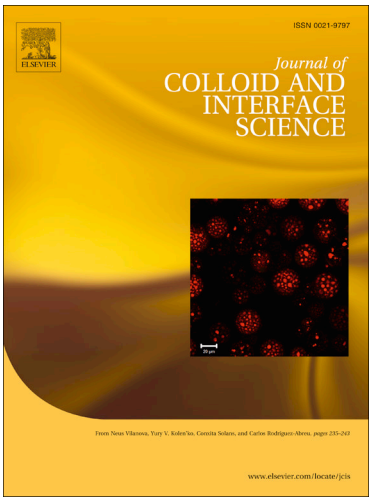

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Atomic-Scale Investigation of Physical Adsorption of Water Molecules and Aggressive Ions to Ettringite's Surfaces

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Abstract

The strength and durability of cementitious composite materials are adversely affected by the ingress of water and aggressive ions into their intrinsic meso- and nano-pore spaces. Among various phases of hydrated cement paste (HCP), the aluminum-rich phases play a critical role in controlling the diffusivity of aqueous solutions containing aggressive ions. To this date, however, there has been no systematic study to understand the adsorption mechanisms and chloride binding capacity of aluminum-rich phases of HCP. This research gap has been the motivation of the current study to investigate the physical adsorption characteristics of ettringite as the main aluminum-rich phase of HCP and the primary hydrated product of calcium solfualuminate cement. Through a set of Molecular Dynamics simulations supported by macro-scale experimental tests, a fundamental insight on the molecular origins of the diffusion of water molecules, as well as sodium and chloride ions, in contact with ettringite is provided. As the primary objective of this study is to evaluate the transport properties at and near the solution/solid interfaces, the molecular mechanisms of adsorption are characterized for inner- and outer-sphere distances from the solid substrate. With an in-depth understanding of the structure and dynamics of water molecules and aggressive ions in contact with ettringite's surfaces, the outcome of this study provides reliable measures of physical adsorption, binding capacity, and self-diffusion coefficient, which can be further employed to introduce strategies to avoid the degradation of a wide variety of cementitious materials exposed to harsh environmental conditions.

Keywords: Cementitious Composite Materials; Ettringite; Chloride Binding Isotherms; Water Mobility; Diffusion Coefficients; Molecular Dynamics Method