Title: Effect of physicochemical properties and structural heterogeneity on reactive transport in saturated porous media

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Abstract

Physicochemical properties serve as crucial indicators on reactive solute transport and soil structure evolution in porous media, meanwhile structural heterogeneity of soil significantly alters physicochemical properties via redirecting solute transport path. Key biogeochemical processes such as precipitation – dissolution (PD) is essential to reactive solute transport in porous media, yet their relation with soil physicochemical properties and how they are influenced by soil heterogeneity remains unknown for years. This study took the PD process of Ca^{2+} and CO_3^{2-} ($Ca^{2+} + CO_3^{2-} \rightleftharpoons CaCO_3$) as an example to study the reactive solute transport behavior with different physicochemical conditions in heterogeneous media by a series of column experiments and numerical simulations. In the meantime, X-ray computed tomography (XCT) and morphological measurement (via ImageJ) were applied to investigate the effects of PD process on structural heterogeneity. Results demonstrate that the salinity, acidity, and flow rates in homogeneous columns significantly altered the reaction rate of PD process, leading to immediate hydraulic conductivity variation, and thus converted reactive transport behavior. Preferential flow paths in heterogeneous columns could lead to early breakthroughs and thereby promoted the transport of calcium carbonate (CaCO₃) in saturated porous media. XCT images revealed that more Ca²⁺ precipitated on flat and concave surface, forming a round coat outside grain particles. The CaCO₃ precipitates could also narrow or even block pore throat, and thus decrease pore connectivity. Our study provided essential experimental data for predictive modeling of Ca²⁺ reactive transport as well as new insights into the changes in soil structural heterogeneity and transport properties during the PD process.