# Supporting Information for "A Mathematical Model for the Release, Transport, and Retention of Per- and Polyfluoroalkyl Substances (PFAS) in the Vadose Zone"

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**Description for the simulation setup for S1**

To verify our numerical implementation of the mathematical model, we compare our code with the commercially available software HYDRUS-1D. We simulate water infiltration into a 1D vadose zone. The water table is fixed at $z = 4.82\,\text{m}$. Initially, water is at a hydrostatic condition with a uniform solute concentration $2\,\text{mg/L}$. Then, water with zero solute concentration is infiltrated from the top boundary at a constant rate of $10\,\text{cm/day}$. The bottom boundary is zero flux for both water and solute. Solid-phase adsorption is included using the Freudlich isotherm. All other parameters are the same as those used

in the Accusand simulation (section 5.2). We simulate this problem using both our code and HYDRUS-1D and present the spatial distribution of the water saturation and solute concentration over a period of 6 days. The results from the two codes are almost identical (Fig. S1), which shows that our implementation of the Richards' equation and the advection-dispersion equation is correct. Note that here we do not consider the change of surface tension and air-water interfacial adsorption because they are not implemented in official version of HYDRUS-1D.

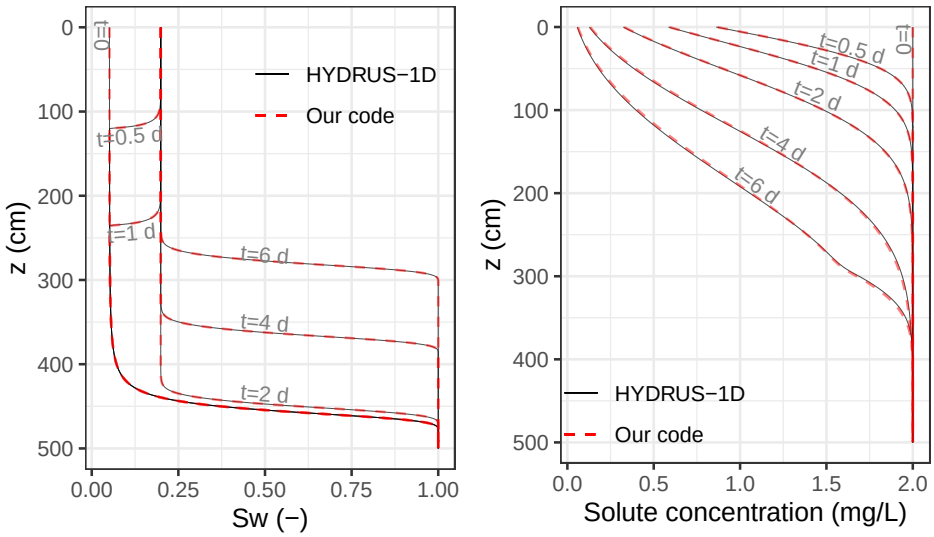


**Figure S1.** Spatial distributions of (left) water saturation and (right) solute concentration over a period of 6 days.

