Zentrum für Technomathematik
Fachbereich 3 – Mathematik und Informatik

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

Adrian Muntean

Report 06–05

Berichte aus der Technomathematik

Report 06–05 Mai 2006

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

Adrian Muntean*

May 31, 2006

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.

2000AMS Classification: 65M15, 65M60, 35R35

Keywords: Reaction-diffusion system, moving-boundary problem, spatial semi-discretization, finite elements, *a priori* estimates, *a posteriori* estimates, concrete carbonation

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

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

*ZeTeM, FB3(Mathematik und Informatik), Universität Bremen, Postfach 330440, 28334 Bremen, Deutschland (Germany), e-mail: muntean@math.uni-bremen.de

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_4 denotes the $Ca(OH)_2(aq)$ concentration. Finally, u_5 represents the moisture concentration produced by (1) in the reacted phase.

The problem reads: Find the concentrations vector $u = u(x,t)$ ($x \in \Omega_1(t) =]0, s(t)[$, 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*

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

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

[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 $\tilde{c} = \tilde{c}(\theta) > 0$ such that

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

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 $\mathbb{R}_h := (R_h^1, R_h^3, R_h^4, R_h^5)^t$ 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 $\theta \in \left[\frac{1}{3}, 1\right[$ 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 $\varphi := (\varphi_1, \varphi_3, \varphi_4, \varphi_5)^t \in \mathbb{V}$ 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.

$$\begin{aligned}
a(s,u,\varphi) &:= \frac{1}{s}\sum_{i\in\mathcal{I}_1}(D_i u_{i,y}, \varphi_{i,y}), &(24)\\
b_f(u,s,\varphi) &:= s\sum_{i\in\mathcal{I}_1}(f_i(u), \varphi_i), &(25)\\
e(s',u,\varphi) &:= \sum_{i\in\mathcal{I}_1} g_i(s', u(1))\varphi_i(1), &(26)\\
h(s',u_y,\varphi) &:= \sum_{i\in\mathcal{I}_1} s'(y u_{i,y}, \varphi_i), &(27)
\end{aligned}$$

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

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

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

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

In (34), we set

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

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 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*

$$\lambda \in W^{1,3}(S_T)^{|\mathcal{I}_1|}, \lambda(t) \geq 0 \ a.e. \ \ t \in \bar{S}_T, \tag{39}$$

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

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

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

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*

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

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

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

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

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 $u_h := (u_{1h}, u_{3h}, u_{4h}, u_{5h})^t \in \mathbb{V}_h$ represents an approximation of $u := (u_1, u_3, u_4, u_5)^t \in \mathbb{V}$. Furthermore, set $v_h := (v_{1h}, v_{3h}, v_{4h}, v_{5h})^t \in \mathbb{V}_h$. The precise definition of the space $\mathbb{V}_h$ is given in section 4.

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

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

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

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

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

A first result is the next theorem:

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

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

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 $P_\Gamma^{1,sd}$ are uniquely solvable. Let (u,s) and (u_h,s_h) be the corresponding solutions. Then the following estimate holds: There exist a $\delta_1 \in]0, \max\{\delta, \tilde{\delta}\}]$ and a strictly positive constant c, which are independent of h, such that*

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

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 $P_\Gamma^{1,sd}$ are uniquely solvable. Let (u,s) and (u_h,s_h) be the corresponding solutions. There exist $\delta_2 \in]0, \max\{\delta, \tilde{\delta}\}]$ and strictly positive constants c_i ($i \in \{1,2,3\}$) and c, which are independent of h and u, such that*

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

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 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* $P_\Gamma^{1,sd}$ *is* <u>*sufficiently regular*</u> *(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 $P_\Gamma^{1,sd}$, 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:

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

$$
\begin{aligned}
&+ \quad (P_2(Q_2(u_{2h}+\lambda_2)-(u_{1h}+\lambda_1)), w_{2h}) \\
&+ \quad \frac{s'}{s}\sum_{i\in I_1}(yu_{i,y}, w_{ih}) - \frac{s'_h}{s_h}\sum_{i\in I_1}(yu_{ih,y}, w_{ih}). \qquad (54)
\end{aligned}
$$

