Computing positive stable numerical solutions of moving boundary problems for concrete carbonation

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ABSTRACT

This paper deals with the construction and computation of numerical solutions of a coupled mixed partial differential equation system arising in concrete carbonation problems. The moving boundary problem under study is firstly transformed in a fixed boundary one, allowing the computation of the propagation front as a new unknown that can be computed together with the mass concentrations of CO_2 in air and water. Apart from the stability and the consistency of the numerical solution, constructed by a finite difference scheme, qualitative properties of the numerical solution are established. In fact, positivity of the concentrations, increasing properties of the propagation front and monotone behavior of the solution are proved. We also confirm numerically the $\sqrt{t}$-law of propagation. Results are illustrated with numerical examples.

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1. Introduction

Environmental impact on concrete parts of buildings and civil engineering works such as bridges, sewage pipes and seawalls results in a variety of chemical and mechanical changes. The bulk of these changes leads to damaging and destabilization of the concrete itself or of the reinforcement embedded in the concrete. It is well known that in all carbonation scenarios, gaseous carbon dioxide is assumed to be supplied from an inexhaustible exterior source to the concrete sample, [1,2]. Carbon dioxide entering the non-saturated concrete sample through the air parts of the pores dissolves into the pore water and forms carbonic acid. This phenomenon, called concrete carbonation, may reduce the durability of reinforced concrete structures, causing the corrosion of the steel bars. The concrete carbonation level is measured throughout the CO_2 mass concentration in air and water phases in the concrete pores, that needs to be calculated. Gradually the process penetrates deeper into de concrete shaping a carbonation front that separates the carbonated zone from the uncarbonated one. A good understanding of the evolution of the carbonation process is crucial to predict the life service of concrete structures and save important amounts of money and energy.

Empirical evidences of the behavior of the carbonation front propagation have shown a dependence on time following the so-called $\sqrt{t}$-law, [3–10]. In the framework of moving-boundary problems, to our knowledge, Tuutti [11] in 1982, was the first appealing to the square root of t-law in the problem of concrete carbonation. Such conclusions were based on the Neumann solution of the two-phase Stefan problem, see Section 13.2.2 of [12].

In recent papers [1,13], the authors studied a one-dimensional free boundary problem modeling the carbonation process. The unknown CO_2 mass concentrations in air and water phases of pores are denoted by $U(t, x)$ and $V(t, x)$ respectively, depending on variables time t and space x. The space variable x is measured from the exposed boundary $x = 0$ to the

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unknown carbonation front $x = S(t)$. In the system (2)–(9) it is assumed that κ_1 and κ_2 are positive diffusion constants ($\kappa_1 \gg \kappa_2$) and the functions $f(U, V)$ and $\psi(r)$ are defined as

$$f(U, V) = \beta(\gamma V - U), \quad \beta > 0, \ \gamma > 0. \tag{1}$$

The continuous model is described by

$$\frac{\partial U}{\partial t} - \frac{\partial}{\partial x}\left(\kappa_1 \frac{\partial U}{\partial x}\right) = f(U, V), \quad 0 < t < T, \ 0 < x < S(t), \tag{2}$$

$$\frac{\partial V}{\partial t} - \frac{\partial}{\partial x}\left(\kappa_2 \frac{\partial V}{\partial x}\right) = -f(U, V), \quad 0 < t < T, \ 0 < x < S(t), \tag{3}$$

together with the left boundary conditions

$$U(t, 0) = G(t), \qquad V(t, 0) = H(t), \quad 0 \le t \le T. \tag{4}$$

The propagation front behavior comes out from the Stefan-like conditions, involving function $\psi(r)$ linked to the chemical reactions:

$$S'(t) = \psi(U(t, S(t))), \quad 0 < t < T, \tag{5}$$

$$-\kappa_1 \frac{\partial U}{\partial x}(t, S(t)) = \psi(U(t, S(t))) + S'(t)U(t, S(t)), \quad 0 < t < T, \tag{6}$$

$$-\kappa_2 \frac{\partial V}{\partial x}(t, S(t)) = S'(t)V(t, S(t)), \quad 0 < t < T. \tag{7}$$

Function $\psi(r)$ is given by

$$\psi(r) = \alpha|r|^p, \quad r \in \mathbb{R}, \ \alpha > 0, \ p \ge 1, \tag{8}$$

where p is the so called order of the chemical reaction.

The bounded initial conditions functions are described by

$$S(0) = S_0, \qquad U(0, x) = U_0(x), \qquad V(0, x) = V_0(x), \quad 0 < x < S_0. \tag{9}$$

Aiki and Muntean [1,13] show qualitative properties of the solutions $U(t, x)$ and $V(t, x)$ of (2)–(9) as positivity and boundedness for fairly well posed initial conditions. Furthermore, they also justify rigorously that the carbonation front $S(t)$ satisfies a long time behavior of the type $C_1\sqrt{t} \le S(t) \le C_2\sqrt{t}$, when the exposed boundary conditions are constant, $G(t) = G^*$, $H(t) = H^*$, and linked by the condition $G^* = \gamma H^*$. Numerical simulations of the solution of carbonation problems using the finite element method have been performed in [14,15].

As the exact solution of the model (2)–(9) is not available and the best model may be wasted with a bad numerical analysis, in this paper we provide conditionally stable positive numerical solutions, apart from preserving the qualitative properties of the theoretical solution.

In Section 2, after a front-fixing transformation approach, the original problem is transformed into another one where the moving boundary becomes a new unknown of the problem, allowing the possibility to compute the expanding front. We propose a coupled finite difference scheme whose unknowns are both CO_2 concentrations, in air and water phases of pores, as well as the square power values of the expanding front. In Section 3, stability and positivity of the numerical solution is treated. The monotone increase in time behavior of the expanding front is shown numerically. We also prove for a fixed time the CO_2 concentrations are spatially decreasing from the exposed front to the carbonation front. Section 4 deals with a numerical conformation of the $\sqrt{t}$-law assumption. Numerical experiments illustrating the shown properties are included in the corresponding sections. Consistency of the proposed numerical scheme with the PDE problem is addressed in Section 5.

2. Front-fixing transformation and discretization

Let us begin this section by transforming the moving boundary problem (2)–(9) into another one with fixed boundary conditions. The Landau transformation, [16,17], suggests the substitution

$$L(t) = S^2(t), \qquad z(t, x) = \frac{x}{\sqrt{L(t)}}, \quad 0 \le t \le T, \ 0 < x < \sqrt{L(t)}. \tag{10}$$

Using substitution (10), the problem (2)–(9) becomes

$$L(t)\frac{\partial W}{\partial t} - L'(t)\frac{z}{2}\frac{\partial W}{\partial z} - \kappa_1\frac{\partial^2 W}{\partial z^2} = L(t)\beta(\gamma Y - W), \quad 0 < t < T, \ 0 < z < 1, \tag{11}$$

$$L(t)\frac{\partial Y}{\partial t} - L'(t)\frac{z}{2}\frac{\partial Y}{\partial z} - \kappa_2\frac{\partial^2 Y}{\partial z^2} = -L(t)\beta(\gamma Y - W), \quad 0 < t < T, \ 0 < z < 1, \tag{12}$$