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Mechanistic modelling of pyrite oxidation during prolonged drought events

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Under changing climate conditions with expected higher risks on long periods of severe drought events, acid sulphate soils have a higher risk for acidification when exposed to oxygen under a falling water table. A regional or continental risk map for acidification under possible future climate scenarios is one of the tools for evaluating agricultural, economic and environmental impacts of acidification. In a first phase of the development of such risk map, a simulation model has to be developed accounting for (i) the effect of changing meteorological boundary conditions on the water dynamics inside the soil and the ground water depth, (ii) diffusion of oxygen inside the soil profile, and (iii) kinetic dissolution of pyrite and geochemical alterations. The objective of this study is to identify key processes, model structures and parameters dominating the acidification during prolonged drought events and the neutralizing capacities after these events.

The simulation tool HPx (Jacques et al., 2018) couples all these processes and enables evaluation of different model structures. Model structures differ in the assumptions on (i) pyrite oxidation scheme, (ii) type of buffer reactions, (iii) competitive processes for oxygen consumption (microbial and root respiration), and (iv) soil boundary conditions. Richards equation is used to simulated water flow, the advection-dispersion-diffusion equations calculate transport of aqueous components; only diffusion in the gas phase is considered. Pyrite oxidation is modelled with kinetic reactions, whereas most buffer reactions (including cation exchange and primary/secondary mineral dynamics) are treated with a thermodynamic model. A first set of simulations is based on a stylized representation of a single drought event over a period of 5 years (including drying and rewetting). These simulations are the basis for (i) the development of a reference model for detailed mechanistic modelling of acidification under different climate scenarios, and (ii) the future development of an abstracted model for the risk map.

Jacques, D., Simunek, J., Mallants, D. and van Genuchten, M.T. (2018) The HPx software for multicomponent reactive transport during variably-saturated flow: Recent developments and applications. JOURNAL OF HYDROLOGY AND HYDROMECHANICS 66, 211-226.