Lattice Boltzmann Modelling of Water and Transport in Hydrate Agglomerates

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Objectives:
In this project, multiphase and multiscale lattice Boltzmann (LB) techniques are used to model microstructural changes in C-S-H hydrate structures experiencing sorption cycles.

Why lattice Boltzmann ?

LB modelling is a useful to understand the flow of fluid on a microstructural level. LB allows 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 structures.

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. Interactions between each node and its neighbours are tracked as a function of time, based on a two-step process of streaming and collision to achieve equilibrium in the form of a relaxed microstructure.

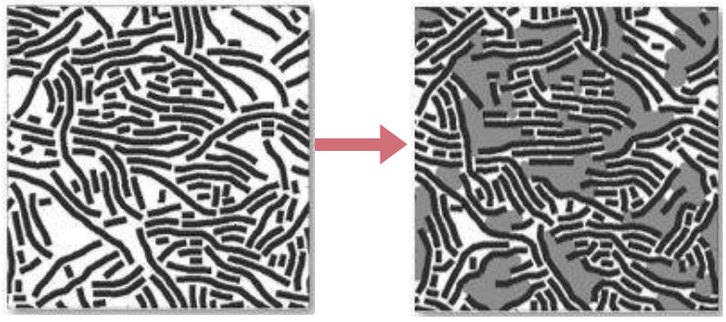
Modelling the Microstructure

Two distinct growth algorithms are developed, replicating quasi-continuous sheet and colloidal C-S-H hydrate structures, filling up the modelling space. The microstructure is analysed once the structure is saturated with fluid, dried, relaxed and resaturated using LB approaches over single or multiple sorption cycles.

How does hydrate relaxation affect the microstructure?

Capillary forces play a significant role in modifying the structure of cement hydrates. The pore size distribution of cementitious materials is a dynamic product of capillary forces. These forces drive gel porosity to a bimodal distribution during desorption, with a larger volume of small 'layer-like' pores and 'interhydrate-like' pores.

The matrix controlled water transport parameters of intrinsic permeability and capillary diffusivity, are observed as a function of time during a sorption cycle. Results are structure and time-dependent, following changes in liquid content. Results strongly mirror each other throught the cycle and broadly support findings of recent spatially and temporally resolved NMR experimental sorption analysis[1].



Quasi-continuous sheet microstructures at full and partial saturation

[1] P.J.McDonald et al., CCR, 133 (2020)

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