



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 NMR relaxometry.

Water in hydrates

Cement hydration involves transport of water and ions at nanoscale. Water can act 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 the NMR experimental results, a novel theoretical model is established through combining NMR theory and molecular dynamic (MD) simulations.

Molecular dynamics

Molecular dynamics 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?

Fe^{3+} is the primary paramagnetic ion in cement, thus it is the major interest in this project. There is also curiosity in Ca^{2+} as the hydration of calcium ions slows the rate of water diffusion.

MD simulations and model parametrisation are being carried out for the mentioned ions so that the NMR signals can be interpreted to describe the water behavior in cementitious materials.

