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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].