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Long-term retention and leaching of PFAS in the vadose zone: controlling processes, mathematical formulation, and practical modeling approaches

Monday, 30 May 2022 11:20 (15 minutes)

PFAS are emergent contaminants of which the fate and transport in the environment remain poorly understood. A growing body of site investigations have demonstrated that vadose zones serve as significant long-term sources of PFAS to contaminate 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. As surfactants, adsorption at air–water and solid–water interfaces leads to complex retention of PFAS in soils. These interfacial behaviors depend strongly on the chemical properties of PFAS such as chain length and functional groups. Concomitantly, PFAS present in pore water can modify surface tension and in turn impact variably saturated flow, which further complicates the fate and transport of PFAS in the vadose zone.

In this talk, I will give an overview of our recent mathematical and numerical modeling studies that aim to understand and quantify the primary processes that control the long-term leaching of PFAS. A few years ago, we have developed a full-process mathematical model that represents a set of PFAS-specific transport processes including concentration-dependent capillary pressure, and rate-limited and nonlinear adsorption at the air–water and solid–water interfaces. The full-process model has been employed to quantify the impact of a variety of factors on long-term PFAS leaching in the vadose zone including surfactant-induced flow, rate-limited and nonlinear air-water interfacial adsorption, PFAS chain length and functional group, pore water chemistry, and subsurface heterogeneity. Insights from the comprehensive analyses then allow us to develop a simplified model with a focus on the primary processes that dominantly control PFAS leaching. We derive new analytical solutions for the simplified model and validate them by application to miscible-displacement experiments under a wide range of conditions and by comparisons to the full-process model under both experimental and field conditions applicable to PFAS-contamination sites. Overall, the simplified analytical model appears to provide an efficient and accurate screening-type tool for quantifying long-term PFAS leaching in the vadose zone.

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References

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Time Block Preference

Time Block C (18:00-21:00 CET)

Participation

Online

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