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Towards a robust reactive transport model to simulate fate and transport of PFAS from surface to groundwater

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The H2020 PROMISCES project aims to promote a zero-pollution circular economy by overcoming the presence of contaminants, notably poly- and perfluoroalkyl substances (PFAS), in the soil-sediment-water system. Hence, a sound understanding of their retention and transport behavior in the soil-aquifer continuum is mandatory. Reactive transport models are suitable tools to tackle this goal albeit their robustness is still questioned, mainly due to their use on a narrow range of experimental dataset. The aim of this study is to test their efficiency to predict PFAS mobility over a broad range of environmental conditions by simulating a large set of column experiments.

A 1D reactive transport model has been based on HYDRUS software. Richards equation was used to simulate variably saturated water flow. Reactive transport were simulated by accounting for advection-dispersion, rate-limited diffusive transfer between mobile-immobile domains and thermodynamic equilibrium and/or kinetically-constraints adsorption processes at solid-water interface (SWI) and air-water interface (AWI). Model calibration and validation have been based on column experiments in saturated and unsaturated conditions carried out on a sandy material and a soil. A mix of 4 PFAS (PFOA, PFOS, PFHxS and PFBS) were used. For each PFAS, concentration in the inlet solution was either 5 mg L^{-1} or 5 µg L^{-1}, hence mimicking a wide range of contaminated environments.

The whole set of PFAS breakthrough curves were accurately simulated. Simulations results illustrate that the amounts of PFAS sorbed at SWI and AWI remained low in regards to the amount in aqueous phases for high PFAS condition. PFAS mobility was controlled by flow rate, dispersivity and transfer between mobile-immobile domains. At low PFAS condition, sorption processes at SWI in saturated conditions and at SWI and AWI in unsaturated conditions play a key-role. We also highlight that calibration of some model parameters associated with sorption processes at AWI and rate-limited diffusive transfer was concentration-dependent. Lower the PFAS concentration is, higher the values of model parameters are. This trend is greater for the compounds with longer carbon-chain. In order to overcome this limit preventing to simulate PFAS mobility over a wide range of contamination conditions, a modified model version is proposed.