Numerical solution of nonlinear moving boundary problems for carbonation in reinforced concrete structures

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1 Concrete carbonation problem and Front-fixing transformation

This work deals with the construction, analysis and computation of a numerical method to solve a moving boundary coupled nonlinear system of parabolic equations, arising in concrete carbonation problems, see [1]. By means of a front-fixing transformation, the domain of the problem becomes fixed, and the position of the moving carbonation front has to be determined together with the mass concentrations of the involved chemical species. Qualitative properties like positivity and stability of the numerical solution are established.

The mass concentrations of the species are represented by the following variables, where time takes values in the interval $0 \leq t \leq T$,

$$\begin{aligned}
&\bar{U}_1(x,t) = [\mathrm{CO_2}(aq)],\ \ \bar{U}_2(x,t) = [\mathrm{CO_2}(g)],\ \ \bar{U}_5(x,t) = [\mathrm{H_2O}], && 0 \leq x \leq S(t),\\
&\bar{U}_3(x,t) = [\mathrm{Ca(OH)_2}(aq)],\ \ \bar{U}_6(x,t) = [\mathrm{H_2O}], && S(t) \leq x \leq L,\\
&\bar{U}_4(t) = [\mathrm{CaCO_3}(aq)], && (1)
\end{aligned}$$

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where $T > 0$ is the time horizon.

Let us consider the suitable transformation of variables:

$$\hat{U}_i(x,t) = \phi\phi_\omega \bar{U}_i(x,t), \quad i \in \{1,3\}, \tag{2}$$

$$\hat{U}_2(x,t) = \phi\phi_a \bar{U}_2(x,t), \quad \hat{U}_4(t) = \phi\phi_\omega \bar{U}_4(t), \tag{3}$$

$$\hat{U}_i(x,t) = \phi \bar{U}_i(x,t), \quad i \in \{5,6\}, \tag{4}$$

where porosity of concrete is given by the parameter ϕ, while air and water fractions in pores are denoted by ϕ_a and ϕ_ω, respectively.

Under the new variables $\hat{U}_i(x,t)$, $i \in \{1,2,3,5,6\}$, $\hat{U}_4(t)$ and using Kronecker's symbol δ_{ij}, the continuous model proposed in [1, 2] is described by a coupled system of five partial differential equations (PDE) and one ordinary differential equation (ODE); together with the initial, boundary and transmission conditions and the velocity law of the moving front:

$$\begin{aligned}&(\delta_{1i} + \delta_{2i} + \delta_{5i})\frac{\partial \hat{U}_i}{\partial t} - D_i \frac{\partial^2 \hat{U}_i}{\partial x^2} = (1-\delta_{5i})(-1)^i P_i(\hat{U}_1 - Q_i \hat{U}_2),\\ &0 \le x < S(t), \quad 0 < t < T, \quad i \in \{1,2,5\},\end{aligned} \tag{5}$$

$$\frac{\partial \hat{U}_i}{\partial t} - D_i \frac{\partial^2 \hat{U}_i}{\partial x^2} = \delta_{3i}(-S_{3,\text{diss}}(\hat{U}_3 - U_{3,\text{eq}})), \quad S(t) < x \le L, \quad 0 < t < T, \quad i \in \{3,6\}, \tag{6}$$

$$\frac{d\hat{U}_4}{dt} = \kappa(\phi\phi_\omega)^{1-p-q}[(\hat{U}_1)^p(\hat{U}_3)^q]_{\Gamma(t)}, \quad 0 < t < T. \tag{7}$$

The transformed initial conditions become $S(0) = S_0 > 0$ and

$$\begin{aligned}&\hat{U}_1(x,0) = \hat{U}_{10}(x) = \phi\phi_\omega \bar{U}_{10}(x), \quad \hat{U}_2(x,0) = \hat{U}_{20}(x) = \phi\phi_a \bar{U}_{20}(x),\\ &\hat{U}_5(x,0) = \hat{U}_{50}(x) = \phi \bar{U}_{50}(x), \; 0 < x < S_0,\end{aligned} \tag{8}$$

$$\hat{U}_4(0) = \hat{U}_{40} = \phi\phi_\omega \bar{U}_{40}, \tag{9}$$

$$\hat{U}_3(x,0) = \hat{U}_{30}(x) = \phi\phi_\omega \bar{U}_{30}(x), \ \ \hat{U}_6(x,0) = \hat{U}_{60}(x) = \phi\bar{U}_{60}(x), \ \ S_0 < x < L, \tag{10}$$

and the transformed boundary conditions are

$$\hat{U}_i(0,t) = \Lambda_i(t), \ \ 0 < t < T, \ \ i \in \{1,2,5\}, \tag{11}$$

$$\frac{\partial \hat{U}_i}{\partial x}(L,t) = 0, \ \ 0 < t < T, \ \ i \in \{3,6\}. \tag{12}$$

