by S_δ (with δ chosen as in (54)) the common time interval $]0, \delta[$ on which the continuous and discrete solutions to (2)-(11) exist. Let $e := u - u_h$ (with $e_i := u_i - u_{ih}$ and $e := (e_1, e_2, e_4, e_5)^t$) and $s - s_h$ be the errors of approximation. For each test function $w_h \in \mathbb{V}_h$ ($w_{ih} \in V_h$, $i \in \mathcal{I}_1$), we subtract the variational formulation in terms of u_h from that one in terms of u and obtain the following equality:

$$\begin{aligned}((u+\lambda)_{,t}, w_h) &- ((u_h+\lambda)_{,t}, w_h) + \frac{1}{s^2}\sum_{i\in\mathcal{I}_1}(D_i u_{i,y}, w_{ih,y}) \\ &- \frac{1}{s_h^2}\sum_{i\in\mathcal{I}_1}(D_i u_{ih,y}, w_{ih,y}) + \frac{1}{s}\left[\eta_\Gamma + s'(u_1(1)+\lambda_1)\right] w_{1h}(1) \\ &- \frac{1}{s_h}\left[\eta_\Gamma^h + s_h'(u_{1h}(1)+\lambda_1)\right] w_{1h}(1) + \frac{s'}{s}(u_2(1)+\lambda_2) w_{2h}(1) \\ &- \frac{s_h'}{s_h}(u_{2h}(1)+\lambda_2) w_{2h}(1) - \frac{1}{s}\eta_\Gamma w_{5h}(1) + \frac{1}{s_h}\eta_\Gamma^h w_{5h}(1)\end{aligned} \tag{55}$$

$$\begin{aligned}&= (P_1(Q_1(u_2+\lambda_2) - (u_1+\lambda_1)), w_{1h}) \\ &- (P_1(Q_1(u_{2h}+\lambda_2) - (u_{1h}+\lambda_1)), w_{1h}) \\ &- (P_2(Q_2(u_2+\lambda_2) - (u_1+\lambda_1)), w_{2h}) \\ &+ (P_2(Q_2(u_{2h}+\lambda_2) - (u_{1h}+\lambda_1)), w_{2h}) \\ &+ \frac{s'}{s}\sum_{i\in\mathcal{I}_1}(y u_{i,y}, w_{ih}) - \frac{s_h'}{s_h}\sum_{i\in\mathcal{I}_1}(y u_{ih,y}, w_{ih}).\end{aligned} \tag{56}$$

Grouping some of the terms in (55), we obtain

$$\begin{aligned}(e_{,t}, w_h) &+ \frac{1}{s^2}\sum_{i\in\mathcal{I}_1}(D_i(u_i - u_{ih})_{,y}, w_{ih,y}) = \left(\frac{1}{s_h^2} - \frac{1}{s^2}\right)\sum_{i\in\mathcal{I}_1}(D_i u_{ih,y}, w_{ih,y}) \\ &- \left(\frac{s'}{s}(u_1(1)+\lambda_1) - \frac{s_h'}{s_h}(u_{1h}(1)+\lambda_1) + \frac{\eta_\Gamma}{s} - \frac{\eta_\Gamma^h}{s_h}\right) w_{1h}(1) \\ &- \left(\frac{s'}{s}(u_2(1)+\lambda_2) - \frac{s_h'}{s_h}(u_{2h}(1)+\lambda_2)\right) w_{2h}(1) - \left(\frac{\eta_\Gamma}{s} - \frac{\eta_\Gamma^h}{s_h}\right) w_{5h}(1) \\ &+ P_1 Q_1(e_2, w_{1h}) - P_1(e_1, w_{1h}) - P_2 Q_2(e_2, w_{2h}) + P_2(e_1, w_{2h}) \\ &+ \frac{s'}{s}\sum_{i\in\mathcal{I}_1}(y e_{i,y}, w_{ih}) + \left(\frac{s'}{s} - \frac{s_h'}{s_h}\right)\sum_{i\in\mathcal{I}_1}(y u_{ih,y}, w_{ih}).\end{aligned} \tag{57}$$

