KINETIC MONTE CARLO SIMULATIONS OF CARBONATION AND SELF-HEALING IN CONCRETE

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The current environmental challenges require concrete production to move away from standard Portland-based concretes and towards a wider portfolio of mixes with diverse, unique, and application-bespoke compositions and properties. However, the adoption of these potentially greener concretes is hindered by the lack of trust in the long-term performance of new mixes. Two ways to reduce uncertainties are to better understand and predict the degradation mechanisms of new concretes, and to develop solutions for increasing their resilience and ensure baseline performance despite the uncertainties. This talk addresses an area that contributes to both these dimensions: microstructural simulations of carbonation in concrete, and application to self-healing concrete.

The talk will present MASKE, which is a software to simulate the microstructural evolution of multi-phase solids, driven by mechanical deformations and by chemical reactions of dissolution and precipitation. The solid is discretized as mechanically interacting nanoparticles, which gives predictive access to the evolution of the stress field while the structure is changing. Notable results published using this software include precipitation-aggregation of C-S-H in cement paste during early hydration [1], and stress-driven dissolution of C_3S near screw dislocations [2]. MASKE is being currently used to simulate the carbonation of C-S-H/$Ca(OH)_2$ pastes in contact with atmospheric CO_2. Recent results cover the temporal evolution of the paste microstructure during carbonation, the corresponding evolution of solution chemistry, and the build-up of crystallization pressure during carbonate precipitation. Finally, the talk will present simulations of carbonation in the presence of pre-existing cracks and also in the presence of bacteria [3] whose metabolism contribute to CO_2 production in the pore solution. For these scenarios, self-healing induced by the mineralization process will be quantified and discussed.

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