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Sensitivity of soil representation in PFAS transport simulations under wetting and drying conditions

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Per- and polyfluoroalkyl substances (PFAS) can enter the vadose zone through episodic infiltration of surface waters, which ubiquitously contain these compounds. Elevated PFAS concentrations in shallow soils are primarily attributed to their accumulation at air-water interfaces, a phenomenon mostly studied near historical point source releases. Atmospheric conditions and infiltrating surface waters impact soil saturation in shallow soils, driving the expansion and contraction of air-water interfaces. Despite the recognized importance of these processes, the long-term impact of fluctuating soil saturation on the fate of PFAS in infiltrating surface waters remains poorly understood.

We simulated the retention and migration of perfluorooctanesulfonic acid (PFOS) from 15 years of periodic ponding of low-concentration (30 ng/L) surface water in a constructed wetland in the Santa Ana River watershed. We used Hydrus to model a 1D heterogeneous (sand–clay) system with boundary conditions informed by local surface water levels, precipitation, and evapotranspiration measurements. We also measured the grain size distribution of sediments from the field site. We used measured water retention curve parameters and permeability of sands and clays with similar texture and porosity to quantify the sensitivity of PFOS transport on soil properties (which are difficult to measure and often overlooked). Infiltration of surface water and atmospheric conditions drive changes in the saturation of shallow soils, which are mediated by soil physical properties. The resulting expansion and contraction of air-water interfaces redistribute PFAS within the pore matrix and control retention and migration of PFOS.
We considered two layering scenarios with the same effective saturated hydraulic conductivity (proportion of sand and clay). We observed differences in the total mass flux, distribution, and front propagation of PFOS for equivalent source concentrations, boundary conditions (precipitation, ponding, and evapotranspiration), and average permeability of the two scenarios. We found that some layered systems with shallow clay layers accumulate a greater mass of PFAS and develop persistently elevated pore water concentrations (up to four times the source concentrations) at shallow depths compared to corresponding layered systems with a top layer of sand. We evaluated multiple realizations of PFOS mass accumulation and will compare observations of the vertical distribution of PFAS in the field.

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References

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