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^{19}F-MRI and numerical modeling as a combined method for the measurement and prediction of fluorinated substances (e.g. PFASs) transport in porous media

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The topic of per- and polyfluoroalkyl substances (PFASs) is a late-breaking issue due to its high environmental relevance (toxicity, persistence and bio accumulation) and due to the detection of PFASs as contaminants in various environmental compartments including groundwater, surface water and soil. PFASs enter the environment for instance through industrial, agricultural, and house-hold activities. Restricted PFASs like PFOA by the Stockholm Convention 2019 have often been replaced by molecules of the same family with shorter carbon chains, and nowadays around 4000 different molecules of PFASs can be found in the environment. Although PFASs have been manufactured since the 1940s, the fate of these chemicals in soils was not studied until the late 1990s.
These studies have shown that the retention of PFASs in soils depends on various factors such as the PFASs type (e.g. molecular structure and carbon chain length), the soil properties (e.g. amount of organic carbon), and the pore water (e.g. degree of saturation, pH). Still, the retention – and release – mechanisms of PFASs on soil constituents are not completely elucidated, and a generic model able to predict the transport of PFASs in the subsoil is not available yet.
In this work, building on a recently developed approach coupling nuclear magnetic resonance (^{19}F - NMR) and modeling [1], we used magnetic resonance imaging (^{19}F - MRI) to obtain quantitative information of the spatial and temporal distribution of a fluorinated substance inside a porous medium during transport experiments. We validated the performance of our approach by comparing MRI profiles obtained during flow-through experiments in sand columns tracing the transport of sodium fluoride (NaF) – a fluorinated non-reactive tracer – with traditional breakthrough curve and numerical simulations. These results pave the way for the application of this innovative MRI/modeling approach PFASs and conclusively to improve our understanding and modeling capability of PFASs fate in porous media.

[1] Courtier-Murias, D., Michel, E., Rodts, S., & Lafolie, F. (2017). Novel Experimental-Modeling Approach for Characterizing Perfluorinated Surfactants in Soils. Environmental Science and Technology, 51(5), 2602–2610. https://doi.org/10.1021/acs.est.6b05671