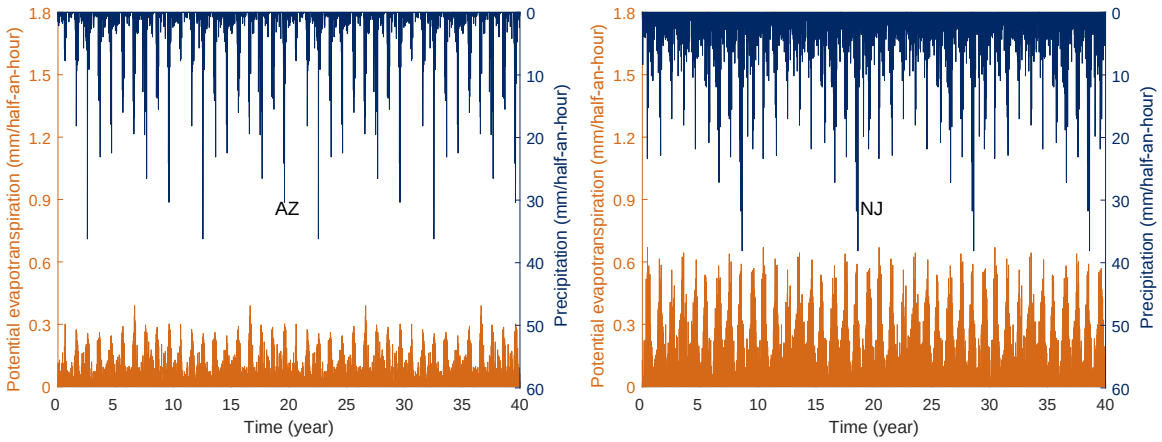


**Figure S2.** Precipitation and evapotranspiration datasets for 40 years. (a) A semi-arid climate (Walnut Gulch Kendall Grasslands site, AZ, U.S.). (b) A humid climate (Silas Little site, NJ, U.S.).

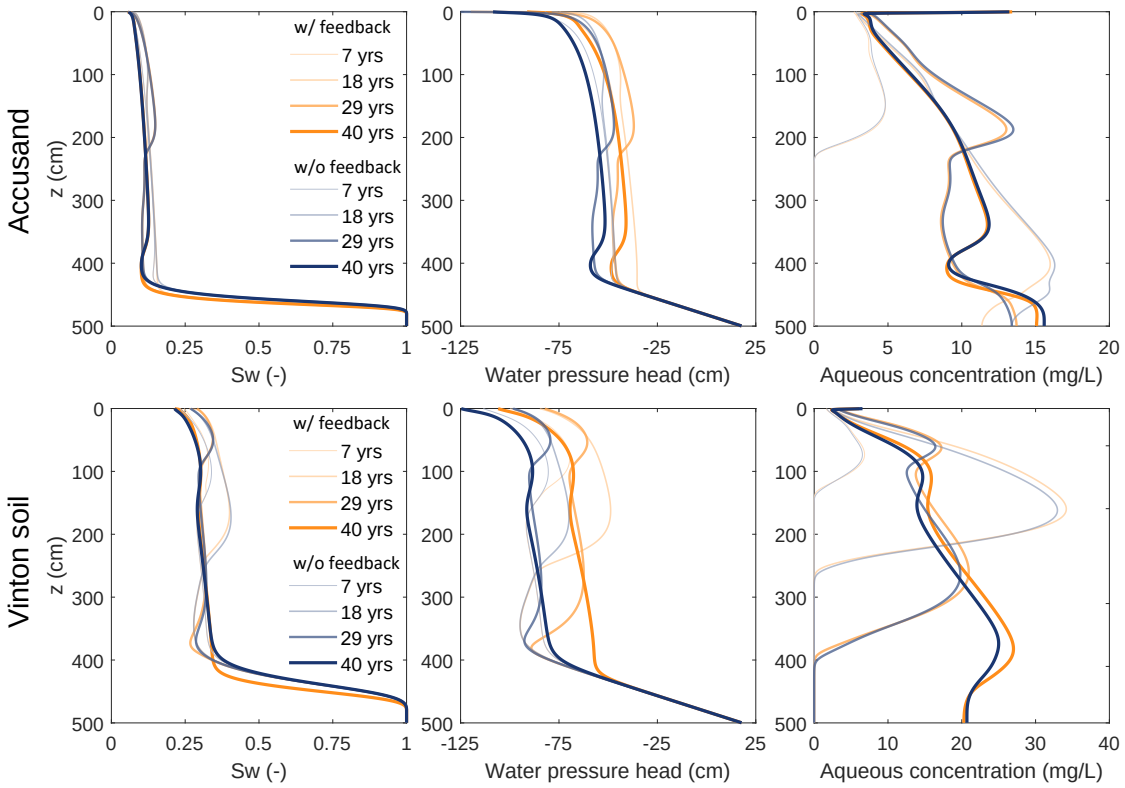


**Figure S3.** Comparison between simulations with constant surface tension (i.e., PFOS does not feedback to flow) and those that have included the impact of PFOS on flow. The first and second rows are for Accusand and Vinton soil, respectively. The three columns are for water saturation, water pressure head, and aqueous concentration of PFOS, respectively. Only the scenario of high PFOS concentration (1000 mg/L) under the humid climate is presented. The scenario under the semi-arid climate has a similar pattern and thus not presented. For the scenario of low PFOS concentration (100 mg/L) (not shown here), the impact of PFOS on flow (and thus the transport of PFOS) is smaller due to less reduction in surface tension.