Therefore, we may write

$$(e_{,t}, w_h) + \frac{\min_{i\in\mathcal{I}_1} D_i}{s^2}(e_{,y}, w_{h,y}) \leq \sum_{\ell=1}^{5} I_\ell, \tag{58}$$

where the terms I_ℓ ($\ell \in \{1,\ldots,5\}$) are given by

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

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

$$\begin{aligned}
\frac{1}{2}\frac{d}{dt}|e|^2 + \frac{d}{s^2}||e||^2 &\leq (e_{,t}, u-u_h)\\
+\frac{d}{s^2}(e_{,y}, (u-u_h)_{,y}) &= (e_{,t}, u-v_h) + \frac{d}{s^2}(e_{,y}, (u-v_h)_{,y})\\
&+(e_{,t}, v_h-u_h) + \frac{d}{s^2}(e_{,y}, (v_h-u_h)_{,y}).
\end{aligned} \tag{59}$$

Note that $w_h = v_h - u_h \in V_h$ decomposes into $w_h = (v_h - u) + e$. Choosing the test function $w_h := v_h - u_h$ in (58), we obtain

$$\begin{aligned}
\frac{1}{2}\frac{d}{dt}|e|^2 &+ \frac{d}{s^2}||e||^2 \leq (e_{,t}, u-v_h) + \frac{d}{s^2}(e_{,y}, (u-v_h)_{,y})\\
&+ \left(\frac{1}{s_h^2} - \frac{1}{s^2}\right)\sum_{i\in\mathcal{I}_1}(D_i(u_{ih})_{,y}, (v_{ih}-u_{ih})_{,y})\\
&+ \left(\frac{\eta_\Gamma}{s} - \frac{\eta_\Gamma^h}{s_h}\right)|(v_{1h}(1) - u_{1h}(1) + v_{5h}(1) - u_{5h}(1))|\\
&+ P_1Q_1(e_2, v_{1h}-u_{1h}) - P_1(e_1, v_{1h}-u_{1h})\\
&- P_2Q_2(e_2, v_{2h}-u_{2h}) + P_2(e_1, v_{2h}-u_{2h})\\
&+ \frac{s'}{s}\sum_{i\in\mathcal{I}_1}(ye_{i,y}, v_{ih}-u_{ih})\\
&+ \left(\frac{s'}{s} - \frac{s_h'}{s_h}\right)\sum_{i\in\mathcal{I}_1}(yu_{ih,y}, v_{ih}-u_{ih}).
\end{aligned} \tag{60}$$

In order to simplify the writing of some of the inequalities, we introduce the strictly positive constants c_ℓ ($\ell \in \{1,\ldots,7\}$), whose precise expression is not explicitly written but can be derived. For each $\ell \in \{1,\ldots,7\}$, we have $c_\ell < \infty$. Before estimating the terms I_ℓ in (58), we point out a few technical facts in Remark 6.1. The proofs are straightforward. They rely on arguments combining the integration by parts, the Cauchy-Schwarz inequality and also on the inequality between the geometric and arithmetic means.

Remark 6.1. (1) *There exists a constant* $c_1 = c_1(\Lambda, s_0) > 0$ *such that*

