Multiscale modelling of chloride ingress in cementitious materials

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Objectives:
This research focuses on modelling the surface interactions between cement hydrates, ionic species and the influence of the microstructure of cement on the transport in order to quantify their effects on the diffusivity of chloride ions.

Chloride Transport

Durability of blended concrete is important to design new cementitious materials with smaller carbon footprints. Chloride ingress is one of the most common durability problems for reinforced concrete, and the relation between ionic transport and microstructure provides many challenges.

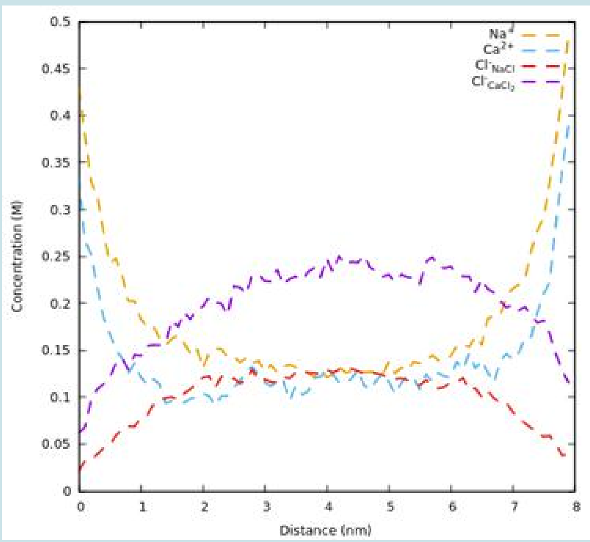
How is Chloride Transport Modelled?

Performing bulk diffusion tests, which reproduce conditions in sea-submerged areas, represents the standard way to characterize and quantify chloride ingress. This experiment consists in leaving mortar or concrete in a known NaCl solution for a period of time.

After drilling, powder grinding, and titrating chloride, a profile of total chloride content can be plotted as a function of depths. The data can be fitted to a diffusion equation, such as the macroscopic Fick's law of diffusion, the apparent diffusion coefficient can be back-calculated.

Nanoscopic modelling of chloride diffusion in cement paste

Hydrates form over time, modifying the microstructure of cement paste. These changes equally affect transport properties which are microstructure dependent, which in turn are a function of w/c ratio. The pore solution content also greatly influences chloride diffusion. To model this, a method based on the coupling of the Grand Canonical Monte Carlo and the Widom algorithm has been implemented. It simulates the Electrical Double Layers that form in gel pores (< 10nm) due to the surface effects dominating the porous C-S-H network.



Distribution of ions in NaCl and $CaCl_2$ solutions at 0.1M in a pore of 8nm diameter

For further information please refer to the following link: https://www.erica-etn.eu/
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