NUMERICAL SIMULATION OF PFAS FATE AT A FORMER FIREFIGHTING TRAINING FACILITY IN KORSØR, DENMARK

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ABSTRACT

The extensive utilization of products containing high concentrations of Per- and Polyfluoroalkyl Substances (PFAS) has resulted in the dispersion of these persistent compounds within soil and groundwater. In specific sites like Korsør in Denmark, a former firefighting training facility, PFAS contamination has been identified in measurable quantities within the vadose zone [1]. This computational model specifically examines the transport dynamics of four PFAS compounds (PFBA, PFOA, PFOS, and PFDA) within the vadose zone, with a focus on potential leaching into groundwater. To achieve this, a 3D domain with dimensions of 8 meters in depth and an area of 100 square meters has been established, comprising multiple soil layers exhibiting varying initial water saturation levels. The diverse range of soil types necessitates heightened model precision [2,3], which is attained through a Python code analyzing the geological strata of the site. In this investigation, the Richards equation is utilized to simulate fluid transport within unsaturated porous media using the COMSOL platform, [4]. This equation is coupled with the van Genuchten approximation [5] to define relative permeabilities as functions of the effective water saturation. In addition to conventional transport mechanisms such as convection, diffusion, and dispersion, PFAS adsorption significantly influences the retention process [6]. This study accounts for PFAS adsorption occurring at both solid grain-water interfaces and air-water interfaces. Sorption coefficients on air/water interfaces are estimated by fitting curves of water/air surface tension as a function of PFAS concentration using the Langmuir-Szyszkowski equation or retrieved from literature [7]. The kinetics of PFAS sorption on solid/water interfaces are estimated through inverse modeling of relevant breakthrough curves from soil column experiments or sourced from literature [8]. Multiple scenarios are examined, encompassing variations in initial soil states (saturated or unsaturated), soil types, initial PFAS concentrations, and precipitation rates ranging from 0 to 5 mm/h. Precipitation is particularly significant as it drives the convection mechanism. Moreover, the retention factor is observed to be substantial, especially with increasing initial PFAS concentrations. The diverse scenarios depicting PFAS movement in the subsurface yield valuable insights into soil treatment strategies.

KEYWORDS: PFAS in soil, PFAS fate, PFAS adsorption

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