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

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

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

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

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

(4) *It holds*

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

(5) *It holds*

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

By Remark 6.1, (59) and (60), we have

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}|e|^2 &+ \frac{d}{s^2}||e||^2 \leq |e_{,t}||u - v_h| + \frac{d}{s^2}||e||||u - v_h|| \\ &+ |s - s_h|\frac{s + s_h}{s^2 s_h^2}\sum_{i \in \mathcal{I}_1}|(D_i u_{ih,y}, (u_h - v_h)_{,y})dy \\ &+ c_1(|s - s_h| + |s' - s_h'|)|v_h(1) - u(1) + e(1)| \\ &+ c_2(|e(1)| + |s - s_h| + |s' - s_h'|)|v_h(1) - u(1) + e(1)| \\ &+ P_1 Q_1|e_2|\left(|v_{1h} - u_1| + |e_1|\right) + P_1|e_1|\left(|v_{1h} - u_1| + |e_1|\right) \\ &+ P_2 Q_2|e_2|\left(|v_{2h} - u_2| + |e_2|\right) + P_2|e_1|\left(|v_{2h} - u_2| + |e_2|\right) \\ &+ \frac{s'}{2s}\sum_{i \in \mathcal{I}_1}[(|e_i(1)|^2 - |e_i|^2) + ||e_i|||v_{ih} - u_{ih}|] \\ &+ c_3(|s - s_h| + |s' - s_h'|)\sum_{i \in \mathcal{I}_1}(|u_{ih}||v_{ih} - u_{ih}| \\ &+ |u_{ih}|||v_{ih} - u_{ih}||).\end{aligned} \tag{61}$$

After elementary manipulations, we gain the next estimates:

$$\begin{aligned}\frac{d}{dt}|e|^2 + \frac{d}{s^2}||e||^2 &\leq |e_{,t}||u - v_h| + \frac{d}{s^2}||e||||u - v_h|| \\ +c_3|s - s_h|||u_h||(||v_h - u|| + ||e||) &+ c_1(|s - s_h| + |s' - s_h'|)\hat{c}||e||^\theta|e|^{1-\theta} \\ &+c_4(|s - s_h| + |s' - s_h'|)\hat{c}||v_h - u||^\theta|v_h - u|^{1-\theta} \\ &+c_2|e(1)|^2 + c_2(|s - s_h| + |s' - s_h'|)\hat{c}||e||^\theta|e|^{1-\theta} \\ +\frac{P_1 Q_1}{2}\left(2|e_2|^2 + |v_{1h} - u_1|^2 + |e_1|^2\right) &+ \frac{P_1}{2}\left(2|e_1|^2 + |v_{1h} - u_1|^2\right) \\ +\frac{P_2 Q_2}{2}\left(2|e_2|^2 + |v_{2h} - u_2|^2\right) &+ \frac{P_2}{2}\left(2|e_1|^2 + |v_{2h} - u_2|^2\right) \\ &+\frac{s'}{2s}\hat{c}||e||^{2\theta}|e|^{2(1-\theta)} + \frac{s'}{s}||e|||v_h - u| \\ &+c_3(|s - s_h| + |s' - s_h'|)|v_h - u| + c_5(||v_h - u|| + ||e||).\end{aligned} \tag{62}$$

We set $v_h = \mathbb{R}_h u$, re-arrange some of the terms in (62), and use Lemma 3.2 to obtain the following estimates:

$$\begin{aligned}
\frac{d}{dt}|e|^2 + \frac{d}{s^2}||e||^2 \leq |e_{,t}|\gamma_1 h^2 |u|_{H^2(0,1)} + \frac{d}{s^2}||e||\gamma_2 h|u|_{H^2(0,1)} \\
+c_3|s-s_h|||u_h||\left(\gamma_2 h|u|_{H^2(0,1)} + ||e||\right) \\
+(c_1+c_2)(|s-s_h|+|s'-s_h'|)\hat{c}||e||^\theta|e|^{1-\theta} \\
+c_4(|s-s_h|+|s'-s_h'|)c\gamma_2^\theta h^\theta \gamma_1^{1-\theta}h^{2(1-\theta)}|u|_{H^2(0,1)} + c_6\left(|e_1|^2+|e_2|^2\right) \\
+c_7\gamma_1^2 h^4\left(|u_1|^2_{H^2(0,1)} + |u_2|^2_{H^2(0,1)}\right) + \frac{s'}{2s}\hat{c}||e||^{2\theta}|e|^{2(1-\theta)} \\
+\frac{\xi}{2}\frac{||e||^2}{s^2} + \frac{s'}{2\xi}\gamma_1^2 h^4|u|^2_{H^2(0,1)} \\
+c_5\left(\gamma_2 h|u|_{H^2(0,1)} + ||e||\right)(|s-s_h|+|s'-s_h'|) = \sum_{\ell=1}^{10} I_\ell.
\end{aligned}$$