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

$$
\begin{aligned}
(e_{,t}, w_h) \quad &+ \quad \frac{1}{s^2}\sum_{i\in I_1}(D_i(u_i-u_{ih})_{,y}, w_{ih,y}) = \left(\frac{1}{s_h^2}-\frac{1}{s^2}\right)\sum_{i\in I_1}(D_iu_{ih,y}, w_{ih,y}) \\
&- \quad \left(\frac{s'}{s}(u_1(1)+\lambda_1) - \frac{s'_h}{s_h}(u_{1h}(1)+\lambda_1) + \frac{\eta_\Gamma}{s} - \frac{\eta_\Gamma^h}{s_h}\right) w_{1h}(1) \\
&- \quad \left(\frac{s'}{s}(u_2(1)+\lambda_2) - \frac{s'_h}{s_h}(u_{2h}(1)+\lambda_2)\right) w_{2h}(1) - \left(\frac{\eta_\Gamma}{s} - \frac{\eta_\Gamma^h}{s_h}\right) w_{5h}(1) \\
&+ \quad P_1Q_1(e_2, w_{1h}) - P_1(e_1, w_{1h}) - P_2Q_2(e_2, w_{2h}) + P_2(e_1, w_{2h}) \\
&+ \quad \frac{s'}{s}\sum_{i\in I_1}(ye_{i,y}, w_{ih}) + \left(\frac{s'}{s}-\frac{s'_h}{s_h}\right)\sum_{i\in I_1}(yu_{ih,y}, w_{ih}). \qquad (55)
\end{aligned}
$$

Therefore, we may write

$$
(e_{,t}, w_h) + \frac{\min_{i\in I_1} D_i}{s(t)}(e_{,y}, w_{h,y}) \le \sum_{\ell=1}^{5} I_\ell, \qquad (56)
$$

where the terms I_ℓ are given by

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

Set $d := \min_{i\in I_1} D_i$. 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

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

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

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

Remark 7.1 *(1) There exists a constant* $c_1=c_1(\Lambda,s_0)>0$ *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

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

$$
\begin{aligned}
&+ \quad c_1(|s-s_h|+|s'-s_h'|)|v_h(1)-u(1)+e(1)| \\
&+ \quad c_2(|e(1)|+|s-s_h|+|s'-s_h'|)|v_h(1)-u(1)+e(1)| \\
&+ \quad P_1Q_1|e_2|\left(|v_{1h}-u_1|+|e_1|\right)+P_1|e_1|\left(|v_{1h}-u_1|+|e_1|\right) \\
&+ \quad P_2Q_2|e_2|\left(|v_{2h}-u_2|+|e_2|\right)+P_2|e_1|\left(|v_{2h}-u_2|+|e_2|\right) \\
&+ \quad \frac{s'}{2s}\sum_{i\in I_1}[(|e_i(1)|^2-|e_i|^2)+||e_i|||v_{ih}-u_{ih}|] \\
&+ \quad c_3(|s-s_h|+|s'-s_h'|)\sum_{i\in I_1}(|u_{ih}||v_{ih}-u_{ih}| \\
&+ \quad |u_{ih}|||v_{ih}-u_{ih}||). \qquad (59)
\end{aligned}
$$

After some elementary manipulations, we directly gain the estimate:

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

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

$$
\begin{aligned}
\frac{d}{dt}|e|^2+\frac{d}{s^2}||e||^2 &\leq |e_{,t}|\gamma_1h^2|u|_{H^2(0,1)}+\frac{d}{s^2}||e||\gamma_2h|u|_{H^2(0,1)} \\
&+c_3|s-s_h|||u_h||\left(\gamma_2h|u|_{H^2(0,1)}+||e||\right) \\
&+(c_1+c_2)(|s-s_h|+|s'-s_h'|)\tilde{c}||e||^{\theta}|e|^{1-\theta} \\
+c_4(|s-s_h|+|s'-s_h'|)c\gamma_2^{\theta}h^{\theta}\gamma_1^{1-\theta}h^{2(1-\theta)}&|u|_{H^2(0,1)}+c_6\left(|e_1|^2+|e_2|^2\right) \\
+c_7\gamma_1^2h^4\left(|u_1|^2_{H^2(0,1)}+|u_2|^2_{H^2(0,1)}\right)&+\frac{s'}{2s}\tilde{c}||e||^{2\theta}|e|^{2(1-\theta)} \\
&+\frac{\xi}{2}\frac{||e||^2}{s^2}+\frac{s'}{2\xi}\gamma_1^2h^4|u|^2_{H^2(0,1)} \\
+c_5\left(\gamma_2h|u|_{H^2(0,1)}+||e||\right)&(|s-s_h|+|s'-s_h'|). \qquad (61)
\end{aligned}
$$

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

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

Owing to $P_T^{1,sd}$, 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:

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

$$
\begin{aligned}
&- \quad e(s', u, e) + h(s', u_{,y}, e) - h(s'_h, u_{h,y}, e) - \left(\frac{1}{s^3} - \frac{1}{s_h^3}\right) \sum_{i\in I_1} (D_i u_{ihy}, v_{,y}) \\
&+ \quad \sum_{i\in J_n} \int_{y_i}^{y_{i+1}} (e - \mathbb{R}e) dy \\
&- \quad \frac{1}{s_h^3} \sum_{i\in J_n} \sum_{\ell\in I_1} \max_{\ell\in I_1} D_\ell \left[u_{\ell h,y} y_{i+1} (e - \mathbb{R}_h e)(y_{i+1}) - u_{jh,y}(y_i)(e - \mathbb{R}_h e)(y_i)\right] \\
&= \quad \sum_{\ell=1}^{5} I_\ell, \qquad (67)
\end{aligned}
$$

