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.

Transport in cement

Concrete is a living material. Hydrates still form through time and the microstructure of cement paste never stops evolving. This also applies to the transport properties that are microstructure-dependent. Quantitatively, ionic effective diffusivity is a function of porosity, pore size distribution, and pore classes which are a function of hydration degree, initial particle size, etc.

Research has shown that pore solution content also has an effect on chloride transport. This is due to three main phenomena: the electroneutrality conservation, the non-ideality of the solution, and the surface effects. On a nanoscopic scale, surface effects in gel pores (<10 nm) dominate through the forming of the 'Electrical Double Layers' on the charged C-S-H surfaces.