

## Early Stage Hydration of Wollastonite: Kinetic Aspects of the Metal-Proton Exchange Reaction

**Authors :** Nicolas Giraud, Peter Thissen

**Abstract :** In this paper we bring up new aspects of the metal proton exchange reaction (MPER, also called early stage hydration): (1) its dependence of the number of protons consumed by the preferential exchanged cations on the pH value applied at the water/wollastonite interface and (2) strong anisotropic characteristics detected in atomic force microscopy (AFM) and low energy ion scattering spectroscopy measurements (LEIS). First we apply density functional theory (DFT) calculations to compare the kinetics of the reaction on different wollastonite surfaces, and combine it with ab initio thermodynamics to set up a model describing (1) the release of Ca in exchange with H coming from the water/wollastonite interface, (2) the dependence of the MPER on the chemical potential of protons. In the second part of the paper we carried out in-situ AFM and inductive coupled plasma atomic emission spectroscopy (ICP-OES) measurements in order to evaluate the predicted values. While a good agreement is found in the basic and neutral regime (pH values from 14-4), an increasing mismatch appears in the acidic regime (pH value lower 4). This is finally explained by non-equilibrium etching, dominating over the MPER in the very acidic regime.

**Keywords :** anisotropy, calcium silicate, cement, density functional theory, hydration

**Conference Title :** ICCCC 2015 : International Conference on Cement and Concrete Chemistry

**Conference Location :** Istanbul, Türkiye

**Conference Dates :** October 26-27, 2015