

Pore-scale chemo-mechanical modelling of dissolution processes in cement paste

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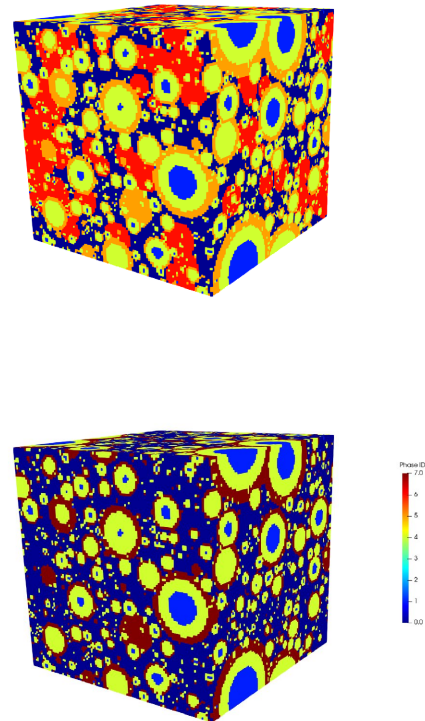
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Cement is one of the key materials to be used in deep geological radioactive waste repositories, both as waste matrix, technical barrier and as a structural component. Therefore, understanding its long-term chemo-mechanical stability, as it evolves due to geochemical reactions which cause changes in the pore structure itself, is essential. Tracking the dissolution of the portlandite (CH) and calcium silicate hydrates (C-S-H) phases through the leaching of Ca^{+} ions provides an insight into the effects of leaching processes on the mechanical properties.

A pore-scale reactive transport Lattice Boltzmann (LB) approach is applied to the Ca^{+} leaching, considering the kinetics of the CH and C-S-H dissolution. The LB model solves in 3D the advection-diffusion equation along with surface dissolution reactions, by tracking the dissolution and transport of Ca^{+} from CH and C-S-H in the pore water. The resulting model is additionally compared to a random sampling dissolution approach [1]. The computational domain is a 3D pore-scale microstructure generated by HYMOSTRUC3D, based on Ordinary Portland Cement (OPC).

Both approaches provide a timeline of the total Ca^{+} leached which is used to estimate the elasticity modulus and Poisson's ratio through a numerical [2] and an analytical [3] homogenization approach. Results are compared with the trends of other numerical and experimental results.

Figure 1: 3D microstructure showing the gradual dissolution as computed by the LB approach (left) initial state, (right) after 50% of CH and C-S-H nodes on the system have dissolved. Colors correspond to the different mineral phases which are considered as follows: 0: water filled micropore; 1: Unhydrated clinkers; 4: High density C-S-H; 5: Low density C-S-H; 6: CH; 7: Silica gel



1. Kamali-Bernard, S., et al. *Hydrate dissolution influence on the Young's modulus of cement pastes*. in *Proc. Fracture Mechanics of Concrete Structures (FraMCoS-V)*. 2004. Vail: Routledge.
2. Hain, M. and P. Wriggers, *Numerical homogenization of hardened cement paste*. Computational Mechanics, 2008. **42**(2): p. 197-212.
3. Shen, W.Q., et al., *A microstructure-based constitutive model for cement paste with chemical leaching effect*. Mechanics of Materials, 2020. **150**: p.