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Imaging the spatial distribution of geochemical heterogeneities in porous media: multidimensional flow-through experiments and inverse modeling

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The spatial distribution of physical and chemical heterogeneities is critical in many subsurface applications. For instance, the location of reactive minerals is a primary factor controlling the fate and transport of organic and inorganic pollutants in groundwater. A number of studies have focused on using hydrologic measurements and inverse modeling techniques to image physical heterogeneity and the spatial distribution of hydraulic conductivity. However, such approaches are not commonly applied to water quality parameters and reactive transport problems. A recent numerical study [1] proposed a methodology to use distributed sensor data and inverse reactive transport modeling to characterize arsenic mobilization and distribution.
In this work we focus on imaging pyrite inclusions in saturated porous media and we combine experiments with forward and inverse reactive transport modeling. We studied the oxidative dissolution of pyrite in different experimental setups, including batch systems, 1-D column setups and 2-D flow-through chambers. Measurements of water quality parameters such as pH, dissolved oxygen, iron and sulfur were useful to formulate and constrain pyrite dissolution kinetics within a reactive transport modeling framework. In particular, spatially-distributed measurements of dissolved oxygen in the 1-D and 2-D setups were instrumental for imaging pyrite inclusions. Non-invasive optode sensors along the column setups and at different cross sections in the 2-D system allowed us to measure oxygen transport and consumption at high spatial resolution (2.5 mm spacing). The oxygen data were combined with inverse reactive transport modeling based on the Principal Component Geostatistical Approach (PCGA) [2]. The results show that the proposed methodology allows imaging both the spatial distribution and the concentration of single and multiple pyrite inclusions in the 1-D and 2-D experimental setups.

References

[1] S. Fakhreddine, J. Lee, P.K. Kitanidis, S. Fendorf and M. Rolle. Imaging geochemical heterogeneities using inverse reactive transport modeling: An example relevant for characterizing arsenic mobilization and distribution. Advances in Water Resources, 88, 186-197, (2016).
[2] J. Lee and P.K. Kitanidis. Large-scale hydraulic tomography and joint inversion of head and tracer data using the Principal Component Geostatistical Approach(PCGA). Water Resources Research, 50, 5410-5427, (2014).

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