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Semi-analytical solutions for nonequilibrium PFAS transport in heterogeneous vadose zones

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We present screening-type models for quantifying the fate and transport of perfluoroalkyl acids and their precursors (PFAS) in a heterogeneous vadose zone. The models represent the heterogeneous vadose zone by one-dimensional dual-porosity, dual-permeability, or tripe-porosity domains. They account for transport mechanisms specific to PFAS and their precursors—including multi-site rate-limited solid-water and air-water interfacial adsorption and biochemical transformation. Assuming steady-state infiltration, linear adsorption, and first-order-rate transformation, we derive semi-analytical solutions for these models under arbitrary initial and boundary conditions. The newly derived solutions have been validated by experimentally measured breakthrough curves of PFAS and other solutes for various soils and wetting conditions. Additionally, we demonstrate the models' capability for analyzing long-term PFAS leaching and mass discharge in a heterogeneous vadose zone beneath a PFAS-contaminated site. Among other findings, the simulations show that the strong retention of PFAS (especially longer-chain PFAS) reduces the mass-transfer limitations and nonequilibrium transport behaviors between the different pore domains. Overall, the semi-analytical models provide practical tools for assessing the long-term fate and transport of PFAS in the vadose zone and for soil screening applications.

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