where we have

$$
\begin{aligned}
I_1 &:= b_f(s, u, e) - b_f(s_h, u_h, e), \\
I_2 &:= e(s'_h, u_h, e) - e(s', u, e), \\
I_3 &:= h(s', u_{,y}, e) - h(s'_h, u_{h,y}, e), \\
I_4 &:= -\left(\frac{1}{s^3} - \frac{1}{s_h^3}\right) \sum_{i\in I_1} (D_i u_{ihy}, e_{,y}), \\
I_5 &:= \sum_{i\in J_n} \int_{y_i}^{y_{i+1}} (e - \mathbb{R}_h e) dy \\
&- \quad \frac{1}{s_h^3} \sum_{i\in J_n} \sum_{\ell\in I_1} \max_{\ell\in I_1} D_\ell \left[u_{\ell h,y} y_{i+1} (e - \mathbb{R}_h e)(y_{i+1}) - u_{jh,y}(y_i)(e - \mathbb{R}_h e)(y_i)\right].
\end{aligned}
\qquad (68)
$$

Simple manipulations of the multiplicative inequality (20) together with Cauchy-Schwarz's and Young's inequalities (17) and (18) lead to the following bounds: We obtain

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

$$
\begin{aligned}
|I_2| \quad &\leq \quad |s - s_h|^2 + |s' - s'_h|^2 + c_\xi \left(\bar{c}^2 (\bar{c} + \bar{c}^2)\right)^{\frac{1}{1-\theta}} s^{\frac{2\theta}{1-\theta}} |e|^2 \\
&+ \quad \xi \frac{||e||^2}{s^2}, \qquad (70) \\
|I_3| \quad &\leq \quad \frac{s'_h}{2s_h} \sum_{i\in I_1} \left(|e_i(1)|^2 - |e_i|^2\right) \\
&+ \quad \frac{1}{s s_h} \left(s_h(s' - s'_h) + s'_h(s_h - s)\right) \left(||e||^2 + |e|^2\right). \qquad (71)
\end{aligned}
$$

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

$$
\begin{aligned}
|I_4| \quad &= \quad -\left(\frac{1}{s^3} - \frac{1}{s_h}\right)^3 \sum_{i\in I_1} (D_i u_{ih,y}, e_{,y}) \\
&\leq \quad |s - s_h| \frac{s + s_h}{s_h^3 s} \sum_{i\in I_1} \left(|D_i u_{ih}(1) e(1)| + |D_i u_{ih}| ||e||\right)
\end{aligned}
$$

$$\leq \quad \hat{c}|s-s_h|||e||^{\theta}|e|^{1-\theta}\frac{s+s_h}{s_h^2 s}\sum_{i\in I_1} D_i|u_{ih}(1)| + |s-s_h|\frac{||e||}{s_h}\frac{s+s_h}{ss_h}\sum_{i\in I_1}|D_i u_{ih}|$$

$$\leq \quad \xi|s-s_h|^2 + c_{\xi}\xi\frac{||e||^2}{s_h^2} + c_{\xi}c_{\bar{\xi}}\left(\hat{c}\frac{(s+s_h)\sum_{i\in I_1} D_i|u_h(1)|}{s_h^{2-\theta}s}\right)^{\frac{2}{1-\theta}}|e|^2. \qquad (72)$$

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 $|I_5|$:

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

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

$$\begin{aligned}
\frac{1}{2}\frac{d}{dt}|e|^2 + \frac{d}{L_0^2}||e||^2 \leq \frac{P_1Q_1+P_2}{2}\left(|e_1|^2+|e_2|^2\right) \\
+|s-s_h|^2+|s'-s_h'|^2+\xi\frac{||e||^2}{s^2}+c_{\xi}(C_c)^{\frac{1}{1-\theta}}|s|^{\frac{2\theta}{1-\theta}}|e|^2 \\
+\left(\frac{1}{s}|s'-s_h'|+\frac{s_h'}{ss_h}|s-s_h|\right)||e||^2+\xi\frac{||e||^2}{s^2} \\
+\left(c_{\xi}\hat{c}^{\frac{2}{1-\theta}}|s|^{\frac{2\theta}{1-\theta}}+\frac{1}{s}|s'-s_h'|+\frac{s_h'}{ss_h}|s-s_h|\right)|e|^2 \\
+\xi\frac{||e||^2}{s^2}(s-s_h)\frac{s+s_h}{s_h^2 s}\max_{\ell\in I_1}D_\ell+\frac{1}{\xi}|s-s_h|\frac{s+s_h}{2s_h^2 s}\max_{\ell\in I_1}||u||^2 \\
+\xi\frac{||e||^2}{s^2}+c_{\xi}c^2s^2\sum_{i\in J_n}||R(u_h)||_{L^2(\mathcal{J}_i)}h_i^2. \qquad (74)
\end{aligned}$$

