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Numerical simulation of chloride transport in concrete

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Penetration of chlorides into concrete causes various types of degradation and it affects durability of concrete. Extraction of chlorides from concrete can be significantly accelerated with the help of electric field. Such extraction is nondestructive and it is relatively very fast.

It is assumed in this work that concrete pores are fully filled with water which is a common case of many structures in wet or sea areas. In saturated pores, the ionic transport is driven by two main driving forces, the concentration gradient and the electromotive force acting on charged ions. The two forces can be considered in the ionic flux which then composes of the diffusion term (Fick's law) and the electrical migration term (Nernst-Planck equation) as

$$\boldsymbol{j} = -D\varrho\nabla c - \frac{DFz\varrho c}{RT}\nabla\phi,\tag{1}$$

where $D \,[\text{m}^2/\text{s}]$ is the diffusion coefficient, F = 96,487 C/mol is the Faraday constant, z is the valence of ions, $\rho \,[\text{kg/m}^3]$ is the total density of concrete, R = 8.314 J/K/mol is the molar gas constant, $T \,[\text{K}]$ is the temperature, $\phi \,[\text{V}]$ is the electric potential. The diffusion coefficient, D, is a function of many variables (concrete type, age, porosity, aggregate size, temperature, humidity and chloride concentration). However, it is assumed to be constant in this work for simplicity. On the other hand, an effect of chloride binding is taken into account. The amount of chlorides in concrete can be decomposed to two parts, the free chlorides (with concentration c_f) that can be transported and bound chlorides (with concentration c_b) that are chemically or physically bound to the concrete pore walls [1, 3]. The two concentrations must satisfy the condition $c = c_b + c_f$. The ratio between the free and bound chlorides is described by a binding isotherm [1–3]. The Freundlich binding isotherm is assumed in this work in the form $c_b = \alpha c_f^{\beta}$, where α and β are experimentally obtained constants. Then, the mass balance equation can be written for free chloride concentration in the form

$$\frac{\partial c_f}{\partial t} \left(1 + \frac{\mathrm{d}c_b}{\mathrm{d}c_f} \right) = \mathrm{div} \left(D\nabla c_f + \frac{DFzc_f}{RT} \nabla \phi - c_f \boldsymbol{v} \right).$$
(2)

The externally applied electric field during accelerated extraction of chloride is taken into account by using the Gauss law of electrostatics as

$$\operatorname{div}(\varepsilon_r \varepsilon_0 \boldsymbol{E}) = -\Delta(\varepsilon_r \varepsilon_0 \phi) = \sigma, \tag{3}$$

where E is the intensity of the electric field, ϕ [V] is the electric potential, σ [C/m³] is the density of charge that is zero for our case, ε_r [–] is the relative permittivity and $\varepsilon_0 = 8.854 \times 10^{-12}$ F/m is the permittivity of the vacuum. The mass balance equation must be complemented with a set of boundary conditions in the form of, e.g., Dirichlet conditions (prescribed concentrations at the boundary, $c_D(\boldsymbol{x},t)$) or Neumann condition of the boundary flux, $j_N(\boldsymbol{x},t)$, and initial condition (prescribed concentrations, $c_0(\boldsymbol{x},t=0)$). A finite element approximation using the Galerkin-Petrov approach was applied to Eq. (2), which leads to the assemblage of a non-symmetric system of ordinary differential equations in the form

$$C\frac{\mathrm{d}\boldsymbol{c}}{\mathrm{d}t} + (\boldsymbol{K} - \boldsymbol{H})\boldsymbol{c} = \boldsymbol{f},\tag{4}$$

where C is the capacity matrix, K is the diffusivity matrix, H is the conductivity matrix and f is the right hand side vector corresponding to the ion flux density normal to the boundary, $j_N(x, t)$.

Fig. 1 shows typical graphs of chloride penetration into concrete due to diffusion and chloride extraction accelerated by an electric field. While the penetration lasts several years, the extraction takes usually only few days.



Fig. 1. (a) Concentration after 10 years of pure diffusion, (b) concentration after 2 days of extraction

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References

- Florea, M.V.A., Brouwers, H.J.H., Chloride binding related to hydration products: Part I: Ordinary Portland Cement, Cement and Concrete Research 42 (2) (2012) 282-290.
- [2] Tang, L., Nilsson, L.O., Chloride binding capacity and binding isotherms of OPC pastes and mortars, Cement and Concrete Research 23 (2) (1993) 247-253.
- [3] Thomas, M.D.A., Hooton, R.D., Scott, A., Zibara, H., The effect of supplementary cementitious materials on chloride binding in hardened cement paste, Cement and Concrete Research 42 (1) (2012) 1-7.