We have

$$\begin{aligned}
I_1 &:= |e_t|\gamma_1 h^2|u|_{H^2(0,1)} \leq \frac{|e_t|^2}{2}h^2 + \frac{\gamma_1^2 h^2}{2}|u|^2_{H^2(0,1)} \\
I_2 &:= \frac{d}{s}||e||\gamma_2 h|u|_{H^2(0,1)} \leq \xi\frac{d}{s^2}||e||^2 + c_\xi d\gamma_2 h^2|u|^2_{H^2(0,1)} \\
I_3 &:= c_3|s-s_h|||u_h||\left(\gamma_2 h|u|_{H^2(0,1)} + ||e||\right) \leq 2\rho|s-s_h|^2 + c_\rho\hat{c}_3^2||e||^2 + c_\rho\hat{c}_3^2|u|^2_{H^2(0,1)} \\
I_4 &:= (c_1+c_2)(|s-s_h|+|s'-s_h'|)\hat{c}||e||^\theta|e|^{1-\theta} = I_{41}+I_{42},
\end{aligned} \tag{63}$$

where I_{41} and I_{42} are defined by

$$\begin{aligned}
I_{41} &:= \hat{c}(c_1+c_2)|s-s_h|\frac{||e||^\theta}{s^\theta}|e|^{1-\theta}s^\theta, \\
I_{42} &:= \hat{c}(c_1+c_2)|s'-s_h'|\frac{||e||^\theta}{s^\theta}|e|^{1-\theta}s^\theta.
\end{aligned}$$

In (63), we have $\rho > 0, c_\rho > 0$, and $\hat{c}_3 := \max\{\gamma_2, 1\}$. Since I_{41} and I_{42} are bounded from above by

$$\frac{\bar{\xi}}{2}|s-s_h|^2 + \xi c_{\bar{\xi}}\frac{||e||^2}{s^2} + c_\xi c_{\bar{\xi}}(\hat{c}(c_1+c_2))^2 s^{2\theta}|e|^2$$

and

$$\frac{\bar{\xi}}{2}|s'-s_h'|^2 + \xi c_{\bar{\xi}}\frac{||e||^2}{s^2} + c_\xi c_{\bar{\xi}}(\hat{c}(c_1+c_2))^2 s^{2\theta}|e|^2,$$

it results that

$$I_4 \leq \frac{\bar{\xi}}{2}\left(|s-s_h|^2 + |s'-s_h'|^2\right) + 2\xi c_{\bar{\xi}}\frac{||e||^2}{s^2} + 2c_\xi c_{\bar{\xi}}(\hat{c}(c_1+c_2))^2 s^{2\theta}|e|^2.$$

Furthermore, we have

$$\begin{aligned}
I_5 &:= cc_4\gamma_2^{\theta}\gamma_1^{1-\theta}cc_4\left(|s-s_h|+|s'-s'_h|\right)h^{2-\theta}|u|_{H^2(0,1)},\\
&\leq \xi\left(|s-s_h|^2+|s'-s'_h|^2\right)+c_\xi\left(cc_4\gamma_2^{\theta}\gamma_1^{1-\theta}\right)^2 h^{2(2-\theta)}|u|^2_{H^2(0,1)},\\
I_6 &:= c_6\left(|e_1|^2+|e_2|^2\right)\leq c_6|e|^2,\\
I_7 &:= c_7\gamma_1^2 h^4\left(|u_1|^2_{H^2(0,1)}+|u_2|^2_{H^2(0,1)}\right)\leq c_7\gamma_1^2|u|^2_{H^2(0,1)}h^4,\\
I_8 &:= \frac{s'}{2s}\hat{c}||e||^{2\theta}|e|^{2(1-\theta)}\leq \xi\frac{||e||^2}{s^2}+c_\xi\hat{c}^{\frac{1}{1-\theta}}\left(\frac{s'}{2}\right)^{\frac{1}{1-\theta}}s^{\frac{2\theta-1}{1-\theta}}|e|^2\\
&= \xi\frac{||e||^2}{s^2}+c_\xi\hat{c}^2\left(\frac{s'}{2}\right)^2|e|^2\left(\text{ for }\theta=\frac{1}{2}\right),\\
I_9 &:= \frac{\xi}{2}\frac{||e||^2}{s^2}+\frac{s'}{2\xi}\gamma_1^2h^4|e|^2_{H^2(0,1)},\\
I_{10} &:= c_5\left(\gamma_2 h|u|_{H^2(0,1)}+||e||\right)\left(|s-s_h|+|s'-s'_h|\right)\\
&\leq \xi\left(|s-s_h|^2+|s'-s'_h|^2\right)+c_\xi(c_5\gamma_2)^2|u|^2_{H^2(0,1)}h^2+\hat{\xi}\frac{||e||^2}{s^2}\\
&+ c_{\hat{\xi}}s^2\left(|s-s_h|^2+|s'-s'_h|^2\right).
\end{aligned}$$