This finally yields

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

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

$$
\begin{aligned}
\mathcal{A}_1 &:= 1,\\
\mathcal{A}_2 &:= 3\xi + c_\xi \xi,\\
\mathcal{A}_3 &:= M(s,s',s_h,s'_h) + \frac{P_1Q_1+P_3}{2} + \left(c_\xi C_c^{\frac{1}{1-\theta}} + c_\xi \hat{c}^{\frac{2}{1-\theta}}\right)|s|^{\frac{2\theta}{1-\theta}}\\
&+ c_\xi c_{\bar{\xi}} \hat{c}^{\frac{2}{1-\theta}} \left(\frac{(s+s_h)\sum_{i\in I_1} D_i}{ss_h^{3-\theta}}|u_h(1)|\right)^{\frac{2}{1-\theta}},\\
\mathcal{A}_4 &:= c_\xi c^3 L^3.
\end{aligned}
\tag{76}
$$

It is worth noting that the right-hand side of (75) depends on u_h but is independent of u, and hence, (75) keeps the *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 $O(h)$ 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.

Acknowledgments: Fruitful discussions with S. Meier, M. Böhm and A. Schmidt are greatly acknowledged. This work was financially supported by the special priority program SPP1122 *Prediction of the course of physicochemical damage processes involving mineral materials* of the German Science Foundation (DFG).

References

[BDJR98] Böhm, M., Devinny, J., Jahani, F. and Rosen, G. *On a moving-boundary system modeling corrosion in sewer pipes.* Appl. Math. Comput. **92**(1998), 247–269

[BKM03a] Böhm, M., Kropp, J. and Muntean, A. *On a Prediction Model for Concrete Carbonation based on Moving Interfaces - Interface concentrated Reactions.* Berichte aus der Technomathematik 03-03, ZeTeM, University of Bremen, 2003

[BKM03b] Böhm, M., Kropp, J. and Muntean, A. *A two-reaction-zones moving-interface model for predicting $Ca(OH)_2$-carbonation in concrete.* Berichte aus der Technomathematik 03-04, ZeTeM, University of Bremen, 2003

[BS96] Brenner, S. C. and Scott, L. R. *The Mathematical Theory of Finite Elements Methods.* Springer Verlag, Berlin, 2nd edition, 1996

[Cha99] Chaussadent, T. *États de lieux et réflexions sur la carbonatation du beton armé.* Technical report, Laboratoire Central de Ponts et Chaussées, 1999

[CR05] Caboussat, A. and Rappaz, J. *Analysis of a one-dimensional free boundary flow problem.* Numer. Math. **101**(2005), 1, 67–86

[Cra84] Crank, J. *Free and Moving Boundary Problems.* Clarendon Press, Oxford, 1984

[Joh94] Johnson, C. *Numerical Solution of Partial Differential Equations by the Finite Element Method.* Cambridge University Press, Cambridge, 5th edition, 1994

[JP95] Jones, L. and Pani, A. K. *On superconvergence results and negative norm estimates for a unidimensional single phase Stefan problem.* Numer. Funct. Anal. and Optimiz. **16**(1995), 1-2, 153–175

[KG87] Kharab, A. and Guenther, R. B. *A free boundary value problem for water invading an unsaturated medium.* Computing **38**(1987), 185–207

[Lan50] Landau, H. G. *Heat conduction in a melting solid.* Quart. Appl. Mech. Math. **8**(1950), 81–94

[LL98] Lee, H. Y. and Lee, J. R. *Error estimates for a single-phase quasilinear Stefan problem in one space dimension.* Applied Numerical Mathematics **26**(1998), 327–348

[LOS02] Lee, H. Y., Ohm, M. R. and Shin, J. Y. *Fully discrete approximation for a quasilinear Stefan problem with forcing term.* Appl. Math. Comput. **133**(2002), 461–478

[LT03] Larsson, S. and Thomée, V. *Partial Differential Equations with Numerical Methods.* Springer Verlag, Berlin, Heidelberg, 2003

[MB06a] Muntean, A. and Böhm, M. *Dynamics of a moving reaction interface in a concrete wall.* In *Free and Moving Boundary Problems. Theory and Applications,* (edited by J. F Rodrigues, L. Santos, I. N. F.). Birkhäuser, Basel, 2006. In press

[MB06b] Muntean, A. and Böhm, M. *A sharp-interface moving-boundary system modeling carbonation penetration in concrete.* Berichte aus der Technomathematik 06-03, ZeTeM, University of Bremen, 2006

[Mun06] Muntean, A. *A Moving-Boundary Problem: Modeling, Analysis and Simulation of Concrete Carbonation.* Ph.D. thesis, Faculty of Mathematics,University of Bremen, Cuvillier Verlag, Göttingen, Germany, 2006

[Nit78] Nitsche, J. *Finite element approximations to the one dimensional Stefan problem.* In *Proceedings on Recent Advances in Numerical Analysis*, (edited by deBoor, C. and Golub, G.), 119–142. Academic Press, N.Y., 1978

