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The influence of chemical activity on transport of ions in cementitious materials of real microstructure

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Thermodynamic characteristics of pore solution influence behavior of porous materials. In case of cement-based materials electrolytic solutions present in pores can be highly concentrated. The activity of ions contained in the pores affects their diffusion inside the material and, consequently, may influence the kinetics of degradation of reinforcement concrete. Many models have been proposed to calculate the activity of ions. In this paper we investigated extended Debye-Hückel, Davies, Truesdell-Jones, Pitzer and MacInnes activity models. We show how the activity obtained from different models influences ion transport in porous concrete material.

A 3D model has been considered to calculate distribution of ions concentration and electric potential in concrete. Four ions, major components of pore solution were considered: Na^+, Cl^-, K^+ and OH^-. The Nernst–Planck–Poisson (NPP) system of equations was used to compute ion fluxes in porous materials in space and time. COMSOL Multiphysics software was used to solve the NPP problem in 3D geometry of a real concrete sample, which has been obtained from X-ray computed tomography. Exemplary results of simulations are shown in Figures 1 and 2. Figures suggest that impact on concentration may be non-negligible when activity is taken into account.

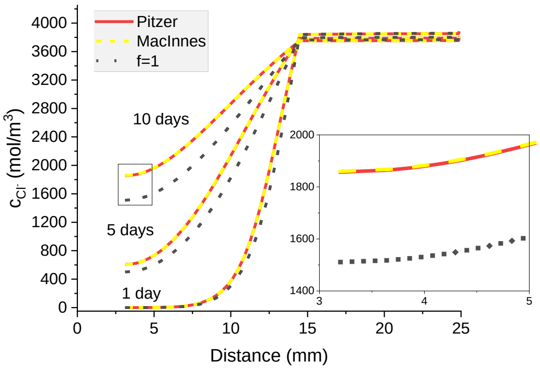

Fig. 1. Calculated concentration distribution of Cl^- in the cement sample after 1200 h of immersion in 20% NaCl water solution assuming Pitzer and MacInnes models compared with ideal solution approximation ($f = 1$).

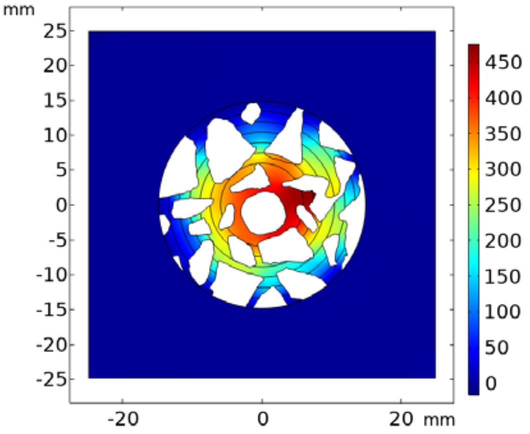

Fig. 2. Difference of chloride concentration (mol/m^3) obtained by Pitzer activity model and ideal solution approximation ($f = 1$) in the concrete sample (3D model) after 1200 h of immersion in 20% NaCl water solution (2D cross-section). White areas correspond to basalt grains.

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