Finally, we obtain

$$\frac{d}{dt}|e|^2+\rho_1||e||^2\leq \rho_2h^2+\rho_3|e|^2+\rho_4\left(|s-s_h|^2+|s'-s'_h|^2\right). \tag{64}$$

We set $u_\infty := |u|_{H^2(0,1)}$ and $\eta_{\Gamma,\max} := |s'|_{L^\infty(S_\delta)}$. In (64), we have

$$\begin{aligned}
\rho_1 &:= \frac{d}{s_0^2}\left[1-\hat{\xi}-2\xi(1+c_{\hat{\xi}})-c_\rho\hat{c}_3^2\right],\\
\rho_2 &:= u_\infty^2\left[(1+c_7)\gamma_1+c_\rho\hat{c}_3+c_\xi cc_4\gamma_2+c_3c_5^2\gamma_2^2\right],\\
\rho_3 &:= 1+c_6+2c_\xi c_{\bar{\xi}}(\hat{c}(c_1+c_2))^2L^{2\theta}+c_\xi\hat{c}^2\left(\frac{\eta_{\Gamma,\max}}{2}\right)^2,\\
\rho_4 &:= 2\rho+\bar{\xi}+2\xi+c_{\hat{\xi}}L^2.
\end{aligned}$$

Since $s'(t)-s'_h(t)\leq \rho_5(u(1,t)-u_h(1,t))=\rho_5\int_0^1 e_y(\zeta,t)d\zeta$, we obtain

$$|s'-s'_h|\leq \rho_5||e||. \tag{65}$$

We insert (65) in (64). We choose $\xi>0,\hat{\xi}>0$ and $c_\rho>0$ sufficiently small such that $(\rho_1-\rho_5^2)||e||^2\geq 0$. In this case, Gronwall's inequality applied in (64) proves the *a priori* estimate (49); (49) shows that the L^2-error of the concentrations vector is governed by the $W^{1,2}$-error of the moving interface position.

By Young's inequality (see also (46) in [6]), we derive

$$\frac{d}{dt}(|s-s_h|^2)\leq ||e||^2+\rho_5^2|s-s_h|^2. \tag{66}$$

By (64) and (66), we have

$$\frac{d}{dt}\left(|e|^2+(\rho_1-\rho_5^2)|s-s_h|^2\right)\leq \rho_2h^2+\rho_3\left(|e|^2+\frac{\rho_4+\rho_1-\rho_5^2}{\rho_3}|s-s_h|^2\right). \tag{67}$$

For sufficiently large $\rho_3>0$ (for instance, such that $\rho_4+(1-\rho_3)(\rho_1-\rho_5^2)=0$), Gronwall's inequality applied to (67) for the quantity $|e|^2+(\rho_1-\rho_5^2)|s-s_h|^2$ gives the estimate

$$|e|^2+(\rho_1-\rho_5^2)|s-s_h|^2\leq ch^2. \tag{68}$$

By integrating (64) on S_δ and by using (21) and (68), it exists a constant $c > 0$ such that

$$||e||^2_{L^2(S_\delta\times]0,1[)} \le ch^2.$$

The latter estimate leads to (50) and (51) of the theorem by noticing that

$$|s' - s'_h|^2 \le \delta\rho_5^2 ||e||^2_{L^2(S_\delta\times]0,1[)} \le c\delta\rho_5^2 h^2.$$

This concludes the proof of Theorem 5.1.