[Nit80] Nitsche, J. *A finite element method for parabolic free boundary problems.* In *Free Boundary Problems: Proceedings of a Seminar held in Pavia*, (edited by Magenes, E.), 277–318. 1980

[Ort94] Ortoleva, P. J. *Geochemical Self-Organization*, volume 23 of *Oxford Monographs on Geology and Geophysics.* Oxford University Press, NY, Oxford, 1994

[Pan93] Pani, A. K. *A finite element method for a diffusion equation with constrained energy and nonlinear boundary conditions.* J. Austral. Math. Soc. Ser. B **35**(1993), 87–102

[PD91a] Pani, A. K. and Das, P. C. *A finite element method for a single phase semilinear Stefan problem in one space dimension.* Numer. Funct. Anal. and Optimiz. **12**(1991), 1-2, 153–171

[PD91b] Pani, A. K. and Das, P. C. *A priori error estimates for a single-phase quasilinear Stefan problem in one space dimension.* IMA J. Num. Anal. **11**(1991), 377–392

[SMB05] Schmidt, A., Muntean, A. and Böhm, M. *Numerical experiments with self-adaptive finite element simulations in 2D for the carbonation of concrete.* Berichte aus der Technomathematik 05-01, ZeTeM, University of Bremen, 2005

[SS05] Schmidt, A. and Siebert, K. *Design of Adaptive Finite Element Software: The Finite Element Toolbox ALBERTA*, volume 42 of *LNCS.* Springer Verlag, Berlin, 2005

[Tho97] Thomée, V. *Galerkin Finite Element Methods for Parabolic Problems.* Springer Verlag, Berlin, Heidelberg, 1997

[Vui90] Vuik, C. *An L^2-error estimate for an approximation of the solution of a parabolic variational inequality.* Numer. Math. **57**(1990), 453–471

Berichte aus der Technomathematik

ISSN 1435-7968

http://www.math.uni-bremen.de/zetem/berichte.html

— Vertrieb durch den Autor —

Reports **Stand: 31. Mai 2006**

98–01. Peter Benner, Heike Faßbender:
An Implicitly Restarted Symplectic Lanczos Method for the Symplectic Eigenvalue Problem, Juli 1998.

98–02. Heike Faßbender:
Sliding Window Schemes for Discrete Least-Squares Approximation by Trigonometric Polynomials, Juli 1998.

98–03. Peter Benner, Maribel Castillo, Enrique S. Quintana-Ortí:
Parallel Partial Stabilizing Algorithms for Large Linear Control Systems, Juli 1998.

98–04. Peter Benner:
Computational Methods for Linear–Quadratic Optimization, August 1998.

98–05. Peter Benner, Ralph Byers, Enrique S. Quintana-Ortí, Gregorio Quintana-Ortí:
Solving Algebraic Riccati Equations on Parallel Computers Using Newton's Method with Exact Line Search, August 1998.

98–06. Lars Grüne, Fabian Wirth:
On the rate of convergence of infinite horizon discounted optimal value functions, November 1998.

98–07. Peter Benner, Volker Mehrmann, Hongguo Xu:
A Note on the Numerical Solution of Complex Hamiltonian and Skew-Hamiltonian Eigenvalue Problems, November 1998.

98–08. Eberhard Bänsch, Burkhard Höhn:
Numerical simulation of a silicon floating zone with a free capillary surface, Dezember 1998.

99–01. Heike Faßbender:
The Parameterized SR Algorithm for Symplectic (Butterfly) Matrices, Februar 1999.

99–02. Heike Faßbender:
Error Analysis of the symplectic Lanczos Method for the symplectic Eigenvalue Problem, März 1999.

99–03. Eberhard Bänsch, Alfred Schmidt:
Simulation of dendritic crystal growth with thermal convection, März 1999.

99–04. Eberhard Bänsch:
Finite element discretization of the Navier-Stokes equations with a free capillary surface, März 1999.

99–05. Peter Benner:
Mathematik in der Berufspraxis, Juli 1999.

99–06. Andrew D.B. Paice, Fabian R. Wirth:
Robustness of nonlinear systems and their domains of attraction, August 1999.

99–07. Peter Benner, Enrique S. Quintana-Ortí, Gregorio Quintana-Ortí:
Balanced Truncation Model Reduction of Large-Scale Dense Systems on Parallel Computers, September 1999.

99–08. Ronald Stöver:
Collocation methods for solving linear differential-algebraic boundary value problems, September 1999.

99–09. Huseyin Akcay:
Modelling with Orthonormal Basis Functions, September 1999.

99–10. Heike Faßbender, D. Steven Mackey, Niloufer Mackey:
Hamilton and Jacobi come full circle: Jacobi algorithms for structured Hamiltonian eigenproblems, Oktober 1999.

99–11. Peter Benner, Vincente Hernández, Antonio Pastor:
On the Kleinman Iteration for Nonstabilizable System, Oktober 1999.

