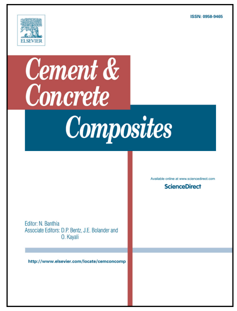

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Pore-scale modeling of chloride ion diffusion in cement microstructures

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Abstract

Understanding the mechanism of chloride ion diffusion in cement is significant to improve the reliability of offshore reinforced concrete structures. The chloride ionic diffusivity in cement-based microstructures is predicted by pore-scale modeling using a modified lattice Boltzmann method. Both the Nernst-Planck equation for ion diffusion and the Poisson equation for electrodynamic effect are fully solved. The predicted effective diffusivities in cement-based microstructures with different porosities are in good agreements with the experiment data. The results show that the pore size distribution and Zeta potential of cement-based microstructures directly influence the effective diffusivities of chloride ions. The cement-based microstructure with smaller pore size and higher negative Zeta potential hinders chloride ions corrosion more effectively. The electrokinetic effect on the chloride ionic transport is negligible when the ratio of the maximum-probability pore size and the Debye length is higher than 32 in the cement-based microstructure. For engineering applications, we provide a predictive and easy-to-use formula by up-scaling to correlate the effective chloride ion diffusivity with electrokinetic effect in cement paste.

***Keywords*:** chloride ion diffusion, cement microstructure, electrokinetic effect, lattice Boltzmann method

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