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Numerical modeling of the PFAS Fate in a Former Firefighting Training Site in Korsør, Denmark

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The extensive use of products containing high concentrations of Per- and Polyfluoroalkyl Substances (PFAS) has led to the spreading of such "forever chemicals"in soil and groundwater In certain locations, like Korsør in Denmark, a former firefighting training site, PFAS have been detected in the vadose zone in measurable amounts 1. Studies in such areas are crucial for understanding the PFAS behavior in subsurface soil layers.
This numerical model focuses on the transport behavior of four PFAS (per-fluoro butanoic acid-PFBA, per-fluoro octanoic acid-PFOA, per-fluoro decanoic acid-PFDA, and per-fluoro octane sulfonic acid-PFOS) in the vadose zone, with emphasis placed also on potential PFAS leaching into groundwater. For this purpose, a 3D domain has been constructed, with dimensions 8 m in depth and area 100m2 consisting of multiple soil layers with various initial water saturation levels (Figure 1). The great variety of soil types necessitates enhanced model accuracy [2], achieved through a Python code that analyzes the geological layers of the site. This code interprets different colors in the geological model (each color representing a distinct soil layer) as layers of varying permeability and effective diffusivity, by utilizing background knowledge from literature [3].

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In this study, the Richards equation is employed to model fluid transport within unsaturated porous media in the COMSOL platform by utilizing the Multiphysics module [4]. This equation is integrated with the van Genuchten approximation [5] for defining relative permeabilities in relation to effective saturation.
In addition to the well-known transport mechanisms, such as convection, diffusion, and dispersion, PFAS adsorption plays a significant role in the retention process [6]. The present approach considers that PFAS adsorption occurs on both the solid grain-water interfaces and the air-water interfaces. The PFAS sorption coefficients on air/water interfaces were estimated by fitting curves of the water/air surface tension as function of PFAS concentration with the Langmuir-Szyszkowski equation or were taken from literature [7]. The kinetics of PFAS sorption on solid/water interfaces was estimated with inverse modeling of the relevant breakthrough curves of soil column experiments or were taken from literature [8].
The spatial-and-temporal distribution of the concentration of four PFAS compounds (PFBA, PFOA, PFOS, and PFDA) is detected as they percolate through the vadose zone until reaching the aquifer by accounting for the unique properties of each PFAS [8]. Multiple scenarios are tested, starting with the initial state of soil (whether saturated or unsaturated) and extending to various soil types, different initial PFAS concentrations, and varying precipitation rates. Precipitation plays a crucial role as it stimulates the convection mechanism. Additionally, the retention factor is estimated to be significant, particularly as the initial PFAS concentration increases. The different scenarios of PFAS motion in subsurface have generated insightful results, regarding strategies for soil treatment.
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