Dynamics of Water and Ions in Hydrates

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Objectives:
This research is conducted to characterise the morphology of cement paste by understanding the behavior of water transport carrying ions through Nuclear Magnetic Resonance (NMR) relaxometry.

Water In Hydrates

Cement hydration involves transport of water and ions at nanoscale. Water can act as a vehicle to transport aggressive ions, leading to concrete deterioration. Therefore, water transport behavior related to ions must be understood at nanoscale stage to predict the effect on the structure of hydrated cement.

Predicting Water Transport

The transport of water-ions in cement is predicted by interpreting the NMR relaxation rate obtained through experiment. To interpret NMR experimental results, a novel theoretical model is established by combining NMR theory and molecular dynamic (MD) simulations.

Molecular Dynamics

Molecular dynamics (MD) are used to test the validity of physics within a theoretical model. Many behavioral properties related to water-ions can be explored through MD simulation including diffusion coefficient, radial density function, desorption time constant, and angle distribution.

What are the ions of interest?

This work focuses on Fe^{3+} and Ca^{2+} ions. Fe^{3+} is an important ion in cement, thus it is the major interest in this project. Attention is also made on Ca^{2+} because the hydration of calcium ions

A new rotational diffusion model has been developed and validated through MD simulations. This model improves the fundamental understanding of the dynamics of aqueous ion complexes leading to an enhanced description of the dipolar interaction between a paramagnetic ion and the ^{1}H spins of water that surrounds it. These results significantly improve the interpretation of experimental results from the NMR relaxometry of cement paste.

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