99–12. Peter Benner, Heike Faßbender:
A Hybrid Method for the Numerical Solution of Discrete-Time Algebraic Riccati Equations, November 1999.

99–13. Peter Benner, Enrique S. Quintana-Ortí, Gregorio Quintana-Ortí:
Numerical Solution of Schur Stable Linear Matrix Equations on Multicomputers, November 1999.

99–14. Eberhard Bänsch, Karol Mikula:
Adaptivity in 3D Image Processing, Dezember 1999.

00–01. Peter Benner, Volker Mehrmann, Hongguo Xu:
Perturbation Analysis for the Eigenvalue Problem of a Formal Product of Matrices, Januar 2000.

00–02. Ziping Huang:
Finite Element Method for Mixed Problems with Penalty, Januar 2000.

00–03. Gianfrancesco Martinico:
Recursive mesh refinement in 3D, Februar 2000.

00–04. Eberhard Bänsch, Christoph Egbers, Oliver Meincke, Nicoleta Scurtu:
Taylor-Couette System with Asymmetric Boundary Conditions, Februar 2000.

00–05. Peter Benner:
Symplectic Balancing of Hamiltonian Matrices, Februar 2000.

00–06. Fabio Camilli, Lars Grüne, Fabian Wirth:
A regularization of Zubov's equation for robust domains of attraction, März 2000.

00–07. Michael Wolff, Eberhard Bänsch, Michael Böhm, Dominic Davis:
Modellierung der Abkühlung von Stahlbrammen, März 2000.

00–08. Stephan Dahlke, Peter Maaß, Gerd Teschke:
Interpolating Scaling Functions with Duals, April 2000.

00–09. Jochen Behrens, Fabian Wirth:
A globalization procedure for locally stabilizing controllers, Mai 2000.

00–10. Peter Maaß, Gerd Teschke, Werner Willmann, Günter Wollmann:
Detection and Classification of Material Attributes – A Practical Application of Wavelet Analysis, Mai 2000.

00–11. Stefan Boschert, Alfred Schmidt, Kunibert G. Siebert, Eberhard Bänsch, Klaus-Werner Benz, Gerhard Dziuk, Thomas Kaiser:
Simulation of Industrial Crystal Growth by the Vertical Bridgman Method, Mai 2000.

00–12. Volker Lehmann, Gerd Teschke:
Wavelet Based Methods for Improved Wind Profiler Signal Processing, Mai 2000.

00–13. Stephan Dahlke, Peter Maass:
A Note on Interpolating Scaling Functions, August 2000.

00–14. Ronny Ramlau, Rolf Clackdoyle, Frédéric Noo, Girish Bal:
Accurate Attenuation Correction in SPECT Imaging using Optimization of Bilinear Functions and Assuming an Unknown Spatially-Varying Attenuation Distribution, September 2000.

00–15. Peter Kunkel, Ronald Stöver:
Symmetric collocation methods for linear differential-algebraic boundary value problems, September 2000.

00–16. Fabian Wirth:
The generalized spectral radius and extremal norms, Oktober 2000.

00–17. Frank Stenger, Ahmad Reza Naghsh-Nilchi, Jenny Niebsch, Ronny Ramlau:
A unified approach to the approximate solution of PDE, November 2000.

00–18. Peter Benner, Enrique S. Quintana-Ortí, Gregorio Quintana-Ortí:
Parallel algorithms for model reduction of discrete–time systems, Dezember 2000.

00–19. Ronny Ramlau:
A steepest descent algorithm for the global minimization of Tikhonov–Phillips functional, Dezember 2000.

01–01. Efficient methods in hyperthermia treatment planning:
Torsten Köhler, Peter Maass, Peter Wust, Martin Seebass, Januar 2001.

01–02. Parallel Algorithms for LQ Optimal Control of Discrete-Time Periodic Linear Systems:
Peter Benner, Ralph Byers, Rafael Mayo, Enrique S. Quintana-Ortí, Vicente Hernández, Februar 2001.

01–03. Peter Benner, Enrique S. Quintana-Ortí, Gregorio Quintana-Ortí:
Efficient Numerical Algorithms for Balanced Stochastic Truncation, März 2001.

01–04. Peter Benner, Maribel Castillo, Enrique S. Quintana-Ortí:
Partial Stabilization of Large-Scale Discrete-Time Linear Control Systems, März 2001.

01–05. Stephan Dahlke:
Besov Regularity for Edge Singularities in Polyhedral Domains, Mai 2001.

01–06. Fabian Wirth:
A linearization principle for robustness with respect to time-varying perturbations, Mai 2001.

01–07. Stephan Dahlke, Wolfgang Dahmen, Karsten Urban:
Adaptive Wavelet Methods for Saddle Point Problems - Optimal Convergence Rates, Juli 2001.

01–08. Ronny Ramlau:
Morozov's Discrepancy Principle for Tikhonov regularization of nonlinear operators, Juli 2001.

