Lattice Boltzmann Modelling of Water Transport in Hydrates Agglomerates

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BACKGROUND
It is well known that sorption hysteresis and first cycle irreversibility exists for cement materials. Experiments show that cement microstructure is dynamic both during and after de/sorption. The Lattice Boltzmann (LB) method is a robust technique to simulate fluid (liquid and vapour) transport in porous materials. This project aims to simulate drying and wetting of model hydrate microstructures through repetitive de/sorption cycles using LB.

METHOD
LB is a partial differential solver method optimised for fluid dynamics. Fluid packets at lattice nodes are repeatedly moved to neighbouring nodes (streaming step) where they relax towards a local equilibrium (collision step), as shown in Figure 1.

An equilibrium function $f_i^\text{eq}$ determines the physics. The function $f_i^\text{eq} = \omega_i \rho \left( 1 + \frac{\mathbf{e}_i \cdot \mathbf{u}}{c_s^2} + \frac{(\mathbf{e}_i \cdot \mathbf{u})^2}{2c_s^2} - \frac{\mathbf{u} \cdot \mathbf{u}}{2c_s^2} \right)$ yields Navier-Stokes equations of fluid dynamics.

- $\omega_i$: Weight factor along direction $i$
- $\mathbf{e}_i$: Lattice velocity vector along direction $i$
- $\rho$: Fluid density
- $c_s^2$: Lattice speed of sound
- $\mathbf{u}$: Macroscopic fluid velocity

- An additional fluid-fluid pressure term within $f_i^\text{eq}$ forces and controls liquid-vapour separation [1].
- A bounce-back rule and fluid-solid term [1] determine the equilibrium contact angle at a solid interface.
- In this work, the fluid capillary pressure is calculated and used to move colloidal particles [2].

CONCLUSIONS AND OUTLOOK
This work provides initial validation of LB methods needed to study the microstructural rearrangement of cement gel during sorption cycles. Future work will compare de/sorption in simulated versions of Jennings colloidal and Feldman & Sereda quasi-continuous sheet structures, whilst introducing effects of solid swelling and mechanical distortion.

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REFERENCES

Figure 1: A Lattice Boltzmann calculation cycle. (a) Fluid located at a lattice node, (b) streams to neighbour nodes and (c) relaxes (collides)

Figure 2: Excess pressure ($\Delta P$) in a liquid drop is inversely proportional to the drop radius ($r$), defined by the Laplace equation

Figure 3: Control of contact angle by varying solid density ($\mu \text{L/u}^2$) at values of 100, 200, 300 and 500, from left to right

Figure 4: Fluid rise in a capillary tube at time steps of 0, 5k, 10k and 15k LB cycles, from left to right

Figure 5: A fluid drop is placed between two wetting particles. Left to right shows capillary forces re-equilibrating the system at time steps of 50, 5k, 10k and 15k LB cycles

Figure 6: Drying of a simple colloidal solution with ten particles at time steps of 0, 4k, 8k and 11.5k LB cycles, from left to right