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A screening model for quantifying PFAS leaching in the vadose zone and mass discharge to groundwater

Bo Guo[1], Jicai Zeng[1], Mark Brusseau[2], and Yonggen Zhang[3]
[1]Department of Hydrology and Atmospheric Sciences, University of Arizona, Tucson, AZ, United States (boguo@arizona.edu)
[2]Department of Environmental Science, University of Arizona, Tucson, AZ, United States
[3]School of Earth System Sciences, Tianjin University, Tianjin, China

A growing body of site investigations have demonstrated that vadose zones serve as significant long-term sources of PFAS to groundwater. Quantifying PFAS leaching in the vadose zone and mass discharge to groundwater is therefore critical for characterizing, managing, and mitigating long-term contamination risks. Recently, mathematical models representing the PFAS-specific transport and retention processes, including surfactant-induced flow, and rate-limited, nonlinear adsorption at solid-water and air-water interfaces, have been developed. While these advanced models provide fundamental insights into the primary processes controlling the long-term retention of PFAS, they are less suitable for screening-type applications due to significant computational cost and the requirement for detailed input parameters. To address this knowledge gap, we develop a simplified model by assuming steady-state infiltration and linear solid-phase and air-water interfacial adsorption; a two-domain model is used to represent kinetic solid-phase adsorption. We derive novel analytical solutions for the simplified model allowing for arbitrary initial conditions. The newly derived analytical solutions are then validated by application to miscible-displacement experiments under a wide range of conditions and by comparisons to a state-of-the-art comprehensive model under both experimental and field conditions applicable to PFAS-contamination sites. Overall, the simplified analytical model provides an efficient and accurate screening-type tool for quantifying long-term PFAS leaching in the vadose zone.