Finally, the transformed interface conditions for $x = S(t)$, $0 < t < T$, become

$$-\left[D_i \frac{\partial \hat{U}_i}{\partial x}\right]_{\Gamma(t)} = (\delta_{5i} - \delta_{1i})(\phi\phi_\omega)^{-p-q}\eta_\Gamma(\hat{U}_1, \hat{U}_3) + S'(t)[\hat{U}_i]_{\Gamma(t)}, \ \ i \in \{1,2,5\}, \tag{13}$$

$$\left[D_i \frac{\partial \hat{U}_i}{\partial x}\right]_{\Gamma(t)} = -(\delta_{3i})(\phi\phi_\omega)^{-p-q}\eta_\Gamma(\hat{U}_1, \hat{U}_3) + S'(t)[\hat{U}_i]_{\Gamma(t)}, \ \ i \in \{3,6\}, \tag{14}$$

and the velocity law is

$$S'(t) = \alpha\kappa(\phi\phi_\omega)^{1-p-q}[(\hat{U}_1)^p(\hat{U}_3)^{q-1}]_{\Gamma(t)}. \tag{15}$$

For the sake of simplicity, and taking advance of the fact that $(S^2(t))' = 2S(t)S'(t)$, in the following we will consider as unknown the square of the free boundary $R(t)$ instead of the free boundary itself $S(t)$ in order to obtain a more simplified PDE system, i.e. $R(t) = S^2(t)$.

In order to transform the PDE problem with moving domain into a fixed domain one, let us consider the following change of spatial variable inspired by the well known Landau transformation:

$$z(x,t) = \begin{cases} \left(x/\sqrt{R(t)}\right) - 1, & 0 \le x < \sqrt{R(t)}, \ \ 0 \le t \le T, \\ 0, & x = \sqrt{R(t)}, \ \ 0 \le t \le T, \\ \left(x - \sqrt{R(t)}\right)/\left(L - \sqrt{R(t)}\right), & \sqrt{R(t)} < x \le L, \ \ 0 \le t \le T. \end{cases} \tag{16}$$

2 Positive and stable numerical scheme

In this section we construct a finite difference scheme for solving numerically the coupled system after applying Landau front-fixing transformation. Let M and N be positive integers, so that the domain $[-1,1]\times[0,T]$ is partitioned in $(2M+1)\times(N+1)$ mesh points denoted by (z_j,t^n), where $z_j = jh$, $-M \le j \le M$ and $t^n = nk$, $0 \le n \le N$. Here the step sizes discretizations h and k verify $hM = 1$ and $kN = T$, respectively. Numerical approximations of the involved variables are denoted by $u^n_{i,j} \approx U_i(z_j,t^n)$, $i \in \{1,2,3,5,6\}$, $u^n_4 \approx U_4(t^n)$, $r^n \approx R(t^n)$, while we denote $\lambda^n_i = \Lambda_i(t^n)$, $i \in \{1,2,5\}$.

Partial derivatives at the interior points are approximated using forward in time and centered in space finite difference expressions. With respect to the discretization of the first derivatives of the transformed transmission conditions at the carbonation front $z=0$, we use one side second order finite difference approximations.

The solutions at the interior points at time level $n+1$ are given by:

$$\begin{aligned} u^{n+1}_{i,j} &= a^n_{i,j}u^n_{i,j-1} + b^n_{i,j}u^n_{i,j} + c^n_{i,j}u^n_{i,j+1} + \delta_{1i}kP_1Q_1u^n_{2,j} + \delta_{2i}kP_2u^n_{1,j}, \\ &-M+1 \le j \le -1,\ \ 0 \le n \le N-1,\ \ i \in \{1,2,5\}, \end{aligned} \tag{17}$$

$$\begin{aligned} u^{n+1}_{i,j} &= a^n_{i,j}u^n_{i,j-1} + b^n_{i,j}u^n_{i,j} + c^n_{i,j}u^n_{i,j+1} + \delta_{3i}kS_{3,\text{diss}}u^n_{3,\text{eq}}, \\ &1 \le j \le M,\ \ 0 \le n \le N-1,\ \ i \in \{3,6\}, \end{aligned} \tag{18}$$

where

$$a^n_{i,j} = \begin{cases} \frac{D_ik}{h^2r^n} - \frac{1+z_j}{4h}\Delta^n_1, & i \in \{1,2,5\}, \\ \frac{D_ik}{h^2\Delta^n_3} + \frac{z_j-1}{4h}r^n\frac{\Delta^n_1\Delta^n_2}{\Delta^n_3}, & i \in \{3,6\}, \end{cases} \tag{19}$$