7. Sketch of the proof of Theorem 5.2

The proof follows the lines of [6]. For all $v \in \mathbb{V}$, we can write

$$\begin{aligned}(e_{,t}, v) \quad &+ \quad \frac{d}{L_0^2}(e_{,y}, v_{,y}) \le (u_{,t}, v) + \frac{1}{s^2}\sum_{i\in\mathcal{I}_1} D_i(u_{iy}, v_{iy}) \\ &- \quad \left[(u_{h,t}, v) + \frac{1}{s^2}\sum_{i\in\mathcal{I}_1} D_i(u_{ihy}, v_{ihy})\right] \le -e(s', u, v) + b_f(s, u, v) \\ &+ \quad h(s', u_{,y}, v) - \left[(u_{h,t}, v) + \frac{1}{s^2}\sum_{i\in\mathcal{I}_1} D_i(u_{ihy}, v_{ihy})\right]. \end{aligned} \tag{69}$$

By (69), we obtain

$$\begin{aligned}(e_{,t}, v) \quad &+ \quad \frac{d}{L_0^2}(e_{,y}, v_{,y}) \le b_f(s, u, v) + h(s', u_{,y}, v) - e(s', u, v) \\ &- \quad \left[(u_{h,t}, v) + \frac{1}{s_h^2}\sum_{i\in\mathcal{I}_1} D_i(u_{ihy}, v_{iy}) + \left(\frac{1}{s^2} - \frac{1}{s_h^2}\right)\sum_{i\in\mathcal{I}_1}(D_i u_{ihy}, v_{,y})\right] \\ &= \quad b_f(s, u, v) + h(s', u_{,y}, v) - e(s', u, v) - b_f(s_h, u_h, v) \\ &- \quad h(s'_h, u_{h,y}, v) + e(s'_h, u_h, v) - \left(\frac{1}{s^2} - \frac{1}{s_h^2}\right)\sum_{i\in\mathcal{I}_1}(D_i u_{ihy}, v_{,y}) \\ &+ \quad \int_0^1 R(u_h) v dy - \frac{1}{s_h^2}\sum_{i\in\mathcal{I}_1}\int_0^1 D_i(u_{ih,y}, v_{i,y}) dy, \end{aligned} \tag{70}$$

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

$$\sum_{i\in J_n}\int_{y_i}^{y_{i+1}} R(u_h) v dy - \frac{1}{s_h^2}\sum_{i\in J_n}\sum_{\ell\in\mathcal{I}_1}\max_{\ell\in\mathcal{I}_1} D_\ell\left[u_{\ell h,y}(y_{i+1})v(y_{i+1}) - u_{\ell h,y}(y_i)v(y_i)\right]. \tag{71}$$

Owing to the structure of $P_\Gamma^{1,\mathrm{sd}}$, (71) vanishes when selecting $v = v_h$ as test function. We rely on this observation to add (71) (in which we take $v := v_h$) to (70). Inserting in the result $v = e \in \mathbb{V}$ and $v_h := R_h e \in \mathbb{V}_h$, we obtain the inequality:

$$\begin{aligned}
(e_{,t}, e) &+ \frac{d}{L_0^2}||e||^2 \leq b_f(s,u,e) - b_f(s_h,u_h,e) + e(s_h', u_h, e) \\
&- e(s', u, e) + h(s', u_{,y}, e) - h(s_h', u_{h,y}, e) - \left(\frac{1}{s^2} - \frac{1}{s_h^2}\right)\sum_{i\in\mathcal{I}_1}(D_i u_{ihy}, v_{,y}) \\
&+ \sum_{i\in J_n}\int_{y_i}^{y_{i+1}}(e - \mathbb{R}e)dy \\
&- \frac{1}{s_h^2}\sum_{i\in J_n}\sum_{\ell\in\mathcal{I}_1}\max_{\ell\in\mathcal{I}_1} D_\ell\left[u_{\ell h,y}(y_{i+1})(e-\mathbb{R}_h e)(y_{i+1}) - u_{jh,y}(y_i)(e-\mathbb{R}_h e)(y_i)\right] \\
(72) \quad &= \sum_{\ell=1}^{5} I_\ell.
\end{aligned}$$

