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Reactive transport modeling based interpretation of humidity cell tests: Challenges and limitations

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Mine waste rocks represent a major issue for the ecosystem conservation and human health because of the possible release of heavy metal(loid)s and acidity in the surrounding aquatic environments. Among the acid rock drainage prediction methods, humidity cell test is widely used for the long-term geochemical evaluation of leachates resulting from mining wastes . However, the reliability of this test remains an open question in terms of adequate sample representation, detailed characterization of experimental conditions, processes acting at different scales and their effects on output results. These aspects can heavily affect the interpretation of the test results, thus, consecutive management of mine workings. This study investigates the leaching behavior of the mine waste rocks collected from the Särkiniemi mine site, Finland, focusing on the impact of cell shapes on the effluent chemistry. Furthermore, the humidity cell tests were quantitively interpreted by means of multiphase and multicomponent reactive transport modeling [1].

The experiments were performed in two cells, packed with the same waste rock and subjected to the same procedure (ASTM D5744-18), with considerably different dimensions [2]. The test results suggest higher weathering rates of the waste rocks and mass loadings of different elements (approximately by two- to threefold) in the long/narrow shaped humidity cell setup compared to the short/broad cell although both experiments were subjected to identical conditions. The numerical simulation allowed detailed examination of the complex interplay between chemical reactions and physical processes, helped distinguishing the dominant mechanisms, and facilitated the identification of the controlling factors. The simulation implies a potential effect of microscale chemical heterogeneity, despite the attempts to homogenize the waste rock samples by crushing and mixing prior to packing, from the differences detected in the ions' concentrations of effluent water. While the experimental results could be reproduced by fitting different conceptual models or by adjusting model parameters, the model suggests that such simulation outcomes cannot be fundamentally treated as predictive without the proper knowledge of the dynamics of water flow and solute/gaseous transport during these tests.

[1] Muniruzzaman et al. (2020) *Appl. Geochem.* **120**, 104677

[2] Pieretti et al. (2022) *J. Geochem. Explor.* (under review)