$$b^n_{i,j} = \begin{cases} 1 - \frac{2D_ik}{h^2r^n} - \delta_{1i}kP_1 - \delta_{2i}kP_2Q_2, & i \in \{1,2,5\}, \\ 1 - \frac{2D_ik}{h^2\Delta^n_3} - \delta_{3i}kS_{3,\text{diss}}, & i \in \{3,6\}, \end{cases} \tag{20}$$

$$c^n_{i,j} = \begin{cases} \frac{D_ik}{h^2r^n} + \frac{1+z_j}{4h}\Delta^n_1, & i \in \{1,2,5\}, \\ \frac{D_ik}{h^2\Delta^n_3} + \frac{1-z_j}{4h}r^n\frac{\Delta^n_1\Delta^n_2}{\Delta^n_3}, & i \in \{3,6\}, \end{cases} \tag{21}$$

and

$$\Delta^n_1 = \frac{r^{n+1}}{r^n} - 1,\ \ \Delta^n_2 = \frac{L}{\sqrt{r^n}} - 1,\ \ \Delta^n_3 = \left(L - \sqrt{r^n}\right)^2,\ \ 0 \le n \le N-1. \tag{22}$$

Finally, the concentration of $CaCO_3$(aq) in the carbonation front at the step $n+1$ is given by

$$u_4^{n+1} = u_4^n + k\kappa(\phi\phi_\omega)^{1-p-q}(u_{1,0}^n)^p(u_{3,0}^n)^q, \quad 0 \leq n \leq N-1. \tag{23}$$

We assume the hypothesis:

$$Q_1\tilde{G}_2 \leq \tilde{G}_1, \;\; \tilde{G}_1 \leq Q_2\tilde{G}_2, \tag{24}$$

where $\tilde{G}_1$ is the upper bound of [CO_2(aq)] and $\tilde{G}_2$ is the upper bound of [CO_2(g)], for both at the exposed boundary and in the carbonated zone at the initial time, together with the condition on the equilibrium concentration of $Ca(OH)_2$(aq):

$$u_{3,\mathrm{eq}}^n \leq \tilde{G}_3. \tag{25}$$

We also assume the existence of an upper bound $\tilde{G}_5$ for the water content for both at the exposed boundary and in the carbonated region at the initial time, and that [$Ca(OH)_2$(aq)] and water content are upper-bounded by $\tilde{G}_3$ and $\tilde{G}_6$, respectively, at the initial time, see [2], Section 3, pp. 239-240.

Taking small enough values of h and imposing the following condition on the temporal step size

$$k < k_0 = \min\{k_i\}, \;\; 1 \leq i \leq 6, \;\; i \neq 4, \tag{26}$$

where

$$k_1 \leq \frac{h^2r^0}{2D_1 + h^2r^0P_1}, \quad k_2 \leq \frac{h^2r^0}{2D_2 + h^2r^0P_2Q_2}, \quad k_5 \leq \frac{h^2r^0}{2D_5}, \quad i \in \{1,2,5\}, \tag{27}$$

$$k_3 \leq \frac{h^2L^2(1-\beta)^2}{2D_3 + h^2L^2(1-\beta)^2S_{3,\mathrm{diss}}}, \quad k_6 \leq \frac{h^2L^2(1-\beta)^2}{2D_6}, \quad i \in \{3,6\}, \tag{28}$$

the following theorem shows that the numerical solution obtained from the scheme (17)-(18) and (23), preserves the qualitative properties of the theoretical solution obtained in Section 3 of [2]:

Theorem 1. *Under hypotheses (24)-(25), for small enough values of the step size h together with the condition (26), the following conclusions hold true:*

i) Concentration solutions $u_{i,j}^n$*,* $i \in \{1, 2, 5\}$ *of the scheme (17) in the carbonated zone, concentration solutions* $u_{i,j}^n$*,* $i \in \{3, 6\}$ *of the scheme (18) in the uncarbonated region, and concentrations* $u_{i,0}^n$*,* $1 \leq i \leq 6$*,* $i \neq 4$*, at the carbonation front are positive and uniformly bounded for* $0 \leq n \leq N$*.*

ii) The solution u_4^n *of the scheme (23) for the calcium carbonate concentration is positive, increasing and bounded, for* $0 \leq n \leq N$*.*

iii) The carbonation front is positive and increasing, $0 < r^0 < r^1 < \ldots < r^N$*.*

As a consequence of the boundedness of the mass concentrations, scheme (17)-(23) is $\|\cdot\|_\infty$-stable under assumptions (24)-(25), for small enough values of h and conditions (26).

References

[1] A. Muntean, M. Böhm, J. Kropp, "Moving carbonation fronts in concrete: A moving-sharp-interface approach", *Chemical Engineering Science*, 66 (2011), no. 3, 538-547.

[2] A. Muntean, M. Böhm,"A moving-boundary problem for concrete carbonation: Global existence and uniqueness of weak solutions", *Journal of Mathematical Analysis and Applications*, 350 (2009), 234-251.