Lattice Boltzmann Modelling of Water and Transport in Hydrate Agglomerates

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Objectives:
In this project, multiphase and multiscale lattice Boltzmann techniques are used to model C-S-H hydrate structures experiencing repetitive sorption and desorption cycles.

Why Lattice Boltzmann (LB)?

To understand the flow of fluid on a microstructural level, modelling with LB is applied. LB allows us to understand the interaction of solid hydrate structures in a single or multiphase fluid (liquid and/or vapour). It can also model arbitrary shapes and complex boundaries, such as those found in a porous hydrate cement structure.

How does Lattice Boltzmann work?

The LB method is based on a network of equidistantly spaced lattice nodes. Each node is assigned a solid, fluid or vapour phase. With time, interactions between each node and its neighbours are tracked based on a two-step process of streaming and collision to achieve equilibrium in the form of a relaxed microstructure.

Modelling the Microstructure

A sheet growth algorithm is created to randomly develop linked C-S-H hydrate sheets to fill the modelling area.
The model will be analysed once the structure is saturated with fluid, dried, relaxed and resaturated using LB approaches. The effects on capillary action and hydrate movement will be compared to experiments.

How does the relaxation of hydrates affect microstructure?

The pore size distribution of cementitious materials is dynamic in nature and critical to understand fluid transport. Research has shown that irreversible changes occur during the first sorption cycle, where large pores are created at the expense of smaller pores after relaxation of the structure.

This work focuses on modelling the behavior of cement during the first and subsequent de/sorption cycles and understanding resulting microstructural changes.