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Image analysis, microstructure generation and effective property estimation of cement-based materials used as radioactive waste confinement barriers

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Transport through cement-based materials depends strongly on their3D microstructure. To evaluate transport and related processes at time and spatial scales beyond experimental data, and to gain in depth understanding of the critical role of the microstructure, numerical simulations are necessary. This, however, requires an accurate description of the 3D microstructures involved. However, for cement paste, 3D imaging techniques such as μCT do not have sufficient resolution to appropriately describe the microstructure. We therefore present a new 3D-multiphase stochastic reconstruction methodology based on simulated annealing. Our methodology uses a single or set of 2D SEM images to calculate different 2D structural descriptors which are then fitted by a multi-phase simulated annealing-based reconstruction algorithm. This approach is easily extendible for generating 3D microstructures, by assuming isotropy. We demonstrate our approach for ordinary Portland cement pastes with different water to cement ratios. We evaluate the reconstruction methodology by calculating diffusion coefficients with a pore-scale transport model using a lattice Boltzmann approach and the generated 3D reconstructions. Results seem to agree very well with the measured diffusion coefficients for the same cement pastes. This builds confidence in the adequacy of the proposed simulated annealing algorithm for generating 3D realizations of cement paste from a 2D image. The approach will further developed to simulate transport properties in evolving porous systems during degradation to evaluate the confinement properties of cement-based materials over larger time scales in e.g. the context of radioactive and hazardous waste management.

References

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