Carbonation in bacteria based self-healing cement: A new modelling approach

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Concrete, with its excellent resilience and strength, is an excellent building material. It is also relatively low-cost, easy to make and durable. However, in recent years, the cement industry is concerned about its colossal carbon footprint (8% of global CO_2), mostly due to the cement production itself. More sustainable cements and decarbonisation have been forefront in cement research worldwide.

Development of sustainable cement/concrete demands a fundamental scale understanding of its reactions, microstructure and transport properties. Self-healing in concrete is an interesting property which has a lot of potential. When a crack forms in concrete it lets in atmospheric air and humidity. The CO_2 present reacts with the calcium in the cement paste forming calcium carbonate, which acts as a healing material. This work is an attempt to develop first simulations coupling together the bio, the organic, and the mineral, to optimise the self-healing strategy (concrete composition, environmental conditions etc.) for a given material and exposure conditions.

The models of carbonation in concrete must handle both the chemical reactions involved and mechanical and transport phenomena. Bacterial activity in concrete also demands the understanding of bacterial cell division, growth, and nutrient metabolism. Traditional continuum scale models adopts a heuristic assumptions on reaction rates and creates uncertainty while considering new systems. Hence, we are proposing the development of a chemo-mechanical model which can handle the large number of inputs, processes and materials involved in this process. The method uses Kinetic Monte Carlo (KMC) for mineral dissolution and precipitation, while bacterial growth and metabolism are also resolved via direct integration of their kinetic equations. This is achieved by combining two complex code bases.

1) MASKE, which is a recently developed Kinetic Monte Carlo framework [1], [2] for the chemo-mechanical evolution of mineral microstructures. In MASKE, the system is discretized representing the mineral phases as agglomerates of nanoparticles which interact via effective potentials (energy as a function of distance) whose spatial derivatives are the interaction forces. The particles can dissolve and precipitate via reaction rates obtained from transition state theory (TST). MASKE has been shown effective in modelling mineral dissolution-precipitation for cementitious systems and autogenous healing forming calcium carbonate. The system is coarse grained to micro-scale so that particle sizes are comparable to the microbe size.
2) NUFEB (Newcastle University Frontier in Engineering Biology), which is an open-source tool for 3D individual-based simulation of microbial communities. The tool is built a user package for the molecular dynamic simulator LAMMPS and extended with features for microbial modelling [3]– [5].

In this work we combine these code bases, both based on LAMMPS to model self-healing in cement with bacteria. The results predict for the first time the progress of calcium carbonate precipitation within a crack, along with the evolution of the bacterial colony producing CO_2 and the deterioration of the crack surfaces following the dissolution of calcium hydroxide.

References

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