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Imaging the spatial distribution of geochemical heterogeneities with inverse reactive transport modeling: The example of pyrite oxidation

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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 the applications of such approaches to water quality and reactive transport problems are still rare. 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 combine experiments with forward and inverse reactive transport modeling to explore the capability of imaging pyrite inclusions in the subsurface. 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 is able to image both the spatial distribution and the concentration of single and multiple pyrite inclusions in the 1-D and 2-D experimental setups.

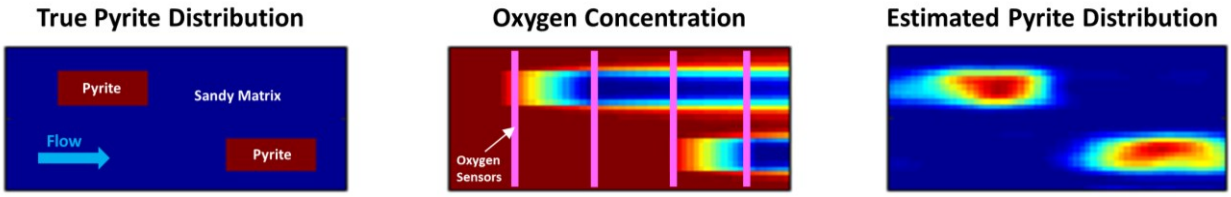

Figure 1: Example of imaging spatial distribution of pyrite in a 2-D setup with two pyrite inclusions.

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