In (72), we have

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

Manipulations of the interpolation inequality (20) together with Cauchy-Schwarz's and Young's inequalities (17) and (18) lead to the following upper bounds:

$$\begin{aligned}
(73) \qquad |I_1| &\leq \frac{P_1 Q_1 + P_2}{2}\left(|e_1|^2 + |e_2|^2\right), \\
|I_2| &\leq |s - s_h|^2 + |s' - s_h'|^2 + c_\xi\left(\hat{c}^2(\bar{c} + \bar{c}^2)\right)^{\frac{1}{1-\theta}} s^{\frac{2\theta}{1-\theta}}|e|^2 \\
(74) \qquad &+ \xi\frac{||e||^2}{s^2}, \\
|I_3| &\leq \frac{s_h'}{2s_h}\sum_{i\in\mathcal{I}_1}(|e_i(1)|^2 - |e_i|^2) \\
(75) \qquad &+ \frac{1}{s s_h}\left(s_h(s' - s_h') + s_h'(s_h - s)\right)\left(||e||^2 + |e|^2\right).
\end{aligned}$$

In (74), the constant $\bar{c}$ only depends on s_0 and L. In order to estimate $|I_4|$, we proceed as follows:

$$
\begin{aligned}
|I_4| &= -\left(\frac{1}{s^2}-\frac{1}{s_h}\right)^2 \sum_{i\in\mathcal{I}_1}(D_i u_{ih,y}, e_{,y}) \\
&\leq |s-s_h|\frac{s+s_h}{s_h^2 s}\sum_{i\in\mathcal{I}_1}(|D_i u_{ih}(1)e(1)| + |D_i u_{ih}|||e||) \\
&\leq \hat{c}|s-s_h|||e||^{\theta}|e|^{1-\theta}\frac{s+s_h}{s_h^2 s}\sum_{i\in\mathcal{I}_1} D_i|u_{ih}(1)| + |s-s_h|\frac{||e||}{s_h}\frac{s+s_h}{ss_h}\sum_{i\in\mathcal{I}_1}|D_i u_{ih}| \\
&\leq \bar{\xi}|s-s_h|^2 + c_{\bar{\xi}}\xi\frac{||e||^2}{s_h^2} + c_{\xi}c_{\bar{\xi}}\left(\hat{c}\frac{(s+s_h)\sum_{i\in\mathcal{I}_1} D_i|u_h(1)|}{s_h^{2-\theta}s}\right)^{\frac{2}{1-\theta}}|e|^2. \qquad (76)
\end{aligned}
$$

To bound above $|I_5|$, we rely on the fact that $\mathbb{R}_h e$ is the Lagrange interpolant of e, and hence, $(e-\mathbb{R}_h)e(y_i)=0$ for all $i\in J_n\cup\{n+1\}$. Additionally, we 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 $|I_5|$:

$$
\begin{aligned}
|I_5| &\leq \sum_{i\in J_n}\int_{y_i}^{y_{i+1}} R(u_h)(e-\mathbb{R}_h e)dy \\
&\leq \sum_{i\in J_n}||R(u_h)||_{L^2(\mathcal{J}_i)}h_i^2||e||_{H^1(\mathcal{J}_i)} \\
&\leq c\left(\sum_{i\in J_n}||R(u_h)||_{L^2(\mathcal{J}_i)}h_i^2\right)^{\frac{1}{2}}||e||_{H^1(0,1)} \\
&\leq \xi\frac{||e||^2}{s^2} + c_{\xi}c^2s^2\sum_{i\in J_n}||R(u_h)||_{L^2(\mathcal{J}_i)}h_i^2|e|^2, \qquad (77)
\end{aligned}
$$

