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Pyrite oxidation in chemically heterogeneous porous media: flow-through experiments and reactive transport modelling

MARIA BATTISTEL¹, MUHAMMAD MUNIRUZZAMAN², FELIX ONSSES¹, JONGHYUN LEE³, MASSIMO ROLLE¹

¹ Department of Environmental Engineering, Technical University of Denmark, 2800 Lyngby, Denmark
(marbat@env.dtu.dk - masro@env.dtu.dk)

² Geological Survey of Finland, 70211 Kuopio, Finland

³ Department of Civil and Environmental Engineering and Water Resources Research Center, University of Hawaii

The spatial distribution of reactive minerals [1] plays an important role for groundwater quality and strongly affects the fate and transport of xenobiotic and geogenic contaminants.

In this study [2] we focus on the oxidative dissolution of pyrite, which is often linked to the geogenic contamination of groundwater from trace elements. We performed well controlled laboratory experiments in three different setups: batch, 1-D column and 2-D flow-through systems. The flow-through experiments were carried out in physically homogeneous but chemically heterogeneous porous media where reactive pyrite inclusions, with different concentration, were embedded at different spatial locations. We monitored the oxidative dissolution of pyrite during the flushing of the system with an oxic solution. The oxygen consumption was measured with a non-invasive optode technique [3], that was used for taking high resolution spatial and temporal measurements. Iron and sulfur were measured during the batch experiments at different times, and at the outlet of the flow-through systems.

The spatial and temporal dynamics of oxygen transport, the kinetics of pyrite oxidative dissolution, and the changes in water quality were modeled coupling a transport code with the geochemical simulator PHREEQC [4].

The results show that the spatial location and concentration of pyrite inclusions impact the reaction rates of pyrite oxidation. The model was instrumental for the quantitative interpretation of the experimental results and allowed us to capture the dynamics of the reactive fronts observed in the heterogeneous flow-through setups.

- [1] Li et al. (2014) *Geochim. Cosmochim. Acta* **126**, 555–573. [2] Battistel et al. (2019) *Appl. Geochemistry* **100**, 77–89. [3] Haberer et al. (2011) *J. Contam. Hydrol.* **122**, 26–39 [4] Muniruzzaman and Rolle (2016) *Adv. Water Resour.* **98**, 1–15