



Modelling of dissolution and precipitation during microbially induced calcium carbonate cementation process using Lattice Boltzmann method

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Cement is the main component of concrete, which is the second most consumed product by society after water. The cement industry is considered a very energy-intensive sector. Also, it is responsible for the emission of a variety of pollutants into the atmosphere, including carbon dioxide, sulfur dioxide, nitrogen oxides, and particulate matters. The BioZement 2.0 project is aimed at developing a product substitution for conventional industrial cement. The method is based on microbially induced calcium carbonate precipitation (MICP). In the first step, microbially induced dissolution of calcium carbonate is performed. In this step, some bacteria are used for acid production in a solution of powdered limestone and substrate. The acid partially dissolves the limestone and releases calcium. In the next step, using the MICP approach, the calcium carbonate is re-precipitated to bind sand grains together, forming a concrete-like construction material which is called bio-cement.

A reactive transport model is developed to simulate the process. A Lattice Boltzmann method is used for coupling bio-geochemical processes at the pore scale. In the first step, the complete set of chemical species, nutrients, and reactions involved in the bio-cementation is explored. To couple the bio-geochemical processes, we consider the microbes as point sources/sinks of reactants.

Because of the dissolution and precipitation, the boundaries of the pore structure are moving. Proper modelling of the geometrical changes of the pore structure is very important for predicting the mechanical characteristics of the final bio-cement. To keep track of such changes, different formulations of boundary conditions based on the diffusion rate and reaction rate during bio-cementation are examined. The dissolution/precipitation regime will be studied over a range of Damköhler numbers. Depending on the computational costs and the accuracy of the surface description, the best approach will be presented.