where the strictly positive constant c only depends on $|J_n|$. Set $C_c := \hat{c}^2(\bar{c}+\bar{c}^2)$. Combining (73)-(77), we obtain

$$
\begin{aligned}
&\frac{1}{2}\frac{d}{dt}|e|^2 + \frac{d}{L_0^2}||e||^2 \leq \frac{P_1Q_1+P_2}{2}\left(|e_1|^2+|e_2|^2\right) \\
&+|s-s_h|^2 + |s'-s_h'|^2 + \xi\frac{||e||^2}{s^2} + c_{\xi}(C_c)^{\frac{1}{1-\theta}}|s|^{\frac{2\theta}{1-\theta}}|e|^2 \\
&+\left(\frac{1}{s}|s'-s_h'| + \frac{s_h'}{ss_h}|s-s_h|\right)||e||^2 + \xi\frac{||e||^2}{s^2} \\
&+\left(c_{\xi}\hat{c}^{\frac{2}{1-\theta}}|s|^{\frac{2\theta}{1-\theta}} + \frac{1}{s}|s'-s_h'| + \frac{s_h'}{ss_h}|s-s_h|\right)|e|^2 \\
&+\xi\frac{||e||^2}{s^2}(s-s_h)\frac{s+s_h}{s_h^2 s}\max_{\ell\in\mathcal{I}_1}D_\ell + \frac{1}{\xi}|s-s_h|\frac{s+s_h}{2s_h^2 s}\max_{\ell\in\mathcal{I}_1}||u||^2 \\
&+\xi\frac{||e||^2}{s^2} + c_{\xi}c^2s^2\sum_{i\in J_n}||R(u_h)||_{L^2(\mathcal{J}_i)}h_i^2. \qquad (78)
\end{aligned}
$$

Finally, we obtain

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}|e|^2 &+ \frac{d}{s^2}||e||^2 \le \mathcal{A}_1\left(|s-s_h|^2+|s'-s_h'|^2\right)+\mathcal{A}_2\frac{||e||^2}{s^2}\\ &+ \mathcal{A}_3|e|^2+\mathcal{A}_4\sum_{i\in J_n}||\mathcal{R}(u_h)||_{L^2(J_i)}h_i^2,\end{aligned} \tag{79}$$

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 positive and uniformly bounded. They are defined by

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

It is worth noting that the right-hand side of (79) depends on u_h but it is independent of u. Hence, (79) keeps the *a posteriori* character. Gronwall's inequality can be applied in order to conclude the proof of Theorem 5.2. The working strategy is very similar to that used to obtain the *a priori* error estimates. We omit to show the calculation details.

8. Summary

The moving-boundary problem discussed in this paper arises in the modeling via moving-reaction interfaces of the concrete carbonation process. The results address the error analysis of the semi-discrete approximation with finite elements of positive weak solutions to this problem and can be summarized as follows:

(1) The *a priori* estimate (51) shows that the approximation by piecewise linear finite elements for the semi-discretization in space converges to the solution of the continuous problem when the discretization grid becomes finer. (51) proves an order of convergence of $\mathcal{O}(h)$ for the semi-discretization method. The *a priori* estimate (49) indicates that the L^2-error of the concentrations vector is governed by the $W^{1,2}$-error of the moving interface position.

(2) An *a posteriori* error estimate has been also obtained, see (52). As soon as the constants c, c_1 and c_2 entering (52) are evaluated quantitatively, the *a posteriori* estimate be employed to calculate adaptively the 1D penetration of the sharp-carbonation inteface in concrete.

Due to the use of the Landau transformation (23), this framework cannot be used to tackle 2D formulations of the model. On the other hand, the way we obtained the error estimates can be applied to a wealth of unidimensional moving-boundary systems in which several internal fixed or moving boundaries may occur, provided positivity and $L^\infty-$ estimates of the weak solution are available.

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