01–09. Michael Wolff:
Einführung des Drucks für die instationären Stokes–Gleichungen mittels der Methode von Kaplan, Juli 2001.

01–10. Stephan Dahlke, Peter Maaß, Gerd Teschke:
Reconstruction of Reflectivity Desities by Wavelet Transforms, August 2001.

01–11. Stephan Dahlke:
Besov Regularity for the Neumann Problem, August 2001.

01–12. Bernard Haasdonk, Mario Ohlberger, Martin Rumpf, Alfred Schmidt, Kunibert G. Siebert:
h–p–Multiresolution Visualization of Adaptive Finite Element Simulations, Oktober 2001.

01–13. Stephan Dahlke, Gabriele Steidl, Gerd Teschke:
Coorbit Spaces and Banach Frames on Homogeneous Spaces with Applications to Analyzing Functions on Spheres, August 2001.

02–01. Michael Wolff, Michael Böhm:
Zur Modellierung der Thermoelasto-Plastizität mit Phasenumwandlungen bei Stählen sowie der Umwandlungsplastizität, Februar 2002.

02–02. Stephan Dahlke, Peter Maaß:
An Outline of Adaptive Wavelet Galerkin Methods for Tikhonov Regularization of Inverse Parabolic Problems, April 2002.

02–03. Alfred Schmidt:
A Multi-Mesh Finite Element Method for Phase Field Simulations, April 2002.

02–04. Sergey N. Dachkovski, Michael Böhm:
A Note on Finite Thermoplasticity with Phase Changes, Juli 2002.

02–05. Michael Wolff, Michael Böhm:
Phasenumwandlungen und Umwandlungsplastizität bei Stählen im Konzept der Thermoelasto-Plastizität, Juli 2002.

02–06. Gerd Teschke:
Construction of Generalized Uncertainty Principles and Wavelets in Anisotropic Sobolev Spaces, August 2002.

02–07. Ronny Ramlau:
TIGRA – an iterative algorithm for regularizing nonlinear ill–posed problems, August 2002.

02–08. Michael Lukaschewitsch, Peter Maaß, Michael Pidcock:
Tikhonov regularization for Electrical Impedance Tomography on unbounded domains, Oktober 2002.

02–09. Volker Dicken, Peter Maaß, Ingo Menz, Jenny Niebsch, Ronny Ramlau:
Inverse Unwuchtidentifikation an Flugtriebwerken mit Quetschöldämpfern, Oktober 2002.

02–10. Torsten Köhler, Peter Maaß, Jan Kalden:
Time-series forecasting for total volume data and charge back data, November 2002.

02–11. Angelika Bunse-Gerstner:
A Short Introduction to Iterative Methods for Large Linear Systems, November 2002.

02–12. Peter Kunkel, Volker Mehrmann, Ronald Stöver:
Symmetric Collocation for Unstructured Nonlinear Differential-Algebraic Equations of Arbitrary Index, November 2002.

02–13. Michael Wolff:
Ringvorlesung: Distortion Engineering 2
Kontinuumsmechanische Modellierung des Materialverhaltens von Stahl unter Berücksichtigung von Phasenumwandlungen, Dezember 2002.

02–14. Michael Böhm, Martin Hunkel, Alfred Schmidt, Michael Wolff:
Evaluation of various phase-transition models for 100Cr6 for application in commercial FEM programs, Dezember 2002.

03–01. Michael Wolff, Michael Böhm, Serguei Dachkovski:
Volumenanteile versus Massenanteile - der Dilatometerversuch aus der Sicht der Kontinuumsmechanik, Januar 2003.

03–02. Daniel Kessler, Ricardo H. Nochetto, Alfred Schmidt:
A posteriori error control for the Allen-Cahn Problem: circumventing Gronwall's inequality, März 2003.

03–03. Michael Böhm, Jörg Kropp, Adrian Muntean:
On a Prediction Model for Concrete Carbonation based on Moving Interfaces - Interface concentrated Reactions, April 2003.

03–04. Michael Böhm, Jörg Kropp, Adrian Muntean:
A Two-Reaction-Zones Moving-Interface Model for Predicting $Ca(OH)_2$ Carbonation in Concrete, April 2003.

03–05. Vladimir L. Kharitonov, Diederich Hinrichsen:
Exponential estimates for time delay systems, May 2003.

03–06. Michael Wolff, Michael Böhm, Serguei Dachkovski, Günther Löwisch:
Zur makroskopischen Modellierung von spannungsabhängigem Umwandlungsverhalten und Umwandlungsplastizität bei Stählen und ihrer experimentellen Untersuchung in einfachen Versuchen, Juli 2003.

03–07. Serguei Dachkovski, Michael Böhm, Alfred Schmidt, Michael Wolff:
Comparison of several kinetic equations for pearlite transformation in 100Cr6 steel, Juli 2003.

