129-ENGR

Modelling the Transport of Emerging PFAS in the Soil and Groundwater

ABSTRACT

Per- and polyfluoroalkyl substances (PFAS) are persistent contaminants with complex transport and retention mechanisms, posing challenges to predictive modeling and remediation strategies. This study evaluates methodologies for simulating PFAS transport, analyzing their strengths and limitations to identify the most effective approach for controlled experimental conditions. Foam fractionation quantifies air-water interfacial adsorption (AWI) at low PFAS concentrations but is limited to static systems and cannot address bulk transport. Machine learning models, like XGBoost, excel in large-scale PFAS detection but lack mechanistic detail. MATLAB-based numerical models offer flexibility for simulating multi-process transport mechanisms but on simplified assumptions and parameters derived from literature rather than direct calibrated experimental data. **This study employs Hydrus-1D, a reactive transport model selected for its ability to integrate key retention processes, including solid-phase sorption and air-water interfacial (AWI) adsorption, with advection-dispersion mechanisms.** To generate the necessary data for model calibration, dynamic soil column experiments are conducted to replicate subsurface conditions and investigate variables such as soil type, moisture content, and PFAS concentrations. The experimental results are essential for calibrating Hydrus-1D, enabling accurate simulation of PFAS transport under varying environmental conditions. Hydrus-1D supports parameter calibration using these results, making it adaptable to various PFAS compounds and soil types. By combining experimental data with modeling, this research addresses critical knowledge gaps and provides a validated framework for understanding PFAS transport mechanisms in subsurface environments.

Keywords: PFAS, Transport Modeling, Hydrus-1D, Retention Mechanisms, Soil Columns