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Quantifying low concentration in-situ field partitioning of PFAS in vadose zone sediments

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Per- and polyfluoroalkyl substances (PFAS) are consistently detected in wastewater treatment plant effluent and urban stormwater runoff at concentrations that exceed federal health advisory levels. Soils and sediments in adjacent wetlands and floodplains may accumulate PFAS due to periodic ponding events. However, our understanding of PFAS transport and partitioning mechanisms in these areas is limited, particularly compared to well-studied sites with known point source releases and orders of magnitude higher concentrations. In this study, we measured the vertical distribution and solid-phase partitioning of perfluorooctanesulfonic acid (PFOS) in sediments collected from a wetland at the outlet of a large (5,0840 km²) urban watershed in semi-arid Southern California. The wetland is episodically ponded with water with some PFAS (e.g., recent PFOS measurements of 9 - 29 ng/l). Quantifying in-situ partitioning of PFAS in vadose zone soils requires knowledge of sorbed and aqueous phase concentrations and estimates of air-water interfacial areas. These are all difficult to measure directly in low permeability soils infiltrated with relatively low concentrations of PFAS.

We combined PFOS field sample measurements, laboratory batch desorption experiments, and partitioning models to quantify in-situ PFAS behavior in vadose zone soils. A batch desorption experiment on an interval directly below the field sample measured with the highest concentration of PFOS (6.53 ng/kg from 1.1 m depth) revealed that both a concentration-dependent Freundlich isotherm and a linear isotherm with an irreversibly adsorbed fraction (17% of the total in-situ mass of PFOS) fit the data well. We estimated in-situ partitioning by integrating the solid-phase partitioning isotherms with the air-water interfacial area and PFAS partitioning models. Pore-water concentrations estimated from a Freundlich air-water partitioning model were below 6 ng/L when paired with either of the solid-phase partitioning models. In contrast, pore-water concentrations estimated from a Langmuir air-water partitioning model ranged from 36.5 to 150.7 ng/L when paired with the linear solid-phase partitioning model, and from 3.9 to 218.7 ng/L when paired with the Freundlich solid-phase partitioning model. The wide range of predicted pore-water concentrations reflects uncertainties in sorption models and estimated air-water interfacial areas (varied by two orders of magnitude, even when constrained by grain size distribution). Finally, to assess possible hysteresis in soil-water partitioning, we performed adsorption/desorption/re-adsorption experiments on samples collected from 1.1 m, 1.9 m, and 2.8 m depths with varying fractions of organic matter and clay content. Mass-labeled PFOS were used to differentiate between field-exposed (PFOS), initial laboratory (M8PFOS), and secondary laboratory (M4PFOS) adsorption-desorption isotherms. This comprehensive study provides a sensitivity analysis of field measurements, partitioning mechanisms, and soil characterization models to evaluate the environmental fate and impact of common, low-concentration PFAS sources.

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References

Primary author: COOKSON, Esther

Co-authors: Dr HAN, Ziwei; DETWILER, Russ; Prof. ADELEYE, Adeyemi (Columbia University)

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