03–08. Volker Dicken, Peter Maass, Ingo Menz, Jenny Niebsch, Ronny Ramlau:
Nonlinear Inverse Unbalance Reconstruction in Rotor dynamics, Juli 2003.

03–09. Michael Böhm, Serguei Dachkovski, Martin Hunkel, Thomas Lübben, Michael Wolff:
Übersicht über einige makroskopische Modelle für Phasenumwandlungen im Stahl,
Juli 2003.

03–10. Michael Wolff, Friedhelm Frerichs, Bettina Suhr:
Vorstudie für einen Bauteilversuch zur Umwandlungsplastizität bei der perlitischen Umwandlung des Stahls 100 Cr6,
August 2003.

03–11. Michael Wolff, Bettina Suhr:
Zum Vergleich von Massen- und Volumenanteilen bei der perlitischen Umwandlung der Stähle 100Cr6 und C80,
September 2003.

03–12. Rike Grotmaack, Adrian Muntean:
Stabilitätsanalyse eines Moving-Boundary-Modells der beschleunigten Karbonatisierung von Portlandzementen,
September 2003.

03–13. Alfred Schmidt, Michael Wolff, Michael Böhm:
Numerische Untersuchungen für ein Modell des Materialverhaltens mit Umwandlungsplastizität und Phasenumwandlungen beim Stahl 100Cr6 (Teil 1),
September 2003.

04–01. Liliana Cruz Martin, Gerd Teschke:
A new method to reconstruct radar reflectivities and Doppler information,
Januar 2004.

04–02. Ingrid Daubechies, Gerd Teschke:
Wavelet based image decomposition by variational functionals,
Januar 2004.

04–03. N. Guglielmi, F. Wirth, M. Zennaro:
Complex polytope extremality results for families of matrices,
März 2004.

04–04. I. Daubechies, G. Teschke:
Variational image restoration by means of wavelets: simultaneous decomposition, deblurring and denoising,
April 2004.

04–05. V.L. Kharitonov, E. Plischke:
Lyapunov matrices for time-delay systems,
April 2004.

04–06. Ronny Ramlau:
On the use of fixed point iterations for the regularization of nonlinear ill-posed problems,
Juni 2004.

04–07. Christof Büskens, Matthias Knauer:
Higher Order Real-Time Approximations In Optimal Control of Multibody-Systems For Industrial Robots,
August 2004.

04–08. Christof Büskens, Roland Griesse:
Computational Parametric Sensitivity Analysis of Perturbed PDE Optimal Control Problems with State and Control Constraints,
August 2004.

04–09. Christof Büskens:
Higher Order Real-Time Approximations of Perturbed Control Constrainted PDE Optimal Control Problems ,
August 2004.

04–10. Christof Büskens, Matthias Gerdts:
Differentiability of Consistency Functions,
August 2004.

04–11. Robert Baier, Christof Büskens, Ilyes Aïssa Chahma, Matthias Gerdts:
Approximation of Reachable Sets by Direct Solution Methods of Optimal Control Problems,
August 2004.

04–12. J. Soares, G. Teschke, M. Zhariy:
A Wavelet Regularization for Nonlinear Diffusion Equations,
September 2004.

05–01. Alfred Schmidt, Adrian Muntean, Michael Böhm:
Numerical experiments with Self-Adaptive Finite Element Simulations in 2D for the Carbonation of Concrete,
April 2005.

05–02. Sebastian A. Meier, Malte A. Peter, Adrian Muntean, Michael Böhm:
Modelling and simulation of concrete carbonation with internal layers,
April 2005.

05–03. Malte A. Peter, Adrian Muntean, Sebastian A. Meier, Michael Böhm:
Modelling and simulation of concrete carbonation: competition of several carbonation reactions,
April 2005.

05–04. Adrian Muntean, Sebastian A. Meier, Malte A. Peter, Michael Böhm, Jörg Kropp:
A note on limitations of the use of accelerated concrete-carbonation tests for service-life predictions,
April 2005.

05–05. Sergey Dashkovskiy, Björn S. Rüffer, Fabian R. Wirth:
An ISS Small-Gain Theorem for General Networks,
Juni 2005.

06–01. Prof. Dr. Christof Büskens, Peter Lasch:
Suboptimal Improvement of the classical Riccati Controller,
März 2006.

06–02. Michael Wolff, Michael Böhm:
Transformation-induced plasticity in steel - general modelling, analysis and parameter identification,
April 2006.

06–03. Adrian Muntean, Michael Böhm:
A sharp-interface moving-boundary system modeling carbonation penetration in concrete,
April 2006.

06–04. Michael Wolff, Michael Böhm,Sebastian Meier:
Modellierung der Wechselwirkung von Kohlenstoff-Diffusion und ferritischen Phasenumwandlungen für einen untereutektoiden unlegierten Stahl,
Mai 2006.

06–05. Adrian Muntean:
Error bounds on a semi-discrete finite element approximation of the weak solution to a one phase moving-boundary system describing concrete carbonation,
Mai 2006.